The Formal Path Integral in Quantum Mechanics

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Subfactor Seminar, UC Berkeley

These slides available at
`http://math.berkeley.edu/~theojf/QMtalk.pdf`

Outline

Introduction

What the path integral should be and why we want it

Motivating the definition: finite-dimensional integrals

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(Lagrangian) Classical Mechanics

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$$U(t, q_0, q_1) = \int_{\substack{\text{paths } \varphi:[0,t]\to\mathcal{N} \\ \varphi(0)=q_0,\, \varphi(t)=q_1}} \exp\left(\frac{i}{\hbar}\mathcal{A}(\varphi)\right) d\varphi$$

where $d\varphi = \prod_{0<\tau<t} d\varphi(\tau) = \prod_{0<\tau<t} d\,\mathrm{Vol}$, and $\hbar \neq 0$ is a real variable.

Physical Motivation for the Path Integral

- For each t, the map $\psi \mapsto \int_{\mathcal{N}} U(t, q_0, -)\, \phi(q_0)\, dq_0$ defines a unitary operator $U(t)$ on $L^2(\mathcal{N})$.

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Therefore $U(t)$ is the quantum-mechanical time evolution operator for $(\mathcal{N}, L)$, and gives a canonical quantization.
But analytic definitions (Wiener measure) don't generalize well.

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But it only works when:

- $L(v, q) = \frac{1}{2}a(q)\cdot v^2 + b(q)\cdot v + c(q)$, where c is a function on $\mathcal{N}$, b is a one-form, and a is a Riemannian metric.

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- $d\,\mathrm{Vol} = \sqrt{|\det a|}$.
- γ satisfies a nondegeneracy condition.

Motivating the Definition: Finite-Dimensional Integrals

Theorem

Let $\mathcal{M}$ be a finite-dimensional manifold with volume form $d\,\mathrm{Vol}$, and $f : \mathcal{M} \to \mathbb{R}$ a Morse function with finitely many critical points and good growth at infinity. Then:

$$\int_{\mathcal{M}} \exp\left(\frac{i}{\hbar} f\right) d\,\mathrm{Vol} = (2\pi i\hbar)^{\dim \mathcal{M}/2} \times$$

$$\times \sum_{\text{critical points } c} \exp\left(\frac{i}{\hbar} f(c)\right) (-i)^{\eta(c)} \left|\det f^{(2)}(c)\right|^{-1/2} (1 + O(\hbar))$$

$\eta(c)$ is the Morse index, and $f^{(2)}(c)$ is the Hessian.

For details, see [Evans and Zworski, 2007].

The Higher-order Asymptotics

To describe the $O(\hbar)$ part:

- Pick coordinates $x : \mathcal{M} \to \mathbb{R}^{\dim \mathcal{M}}$ near c so that $x(c) = 0$ and $d\,\mathrm{Vol} = dx$.
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$$f(x) = \sum_{n=0}^{\infty} f^{(n)} \cdot \frac{x^{\otimes n}}{n!} + O(x^{\infty})$$

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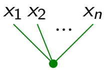
$$f(x) = \sum_{n=0}^{\infty} f^{(n)} \cdot \frac{x^{\otimes n}}{n!} + O(x^{\infty})$$

Each $f^{(n)}$ is a symmetric linear map $(\mathbb{R}^{\dim \mathcal{M}})^{\otimes n} \to \mathbb{R}$.
$f^{(1)} = 0$ and $f^{(2)}$ is invertible as a map $\mathbb{R}^{\dim \mathcal{M}} \to (\mathbb{R}^{\dim \mathcal{M}})^*$.

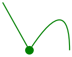
Feynman Diagrams

Define the graphical calculus:



$$= -f^{(n)} \cdot (x_1 \otimes \cdots \otimes x_n)$$

$$= \left(f^{(2)}\right)^{-1}, \text{ i.e.}$$



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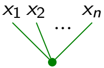

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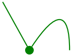

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Definition

A Feynman diagram is a combinatorial graph Γ (possibly empty, disconnected, etc.). $\mathrm{ev}(\Gamma)$ evaluates the diagram with respect to the above Feynman rules. $\chi(\Gamma) = |V| - |E|$ is its Euler characteristic. $|\mathrm{Aut}\,\Gamma|$ is its number of symmetries.

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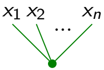

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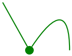

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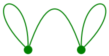
Example

$\mathrm{ev}\Bigg($  $\Bigg) = \left(f^{(3)}\right)^{\otimes 2} \circ \left(\left(f^{(2)}\right)^{-1}\right)^{\otimes 3}$. $\chi = -1$. $|\mathrm{Aut}| = 8$.

