Formal calculus, with applications to quantum mechanics

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Abstract

"Formal" or "Feynman diagrammatic" calculus is nothing more nor less than the differential and integral calculus of formal power series. The latter name is because Feynman's diagrams provide a convenient notation for manipulating formal power series and for understanding their combinatorics. In this talk, I will outline the formal calculus, and then use it to write out the "path integral" description of the asymptotics of the time-evolution operator in quantum mechanics. The diagrammatics make it much easier to prove that the "path integral" is well-defined and satisfies the necessary requirements.

1

I'd like to begin by describing the category of infinitesimal pointed manifolds. The definition starts with the category of $\mathbb{R}$ vector spaces. The construction works more generally, but I'll leave it to the experts to think about how much more generally.

Definition. The objects of InfMan are the same as the the objects of $\mathbb{R}$-Vect. Given $X, Y \in$ InfMan, we misuse notation (better would be "$\mathcal{C}^{\infty,\text{formal}}$") and define

$$\mathcal{C}^\infty(X,Y) = \prod_{n=0}^{\infty} S_n\text{-invariant}\,\mathrm{Hom}_{\mathbb{R}\text{-}\mathrm{Vect}}(X^{\otimes n}, Y)$$

For comparison, $\mathrm{Poly}(X,Y)$ uses $\coprod$.

There is no good composition for $\mathcal{C}^\infty$ maps. Instead, we define

$$\mathrm{Hom}_{\mathrm{InfMan}}(X,Y) = \mathcal{C}^\infty_{\text{pointed}}(X,Y) = \prod_{n=1}^{\infty}$$

I.e. the formal power series that begin in degree 1. This gives the word "pointed" in "infinitesimal pointed manifolds".

Let $f = (f^{(0)}, f^{(1)}, f^{(2)}, \dots) \in \mathcal{C}^\infty(X,Y)$. The idea is that the nth piece $f^{(n)}$ should be thought of as the nth Taylor coefficient. With this in mind, we define the composition

$$\mathcal{C}^\infty_{\text{pointed}}(X,Y) \times \mathcal{C}^\infty(Y,Z) \to \mathcal{C}^\infty(X,Z)$$

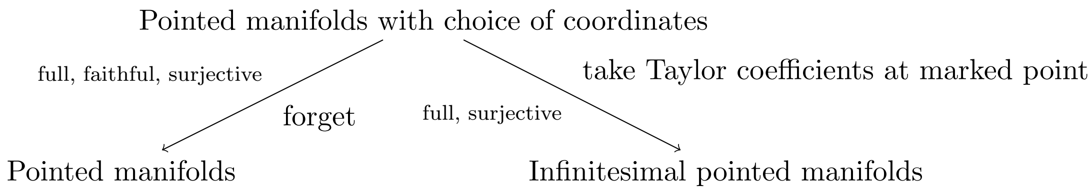
by the Faà di Bruno formula:

$$(g\circ f)^{(n)} = \sum_{\substack{\text{(unordered) partitions}\\ \text{of } \{1,\dots,n\}}} g^{(\#\text{ of blocks})} \underset{\substack{\uparrow\\ \text{composition}\\ \text{of tensors}}}{\circ} \bigotimes_{\text{blocks}} f^{(\text{block})}$$

By this I mean: feed in a pure tensor $x = x_1 \otimes \cdots \otimes x_n$. Then $f^{(\{2,3,5\})}(x) = f^{(3)}(x_2 \otimes x_3 \otimes x_5)$.

The sum truncates because f is pointed, so partitions with empty blocks don't contribute.

There are functors:



2

There is a better notation and description of composition. Recall that a *groupoid* is a category with all morphisms invertible. If $\mathscr{G}$ is a groupoid, let $\pi_0\mathscr{G}$ denote its set of isomorphism classes of objects. A *class function* $\mathscr{G} \to A$ is a function $\pi_0\mathscr{G} \to A$, or equivalently a functor $\mathscr{G} \to A$ where A is given a groupoid structure with no nonidentity morphisms. For example, $|\mathrm{Aut}(-)|$ is a class function. (The name comes from the example where the objects of $\mathscr{G}$ are the elements of a group, and the morphisms are conjugations. Then $\pi_0\mathscr{G}$ are the conjugacy classes.)

Definition (Baez and Dolan). Let $\mathscr{G}$ be a groupoid, A a $\mathbb{Q}$-module, and $F : \mathscr{G} \to A$ a class function. The *groupoid integral* is

$$\int_{\mathscr{G}} F = \sum_{x \in \pi_0\mathscr{G}} \frac{F(x)}{|\mathrm{Aut}\, x|}$$

As with any integral, it may not converge.

