Feynman Diagrams for Quantum Mechanics

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§ WKB

Recall from Kolya's Lectures: we have an operator $H = -\frac{\hbar^2}{2m}\Delta + V(q)$ acting on some function space $C(\mathbb{R}^n)$ — probably L^2, but then its unbounded, and in general any particular choice for this type of thing probably won't work. Anyway, we get the ~~[illegible]~~ unitary operator $U^\hbar(t) = \exp(\frac{i}{\hbar}\hat{H}t)$ and its kernel

$$U^\hbar(t, q_0, q_1) = \langle q_1 | U(t) | q_0 \rangle = \left(U^\hbar(t)(\delta_{q_0})\right)(q_1),$$

which is distributional and satisfies:

(1) Initial value: as $t \to 0$, $U^\hbar(t, q_0, q_1) \to \delta(q_0 = q_1)$ as di

(2) Schrödinger: $-i\hbar \frac{\partial}{\partial t} U^\hbar(t, q_0, q_1) = \hat{H}_{q_1} U^\hbar(t, q_0, q_1)$

(3) Semi-group: $U^\hbar(t_1 + t_2, q_0, q_2) = \int_{\mathbb{R}^n} U^\hbar(t_1, q_0, q_1) U^\hbar(t_2,$

As $\hbar \to 0$, we can ask two important "perturbative" questions:

(a) Analytical: As $\hbar \to 0$, does $U^\hbar(t, q_0, q_1)$ have an asymptotic expansion?

(b) Algebraic: What is it?

I'll make a few comments about (a) but basically ignore it, and focus on (b).

Let's take as an ansatz that $U^\hbar = \exp(\frac{i}{\hbar} S(t, q_0, q_1)) \cdot O(1)$

Then S satisfies the Hamilton-Jacobi equation $\frac{1}{2m}\frac{\partial^2 S}{(\partial q_1)^2} + V(q) = 0$.

We have a favorite solution for this, namely Hamilton's principal function:

~~Defn: Recall that {maps $[0,t] \to \mathbb{R}^n$ satisfying~~

Euler

<u>Defn</u>: Recall that the Euler-Lagrange equations are non-degenerate 2^{nd}
Then:

$$\begin{array}{c}\{\text{classical paths of duration } t\} \xrightarrow{\gamma \mapsto (\dot\gamma(0), \gamma(0))} T\mathbb{R}^n \text{ is an open submanifold} \\ \| \\ \{\text{paths } [0,t] \to \mathbb{R}^n \text{ satisfying EL}\}\end{array}$$

We can also take boundary conditions: $\{\text{classical paths of duration } t\} \to \mathbb{R}^n \times \mathbb{R}^n$ by $\gamma \mapsto (\gamma(0), \gamma(t))$. Say that γ is <u>non-focal</u> if this latter map is locally a diffeomorphism near γ.

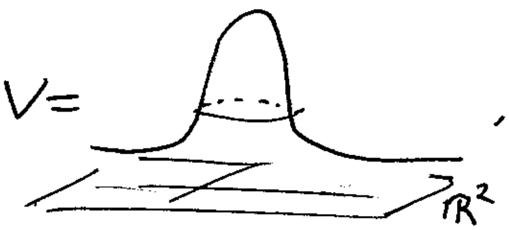
<u>Defn</u>: A 2nd-order classical mechanical system on a manifold M is <u>globally hyperbolic</u> if

$$\{\text{classical paths}\} \longrightarrow M \times M$$
$$\gamma \longmapsto (\gamma(0), \gamma(t))$$

is an isomorphism for all $t > 0$.

<u>Remark</u>: The analysis in 1a) is much simpler in the globally hyperbolic case.

<u>Counter example</u>: If $n=2$ and $V =$



, then not globally hyperbolic.

Anyway, <u>Defn</u>: Given a non-focal γ, extend to a family depending on $\gamma(0) = q_0$, $\gamma(t) = q_1$. Then the <u>Hamilton principal function</u> is $S_\gamma(t, q_0, q_1) = \int_{\tau=0}^{t} \text{action}(\gamma_{cl}(q_0, q_1 \ldots$

It is a partial function on $M \times M$ depending on a choice of γ, but I will suppress this.