Full Asymptotics of Finite-Dimensional Integrals

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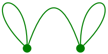
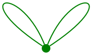
$$= \sum(\dots) \times \Bigg(1 + \frac{i\hbar}{8}$$  $$+ \frac{i\hbar}{12}$$  $$+ \frac{i\hbar}{8}$$  $$+ \dots \Bigg)$$

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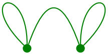
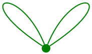
$$= \sum(\dots) \times \Bigg(1 + \frac{i\hbar}{8}$$  $$+ \frac{i\hbar}{12}$$  $$+ \frac{i\hbar}{8}$$  $$+ \dots \Bigg)$$

Exercise

For $\mathcal{M} = \mathbb{R}$ and $f(x) = \frac{x^2}{2} + \frac{x^3}{6}$, find the sum explicitly; show it has zero radius of convergence in $\hbar$.

Defining the Formal Path Integral

Recall

We want to define:

$$U(t, q_0, q_1) = \int_{\substack{\text{paths } \varphi:[0,t]\to\mathcal{N} \\ \varphi(0)=q_0,\, \varphi(t)=q_1}} \exp\left(\frac{i}{\hbar}\mathcal{A}(\varphi)\right) d\varphi$$

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We will define it as a sum over classical paths γ of contributions U_γ. Each of these we will define as a formal series in analogy with the finite-dimensional case.

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Problem

We need a notion of the Taylor expansion of $\mathcal{A}$ near a path γ.

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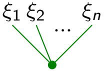
Solution

Pick local coordinates q on $\mathcal{N}$ and induced fiber coordinates v on $\mathrm{T}\mathcal{N}$. Assume that γ is contained entirely within the coordinate patch. Recall: $\mathcal{A}(\varphi) = \int_{\tau=0}^{t} L\big(\dot\varphi(\tau), \varphi(\tau)\big)\, d\tau$. Then:

$-$ 

$$= \mathcal{A}^{(n)}(\gamma) \cdot (\xi_1 \otimes \cdots \otimes \xi_n) =$$

$$= \int_0^t \prod_{k=1}^{n} \sum_{i_k=1}^{\dim \mathcal{N}} \left(\dot\xi_k^{i_k}(\tau) \frac{\partial}{\partial v^{i_k}} + \xi_k^{i_k}(\tau) \frac{\partial}{\partial q^{i_k}} \right) L \Big|_{(v,q)=(\dot\gamma(\tau),\gamma(\tau))} d\tau$$

$\xi_1, \dots, \xi_n : [0,t] \to \mathbb{R}^{\dim \mathcal{N}}$ are continuous piecewise-smooth. The partial derivatives act only on $L(v,q)$.

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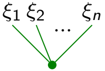
$-$ 

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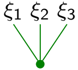
Example

Let $L(v,q) = \frac{1}{2}|v|_a^2 = \sum_{ij} \frac{1}{2} a_{ij}(q)\, v^i v^j$ where a is a Riemannian metric. Then, summing all repeated indices:



$$= -\int_0^t \Bigg(\dot\xi_1^{i_1}(\tau)\,\dot\xi_2^{i_2}(\tau)\,\xi_3^{i_3}(\tau)\,\frac{\partial a_{i_1 i_2}}{\partial q^{i_3}}(\gamma(\tau)) + \text{permutations} +$$

$$+\, \dot\xi_1^{i_1}(\tau)\,\xi_2^{i_2}(\tau)\,\xi_3^{i_3}(\tau)\,\frac{\partial^2 a_{i_1 j}}{\partial q^{i_2}\partial q^{i_3}}(\gamma(\tau))\,\dot\gamma^j(\tau) + \text{permutations} +$$

$$+\, \xi_1^{i_1}(\tau)\,\xi_2^{i_2}(\tau)\,\xi_3^{i_3}(\tau)\,\frac{\partial^3 a_{j_1 j_2}}{\partial q^{i_1}\partial q^{i_2}\partial q^{i_3}}(\gamma(\tau))\,\frac{\dot\gamma^{j_1}(\tau)\,\dot\gamma^{j_2}(\tau)}{2}\Bigg)\, d\tau$$

When a is not constant, these are non-zero. Integrating by parts, the first derivatives are the Christoffel symbols.

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$\mathcal{A}$ is not necessarily a Morse function on fibers of $\{\text{paths}\} \to \mathcal{N} \times \mathcal{N}$. I.e. $\mathcal{A}^{(2)}$ might have zero-modes among ξs with $\xi(0) = 0 = \xi(t)$.

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Solution

A classical path $\gamma : [0, t] \to \mathcal{N}$ is nondegenerate if $\mathcal{A}^{(2)}|_{\xi(0)=0=\xi(t)}$ has trivial kernel. Only try to integrate near nondegenerate paths.

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A classical path γ is nondegenerate if and only if it is a member of a family of classical paths that depend smoothly on the boundary conditions $\gamma(0) = q_0$, $\gamma(t) = q_1$.

The Nondegeneracy Condition

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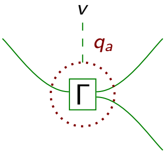
Always extend to families, so everything depends on t, q_0, q_1.