Consider, then, the groupoid $\mathscr{G}_1$ whose objects are directec graphs with one vertex, one outgoing edge, and finitely many incoming edges, with leaves labeled $\{1, \ldots, n\}$. So there are no automorphisms. A choice of $f \in \mathcal{C}^\infty(X, Y)$ determines a class function $F : \mathscr{G}_1 \to \mathcal{C}^\infty(X, Y)$ by assigning the vertex with n incoming edges the value $f^{(n)}$. Then $f = \int_{\mathscr{G}_1} F$.

There is a different basis for $\mathcal{C}^\infty(X, Y)$, where we rescale the nth piece by $n!$, so that we think of the pieces as $f^{(n)}/n!$ rather than as $f^{(n)}$. In characteristic 0, these are the same; we picked the one we did for the convenience of writing out the Faà di Bruno formula. But you can work with this "ordinary generating function" picture instead of our "exponential generating function" picture. Then consider the groupoid whose objects are graphs with one vertex, one outgoing edge, and finitely many *unlabeled* incoming edges. Then a similar class function still has $f = \int_{\mathscr{G}_1} F$.

Lemma. Consider the groupoid $\mathscr{G}_2$ consisting of finite directed graphs of the following form. The vertices live on two rows. On the bottom row is a unique vertex, with a unique outgoing edge. On the top row are some vertices, each with a unique edge pointing towards the bottom row. Each top vertex has some number of incoming edges, and the incoming edges are labeled $\{1, \ldots, n\}$. Given $f \in \mathcal{C}^\infty(X, Y)$ and $g \in \mathcal{C}^\infty(Y, Z)$, we can make a class function $GF : \mathscr{G}_2 \to \mathcal{C}^\infty(X, Z)$, by "evaluating" the diagram by interpreting the bottom most edge as being labeled by Z, the bottom vertex as labeled by g, the middle edges labeled by Y, the top vertices labeled by f, and the top edges labeled by X. Then $\int_{\mathscr{G}_2} GF = g \circ f$, and converges if f is pointed.

3

So much for differential calculus. What about integrals? The *formal gaussian integral* of $f \in \mathcal{C}^\infty(X, Y)$ is

$$
\begin{aligned}
\text{“}\int_X f(x) e^{-a^{-1}x^2/2} \frac{\mathrm{d}x}{\sqrt{\det(2\pi a)}}\text{”} &= \text{“}f \circ \frac{a}{2}\text{”} \\
&= \text{groupoid} \int \text{for} \left\{ \begin{array}{l} \text{graphs with one bottom vertex (and} \\ \text{unique outgoing edge) labeled } f; \\ \text{and some top vertices, labeled } a, \text{ each} \\ \text{with two edges pointing towards } f \end{array} \right\}
\end{aligned}
$$

When $\mathrm{Re}(a)$ is positive-definite and f is a polynomial, then it's easy to see that the RHS converges absolutely as a Riemann integral, and agrees with the LHS. When f is (represented by) a smooth function, the LHS computes the $a \to 0$ asymptotics of the RHS. When a is pure imaginary (and still invertible), then LHS can converge conditionally, and again RHS computes the correct asymptotics, c.f. [Evans and Zworski].

There is a problem, however. $a \in \mathcal{C}^\infty(\mathrm{pt}, X^{\otimes 2})$ is not a pointed map, so RHS does not converge. There are two fixes. One is to consider $\int f \in \mathcal{C}^\infty(X^{\otimes 2}, Y)$, i.e. read a as a variable. The other, which we prefer, is to pick some new infinitesimal parameter $\hbar$, and rescale $a \mapsto \hbar a$. Then for fixed a, f, the RHS converges in $\mathbb{R}[[\hbar]]$.

Now suppose that $f \in \mathcal{C}^\infty(X, \mathbb{R})$ with $f^{(1)} = 0$ and $f^{(2)}$ invertible. Then

$$
\int \exp(-\hbar^{-1} f(x)) = \exp(-\hbar^{-1} f^{(0)}) \int e^{-\hbar^{-1} f^{(2)} x^2/2} \exp(-\hbar^{-1} \sum_{n \geq 3} f^{(n)} x^n / n!)
$$

and expand the exp in Taylor series. Then we can still define the integral, and hope it converges. Does it? Use that

$$
\exp(\star) = \text{groupoid} \int \text{for } \{\text{disjoint copies of } \star\}
$$