Recall / Exercise:

If γ is non-focal, then $\dfrac{\partial^2 S_\gamma}{\partial \xi_0^i \partial \xi_1^j}$ is an invertible matrix, and to 1st-order in $\hbar$ a solution to Schrödinger's equation (2) is

$$\mathcal{U}^\hbar(t, \xi_0, \xi_1) \propto \exp\left(\frac{i}{\hbar} S_\gamma(t, \xi_0, \xi_1)\right) \cdot \sqrt{\left|\frac{\partial^2 S_\gamma}{\partial \xi_0 \partial \xi_1}\right|} \cdot (1 + \dots$$

Actually, to get (1), we should correct this by $\sqrt{2\pi\sqrt{-1}\hbar}^{\,n}$, at least when γ does not contain a focal subpath, so that the family can be continued to $t \to 0$.

Transfer equation:

So we take as an ansatz that

$$\mathcal{U}^\hbar = \exp\left(\frac{i}{\hbar} S\right) \cdot \sqrt{\left|\frac{\partial^2 S_\gamma}{\partial \xi_0 \partial \xi_1}\right|} \cdot \left(1 + \sum_{k \geq 1} (i\hbar)^k a_k(t, \xi_0, \xi_1) + O(\hbar^\infty)\right)$$

Then the a_k's satisfy an eikonal equation:

$$\left(+\frac{\partial}{\partial t} + \frac{1}{m}\sum_j \frac{\partial S}{\partial \xi_1^j}\frac{\partial}{\partial \xi_1^j}\right) a_k = \left(\frac{1}{2m}\Delta + \frac{1}{m}\sum_j \frac{\partial}{\partial \xi_1^j} \log \det\left|\frac{\partial^2 S}{\partial \xi_0 \partial \xi_1}\right| \frac{\partial}{\partial \xi_1^j}\right) a_{k-1}$$

$$+ \frac{1}{\ } \Delta(\sqrt{\ }) \dots$$

The goal of the remainder of this lecture and next is to give a heuristic derivation, and then a verification, of explicit integral expressions for the a_k functions.

Remark: Actually, everything works with time-varying m, V, and with a magnetic term $\sum_j B_j(q)\, \dot{q}^j$ in the Lagrangian. Oh, and with curved metrics on arbitrary manifolds, although that introduces subtleties that I hope to get to next time.

$\boxed{\S \text{ Path Integrals}}$

The way we will predict explicit integral formulas for the a_ks is by thinking about Quantum Mechanics from a very different perspective, namely Feynman's path integral. Recall that $U^\hbar(t, q_0, q_1)$ satisfies a gluing equation:

$$\int_{\mathbb{R}^n} U^\hbar(t_1, q_0, q_1)\, U^\hbar(t_2, q_1, q_2)\, dq_1 = U^\hbar(t_1+t_2, q_0, q_2)$$

If we subdivide $[0,t]$ into many small pieces, then

$$U(t, q_0, q_1) = \int_{\text{maps}: \gamma: \{\frac{t}{N}, \frac{2t}{N}, \ldots, \frac{(N-1)t}{N}\} \to \mathbb{R}^n} \prod U\left(\tfrac{t}{N}, \gamma(\tau), \gamma(\tau + \tfrac{t}{N})\right) d\gamma$$

where the product ranges over $\tau = \{0, \frac{t}{N}, \frac{2t}{N}, \ldots, \frac{(N-1)t}{N}\}$, and $d\gamma = \prod_{\tau \in \{\frac{t}{N}, \ldots, \frac{(N-1)t}{N}\}} d\gamma(\tau)$. Writing $U^\hbar = \exp(\frac{i}{\hbar} S^\hbar)$, we have

$$= \int_{\text{maps}} \exp\left(\frac{i}{\hbar} \sum_\tau S^\hbar\left(\tfrac{t}{N}, \gamma(\tau), \gamma(\tau + \tfrac{t}{N})\right)\right) d\gamma.$$

Now, if the potential $V(q)$ ~~[illegible]~~ satisfies some conditions, then we can estimate $\mathcal{U}^{\hbar}(\frac{t}{N}, q_0, q_1)$ for $N \to \infty$ to be supported only when $|q_1 - q_0| = O(\frac{1}{N})$, and then $S^{\hbar} \approx S_{cl}(\frac{t}{N}, q_0, q_0 + \frac{t}{N} v_0) \approx \frac{t}{N} \cdot L(q_0; v_0)$. Warning: these estimates break down in many interesting cases.