Then expanding the exp in the integral gives a bunch of trivalent-and-higher vertices, where an n-valent vertex is labeled $-\hbar^{-1} f^{(n)}$. Then integrating connects everything up with edges labeled by $(\hbar^{-1} f^{(2)})^{-1}$. So for a given graph, there are $\#(\text{edges}) - \#(\text{vertices}) =$ euler characteristic many $\hbar$s, and as all vertices are trivalent and higher, this number is nonnegative and there are finitely many graphs for a given number. Thus:

$$
\begin{aligned}
\int \exp(-\hbar^{-1} f(x)) \mathrm{d}x = \exp(-\hbar^{-1} f^{(0)}) \sqrt{\det\big(2\pi\hbar (f^{(2)})^{-1}\big)} \times \\
\times \text{ groupoid int for all trivalent-and-higher diagrams}
\end{aligned}
$$

The point is, this has a hope of being generalizable to infinite-dimensional spaces, where analytic definitions are hopeless. For the generalization to be good, we should do two exercises — I know how to do them, but don't have time in the talk right now:

(a) Just from the diagrams, check the u-substitution formula. If you do a non-volume-preserving change of coordinates (jacobian $\neq 1$), you'll need to think about traces and determinants diagrammatically.

(b) Just from the diagrams, check the Fubini theorem. This requires that $\partial \log \det A = \mathrm{tr}\, A^{-1} \partial A$, where LHS is the det that appears in the integral, and RHS is diagrammatic.

Now, let's say you have an actual manifold N and an actual smooth function $f : N \to \mathbb{R}$, and want the asymptotics of the integral $\int_M \exp(-\hbar^{-1} f)$. Well, if it has only one critical point, and if it's nondegenerate, then you can do this: pick that point as the marked point, apply the functor that remembers only the infinitesimal neighborhood, and use the diagrammatics.

4

With the remaining time, I'd like to talk about quantum mechanics. Let M be a manifold. A *path* is a continuous, piecewise smooth function $[0,1] \to M$. Then $\{\text{paths}\}$ is an infinite-dimensional smooth manifold. Pick $L : \mathrm{T}M \to \mathbb{R}$. It defines an *action* $\mathcal{A} : \{\text{paths}\} \to \mathbb{R}$ given by

$$\mathcal{A}(\gamma) = \int_0^1 L\big(\dot\gamma(t), \gamma(t)\big)\mathrm{d}t$$

Given coordinates on M (to identify jet bundles with powers of tangent bundle), the derivatives of A are

$$\mathcal{A}^{(n)}(\gamma) \cdot \xi_1 \cdots \xi_n = \int_0^1 \prod_{k=1}^n \left(\dot\xi_k \frac{\partial}{\partial v} + \xi_k \frac{\partial}{\partial q} \right) L \Big|_{(v,q)=(\dot\gamma,\gamma)} \mathrm{d}t$$

Here $\xi_k \in \mathrm{T}_\gamma\{\text{paths}\} = \text{sections of}\{\gamma^* \mathrm{T}M \to [0,1]\}$, the pull back of $\mathrm{T}M \to M$ along $\gamma : [0,1] \to M$.

We have a fiber bundle $\text{Endpoints} : \{\text{paths}\} \to M \times M$. Feynman says the time evolution operator for QM is $\psi \mapsto \int_M \psi(q_0)\, U(q_0, q_1)\, \mathrm{d}q_0$ (we pick a volume form on M), where

$$U(q_0, q_1) = \int\limits_{\gamma \in \text{Endpoints}^{-1}(q_0,q_1)} \exp\big(-(i\hbar)^{-1}\mathcal{A}(\gamma)\big)\mathrm{d}\gamma$$

where $\mathrm{d}\gamma = \prod_{0<t<1} \mathrm{d}\gamma(t)$ is a meaningless infinite product of volume forms. We have switched $\hbar \mapsto i\hbar$, and $\hbar = 10^{-34} \neq 1/\infty$ but no matter; let's try to define this integral diagrammatically.

We run into some challenges.

(a) First a non-challenge. The critical points of $\mathcal{A}$ on $\text{Endpoints}^{-1}(q_0, q_1)$ are precisely the classically-allowed trajectories connecting q_0 to q_1.

(b) When is the critical point nondegenerate, in the sense that $\ker \mathcal{A}^{(2)} \cap \mathrm{T}\big(\text{Endpoints}^{-1}(q_0, q_1)\big) = 0$? Exactly when the path is *nonfocal*: the corresponding classical flow is a local diffeomorphism. WARNING: if $\frac{\partial^2 L}{\partial v^2}$ is not positive definite, there might not be very many nonfocal paths. If we do have this convexity condition, then nonfocal paths are dense open among all classical paths.