~~Also~~ So then we can make a huge leap of faith that these estimates are sufficiently uniform to survive in the ~~[illegible]~~ limit as $N \to \infty$ of the $\overset{N}{\prod}$. If they do, we would have:

<u>Prediction (Feynman):</u>

$$(*) \qquad \mathcal{U}^{\hbar}(t, q_0, q_1) = \int\limits_{\substack{\text{Maps } \gamma : [0,t] \to \mathbb{R}^n \\ \text{s.t. } \gamma(0) = q_0,\ \gamma(1) = q_1}} \exp\left(\frac{i}{\hbar} \int_{\tau=0}^{t} L(\gamma(\tau), \dot\gamma(\tau))\, d\tau\right)$$

what kind of maps? Who knows?

There are ways to define this integral analytically, at least when $V(q)$ allows the above estimates (say, grows not worse than quadratically in q, ...), essentially by approximating paths by piecewise lines. ~~[illegible]~~ ~~[illegible]~~ The answer is ~~very~~ quite sensitive to the details of the approximation used, and I will ~~try~~ ignore it. Instead, let's try to get the $\hbar \to 0$ asymptotics.

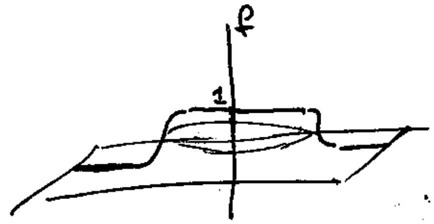
§ Asymptotics of oscillating integrals

What we will do is to pretend that the RHS of (*) is well-defined, and that infinite-dimensional oscillating integrals enjoy the same asymptotics as do finite-dimensional ones. So let's study:

$$\int_{\mathbb{R}^N} \exp\left(\frac{i}{\hbar} A(x)\right) dx, \qquad A \text{ a smooth function.}$$

Of course, this integral is not absolutely convergent, but it might be conditionally convergent. But then the method used to approximate it matters. We will take:

$$= \lim_{(\operatorname{supp} f \to \infty)} \int_{\mathbb{R}^N} f \exp\left(\frac{i}{\hbar} A(x)\right) dx, \qquad f \text{ a compactly-supported bump function.}$$



In particular, we will use <u>smooth</u> cut-offs.

<u>Fundamental Theorem of oscillating integrals</u>

Let f be a <u>compactly supported</u> <u>smooth</u> function and A smooth. If A has <u>no</u> critical points within the support of f, then

$$\int f \exp\left(\frac{i}{\hbar} A\right) = O(\hbar^{\infty}).$$

<u>Remark</u>: the coeffs in the estimates depend on $|f'|$,

Cor: Modulo $O(\hbar^\infty)$, we only care about the germ of A near its critical locus $\{dA = 0\}$.

Now let's make a strong assumption:

(i) $\{dA=0\}$ is finite

(ii) at each critical point, the hessian $\dfrac{\partial^2 A}{\partial x^i \partial x^j}$ is a nondegenerate matrix.

Using (i) and the corollary, we have:

$$\int \exp(\tfrac{i}{\hbar}A) = \sum_{p \in \{dA=0\}} \int f_p \exp(\tfrac{i}{\hbar}A) + O(\hbar^\infty)$$

where f_p is a bump function around p with $\operatorname{supp}(f_p) \cap \{dA=0\} = \{p\}$.

So now we study just $\int f_p \exp(\frac{i}{\hbar}A)$, and translate coords s.t. $p=0$.

Fact: Given (ii), we can work in a formal nbhd of p, not just a small one. I.e. we can replace A by its Taylor expansion.

What I mean is, let's be physicists, derive a formulas and then later do the estimates to see if it works. Actually, … but refer instead to the notes by Evans + Zworski.

So, we want:

$$\int_{\mathbb{R}^N} \exp\left(\frac{i}{\hbar} \sum_{k=0}^{\infty} \frac{A^{(k)}}{k!} x^k \right) dx.$$

note: $A^{(1)} = 0$, since we said $p=0$ is a critical point.

$$= \exp\left(\frac{i}{\hbar} A^{(0)}\right) \int \underbrace{\exp\left(\frac{i}{\hbar} A^{(2)} \frac{x^2}{2}\right) \exp\left(\sum_{k\geq 3}\right) dx}_{\uparrow \text{ a Gaussian!}}$$

change coordinates $\xi = \frac{x}{\sqrt{\hbar}}$.

$$= \exp\left(\frac{i}{\hbar} A^{(0)}\right) \int \exp\left(i A^{(2)} \frac{\xi^2}{2}\right) \overbrace{\exp\left(i \underbrace{\sum_{k\geq 3} \hbar^{\frac{k}{2}-1} A^{(k)} \frac{\xi^k}{k!}}_{= O(\sqrt{\hbar}),\ \text{justifying the use of Taylor expansion...}} \right)} d\xi \sqrt{\hbar}^{N}.$$

$$\overbrace{= \sum_{l\geq 0} \frac{i^l}{l!} \left(\sum_{k\geq 3} \hbar^{\frac{k}{2}-1} A^{(k)} \frac{\xi^k}{k!} \right).}$$

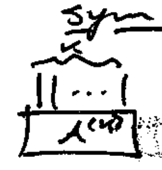
Who knows how to compute Gaussian integrals?
First, we need to make the integral converge. What we do is to push the contour into the complex plane s.t. $iA^{(2)}$ has negative-definite real part.

<u>Exercise:</u> If $A^{(2)}$ is a real symmetric nondegenerate 2-ten[sor]

then $$\int_{\mathbb{R}^N} \exp\left(i A^{(2)} \xi^2/2\right) d\xi = \sqrt{2\pi i}^{\,N} \cdot \frac{1}{\sqrt{|\det A^{(2)}|}} \cdot i^{-\eta(A^{(2)})}$$

~~Know How to~~ Here "$\sqrt{i}^N$" $= e^{i\frac{N\pi}{4}}$, and $\eta(A^{(2)}) \overset{\text{def}}{=}$ the number of negative eigenvalues of $A^{(2)}$ = maximal dimension of any subspace of $\mathbb{R}^N$ on which $A^{(2)}$ is neg. def = dim of any maximal subspace of $\mathbb{R}^N$ on which $A^{(2)}$ is negative definite.

Now, what about all the other terms? First, how to represent them? We have
$$\sum_{l=0}^{\infty} \frac{1}{l!}\left(\sum_{k=3}^{\infty} A^{(k)} \frac{x^k}{k!}\right)^l.$$

<u>Remember:</u> x is really a <u>vector</u> of variables, i.e. a $(1,0)$-tensor, so $x^k = x^{\otimes k}$ is a $(k,0)$ tensor, and $A^{(k)}$ is a sym. $(0,k)$-tensor. So we can think of $A^{(k)} =$ , $x =$ .

How to go from boxes to $\sum A^{(k)} \frac{x^k}{k!}$? ~~take~~ The function A picks out a map

$$\{\text{vertices}\} \longmapsto \text{functions on } \mathbb{R}^N$$

 $\longmapsto A^{(k)} x^k$.

~~But~~ LHS is a groupoid $\mathcal{G}$, and this ~~map~~ function is equivariant: $\mathcal{G} \longrightarrow \mathcal{O}(\mathbb{R}^N)$. Anyway,

$$\cancel{A(x)} \sum A^{(k)} \frac{x^k}{k!} = \int_{\mathcal{G}} (\text{this assignment}).$$

Or, if we just want the sum to start w/ cubics, set

$$\mathcal{G} = \{\text{vertices w/ valence} \geq 3\}.$$

<u>Exercise:</u> Consider the groupoid "$\exp(\mathcal{G})$" w/ objects = disjoint unordered collections of vertices. and obvious symmetries. E.g. $\emptyset$, 