Then $(\mathcal{A}^{(2)})^{-1}$ makes sense as a map $[0,1]^{\times 2} \to \mathrm{T}^{\otimes 2}M$, is given explicitly in terms of $\partial\gamma_{\text{classical}}/\partial(q_0, q_1)$, and has a discontinuity like $|s-t|$.

(c) We needed to define $\sqrt{\det\big(2\pi i\hbar (A^{(2)})^{-1}\big)}$. In finite dimensions, we have $\sqrt{\det(2\pi i \hbar)} = (2\pi i\hbar)^{\dim/2}$. What is the dimension of $\text{Endpoints}^{-1}(q_0, q_1)$? Well, dim(functions from n points to M) $= n \dim M$, and $\text{Endpoints}^{-1}(q_0, q_1)$ is roughly the functions from an open interval to M. But two open intervals and one point together make an open interval, so we set $\dim \text{Endpoints}^{-1}(q_0, q_1) = -\dim M$.

(d) How about the other part? For Fubini, etc., we need some relation between $\det \mathcal{A}^{(2)}$ and diagrams. In good situations, it works to take $\left|\det \mathcal{A}^{(2)}\right|^{-1} = \left|\det \frac{\partial^2 A^{(0)}}{\partial q_0 \partial q_1}\right|$, which is a bit ad hoc. For the sign, we again compare with finite dimensions. In finite dimensions, $\int \exp(iax^2/2)[\dots]$ has a sign like $\sqrt{\det 2\pi i} \times (-i)^{\text{morse index of } a}$. If $\frac{\partial^2 L}{\partial v^2}$ is positive definite, then the Morse index of $\mathcal{A}$ is always finite (and not otherwise).

(e) This biggest problem is that THE DIAGRAMS MIGHT DIVERGE. The intuition is that loops are like traces, and we're in infinitely many dimensions. The details are that $(\mathcal{A}^{(2)})^{-1}$ has a singularity like $|s-t|$, whereas vertices can differentiate the incoming edges — these correspond to the v dependence of L. Now, since L is a function of v, q, and not, say, acceleration, any given vertex differentiates any given edge at most once. But an edge can still be differentiated at each end, and $\frac{\partial^2 |s-t|}{\partial s \partial t} \sim \delta(s-t)$. But this isn't much of a problem: we'll do $\int \mathrm{d}s\mathrm{d}t$. So it's only a problem if there is a complete loop of edges, all of which are differentiated at both ends.

Now, if L is (inhomogeneous) quadratic in v, so that $L(v,q) = \frac{1}{2}a(q)\,v^2 + b(q)\,v + c(q)$, then any vertex differentiates at most two of its edges. And so divergent loops do not intersect. Let's take all our graphs, and pull the divergent loops far apart, and consider a sum of divergent loops. I.e. consider "wagon wheels" with n spokes, or rather the groupoid integral over all such things (fixed n). Then it turns out that

$$\text{groupoid} \int \text{ for wagon wheels with } n \text{ spokes} =$$

$$= \int_0^1 \left(\delta(0)\, \frac{\partial^n}{\partial q^n} \det a(q) \times [\dots] \Big|_{q=\gamma_{\text{classical}}(t)} + [\text{bounded}] \right) \mathrm{d}t$$

What do I mean by "$\det a$"? We've picked a volume form dVol on M. And a is a metric on M. A choice of volume form determines a "determinant" on metrics. For example, pick coordinates compatible with the volume form, and take the determinant of the representing matrix for a in these coordinates. Equivalently,

$$\det a = \frac{\text{volume determined by } a}{\mathrm{dVol}}$$

So we win if $\det a$ is constant, i.e. if dVol is the volume determined by a.

(f) Finally, everything we did depends on coordinates, because Taylor coefficients don't make sense coordinate-free — the jet space $\mathscr{J}^\infty M \cong \bigoplus \mathrm{T}^{\vee n} M$, but not canonically: picking an isomorphism is essentially equivalent to picking coordinates. So you use the "formal u-sub" to prove the coordinate invariance for paths that can be contained within coordinate patches. Then you use the "formal Fubini theorem" to cut long paths apart, compute, and glue back together.

Also, in the quadratic case, $U(q_0, q_1)$ formally satisfies Schrödinger's equation with correct initial values (allow paths of different durations). I'm definitely out of time, so for the proofs, I have articles on the arXiv, and I'll stop here.

Thank you.