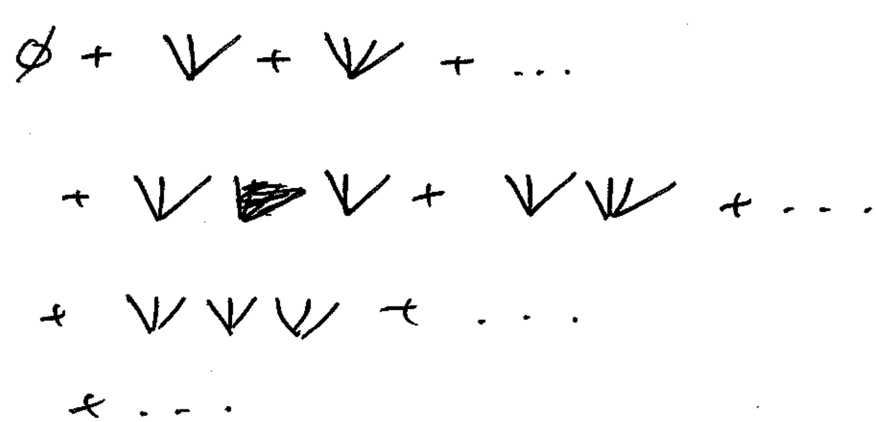
Then $\int_{\exp(\mathcal{G})} (\text{this assignment}) = \exp\left(\int_{\mathcal{G}} (\cdots)\right)$

extend by $\sqcup \mapsto \cdot$

Remark: If we used ordered ~~set~~ collections, you'd get $\frac{1}{1-}$

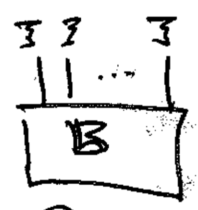
So, we want to compute

$$\int d\xi \, \exp\left(i\lambda^{(2)}\frac{\xi^2}{2}\right)\cdot \underbrace{\sum_{l\geq 0}\frac{1}{l!}\left(\sum_{k\geq 3}\lambda^{(k)}\frac{\xi^k}{k!}\right)^{l}}_{\|}$$



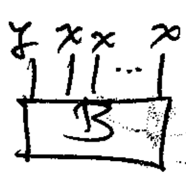
At each summand, we don't naturally have a symmetric tensor, but just some tensor,
So we need to understand

$$\int d\xi \, \exp\left(i\lambda^{(2)}\frac{\xi^2}{2}\right)\cdot$$



$B\cdot\xi^m$.

Prop: Given a tensor B, consider the function of two variables $B\cdot y x^{m-1} =$



($y, x \in \mathbb{R}^N$ Then

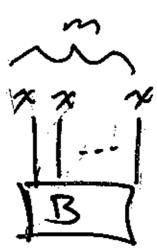
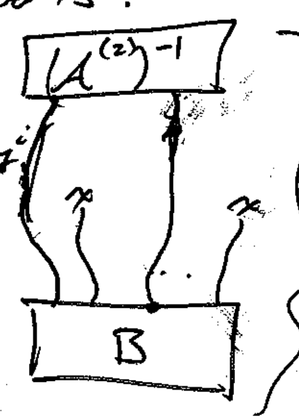
$$\int_{\mathbb{R}^N} dx \, \exp\left(\sqrt{-1}\, A^{(2)} \frac{x^2}{2}\right) \; B x^m$$

$$= \int_{\mathbb{R}^N} dx \, \exp(\;) \sum_{i,j} \frac{\partial}{\partial x^i}\frac{\partial}{\partial y^j}\left(B y x^{m-1}\right) \cdot \left(\left(A^{(2)}\right)^{-1}\right)^{\{i,j\}} \cdot (\ldots$$

$\sqrt{-}$

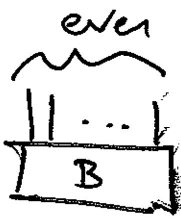
$(i,j) = 1, \dots, N$

Proof: Exercize. Hint: $\int$ by parts.

$\int \exp(\,) \cdot \Bigg($  $\Bigg) = \int \exp(\,) \cdot$  ← degree m x

Σ choices of the second so

Cor: $\int \exp() \cdot (\text{odd degree}) = 0.$

$\int \exp() \cdot$  $= \left(\int \exp()\right) \cdot \sum$ choices: 

$= \left(\int \exp\right) \cdot$ ~~…~~ groupoid integral over

Cor:

$$\int_{\mathbb{R}^N} d\xi \, \exp\left(iA^{(2)}\frac{\xi^2}{2}\right) \cdot \sum_{\ell\geq 0} \frac{1}{\ell!}\left(\sum_{k\geq 3} i\hbar^{\frac{k}{2}-1} A^{(k)} \frac{\xi^k}{k!}\right)^{\ell}$$

$$= \left(\int_{\mathbb{R}^N} d\xi \, \exp\left(iA^{(2)}\frac{\xi^2}{2}\right)\right) \cdot \int_{\mathcal{G}} (\text{Feynman rules})$$

where $\mathcal{G}$ = groupoid of closed diagrams, all vertices trivalent or higher.

(Feynman rules) =  $\longmapsto i\hbar^{\frac{k}{2}-1} A^{(k)}$

$\frown \longmapsto (+i)\cdot \left(A^{(2)}\right)^{-1}$

extend $\sqcup \mapsto \otimes$, contraction of diagrams $\mapsto$ contraction of tensors

[Aside: Cat$^{\vee}$ of graphs, sym$\otimes$, (Feynman rules) = $\overset{\text{sym}\otimes}{\text{functor}}$ Graphs $\to$ Ve…
enriched in groupoids.
$\mathcal{G} = \mathrm{Hom}(\emptyset, \emptyset)$

Slight rewriting:  $\mapsto -A^{(k)}$, so $\hbar$=…

$\frown \mapsto \left(A^{(2)}\right)^{-1}$

All together:

smooth bump picking out c.p. at 0.

$$\int_{\mathbb{R}^N} f \exp\left(\frac{i}{\hbar} A(x)\right) dx = O(\hbar^\infty) +$$

$$+ \exp\left(\frac{i}{\hbar} A^{(0)}\right) \cdot \sqrt{2\pi\hbar i}^{\,N} \cdot \frac{1}{\sqrt{|\det A^{(2)}|}} \cdot (-i)^{Z(A}$$

$\cdot$ Sum of diagrams w/ all vertices valence ≥ 3

 $\longmapsto (A^{(2)})^{-1}$

 $\longmapsto -A^{(k)}$

each diagram is weighted by $(i\hbar)^{\text{Euler}}$

Thm: RHS computes asymptotics of LHS. See Evans+Zwo
or Exercise

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§ Comparison with WKB

Finally, recall the WKB expansion

$$U = \exp\left(\frac{i}{\hbar} S\right) \cdot \sqrt{2\pi\hbar i}^{\,-n} \cdot \sqrt{\left|\det \frac{\partial^2 S}{\partial q_0 \partial q_1}\right|} \cdot (-i)^{\#} \cdot \left(1 + O(\hbar)\right).$$

The function $S = S(t, q_0, q_1)$ is nothing but $A^{(0)}$ as now "x" ranges over paths $[0,t] \to \mathbb{R}^n$ sending $0 \mapsto q_0$ and $t \mapsto q_1$, and ~~that the~~

$$A(x) = \int_0^t L(\dot{x}, x)\, d\tau$$

is the classical action.

The comparison suggests that

$$\text{"}\dim\{\text{paths}\}\text{"} = -n,$$

whatever that is supposed to mean, and that

$$\left|\det A^{(2)}\right| = \left|\det \frac{\partial^2 S}{\partial q_0 \partial q_1}\right|^{-1},$$

where $A^{(2)}$ ~~is~~ can be interpretted as the differential operator for Jacobi fields — this equation at least can be justified using zeta regularization. There is a Morse-Maslov term which vanishes when there is a unique classical path connecting any two points; otherwise it makes sense and is finite.

Finally, there is the $(1+O(\hbar))$ corrections. In fact, one can make sense of Feynman diagrams for A=action, and the diagrams do satisfy Schrodinger and are the asymptotics of WKB.