Feynman Rules for Derivatives

We introduce a new Feynman rule. We have defined ev(vertices), and we will later define ev(edges). If Γ is a Feynman diagram, $a = 0, 1$, and $v \in \mathrm{T}_{q_a}\mathcal{N}$, we define:



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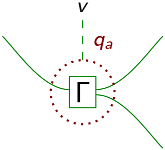

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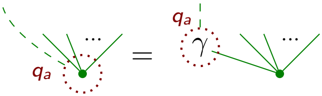

Back to the definition of a vertex

One More Feynman Rule

Definition

Let γ be a family of classical paths depending smoothly on the boundary conditions $\gamma(0) = q_0$, $\gamma(t) = q_1$. The Hamilton-Jacobi function is:

$$S_\gamma(t, q_0, q_1) = -\bullet = \mathcal{A}^{(0)} = \int_0^t L\big(\dot{\gamma}(\tau), \gamma(\tau)\big)\, d\tau$$

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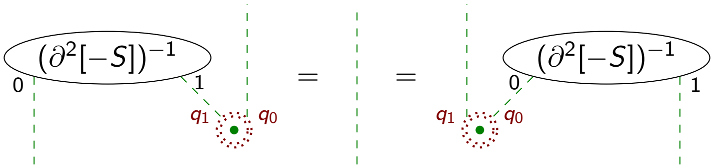

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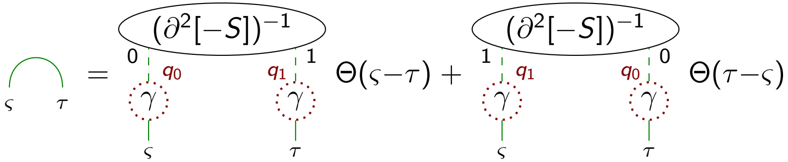

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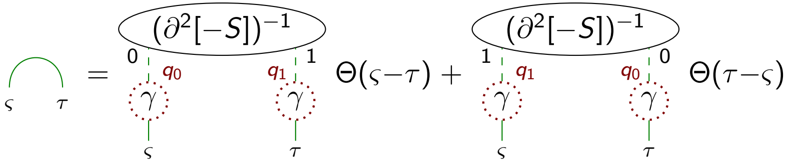

$$= \Theta(\varsigma - \tau) \sum_{i,j=1}^{\dim \mathcal{N}} \frac{\partial \gamma}{\partial q_0^i}(\varsigma) \left(\left(\frac{\partial^2 (-S_\gamma)}{\partial q_0 \partial q_1} \right)^{-1} \right)^{ij} \frac{\partial \gamma}{\partial q_1^j}(\tau) +$$

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So, in:

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By thinking about units, declare: $\dim\{\text{paths}\} = -\dim\mathcal{N}$.

Ultraviolet Divergences

Problem

Individual diagrams may represent divergent integrals.

Exercise

Compute the path integral for $L(v, q) = \frac{v^2}{2q^2}$ on $\mathcal{N} = \mathbb{R}_{>0}$.

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Solution

Theorem

Suppose that $L(v,q) = \frac{1}{2}\sum_{ij} a_{ij}(q)\cdot v^i v^j + \sum_i b_i(q) v^i + c(q)$ *and* $\det a(q) = 1$ *for all* q*. Then divergences cancel at each order in* $\hbar$*.*

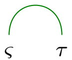
Our proposed definition is justified only if $d\,\mathrm{Vol} = dq$. The condition on the determinant is the compatibility condition $d\,\mathrm{Vol} = \sqrt{|\det a|}$.

▸ Skip Proof

Proof of Cancelation of Divergences

Proof

- Divergences arise because the Green's function is $\sim |\varsigma - \tau|$, so if you take two derivatives, you get $\sim \delta(\varsigma - \tau)$. More precisely:



$$\frac{\partial^2}{\partial\varsigma\partial\tau}\left[\quad \right] = a^{-1}\big(\gamma(\tau)\big)\,\delta(\varsigma-\tau) + \text{finite}$$

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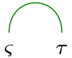

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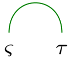

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- Mostly, this just identifies integration variables. The only problem is when vertices are identified too many times: divergences live on loops in Feynman diagrams.
- Because $L(v, q)$ is quadratic in v, no vertex differentiates more than two incoming edges: divergent loops do not intersect.

Proof of Cancelation of Divergences

- An n-valent vertex in a divergent loop must be contributing $-\frac{\partial^{n-2} a(q)}{\partial q^{n-2}}$, evaluated at $q = \gamma(\tau)$, to the integral.

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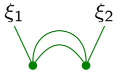

$$= \sum\!\!\!\!\!\!\int_{\substack{\tau \in [0,t] \\ i_1, i_2, i_3, i_4 \in \{1,\dots,\dim \mathcal{N}\} \\ j_1, j_2 \in \{1,\dots,\dim \mathcal{N}\}}} \Bigg(\delta(\tau - \tau)\, \xi_1(\tau)^{j_1}\, \xi_2(\tau)^{j_2} \times$$

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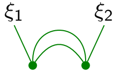

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- So each divergent loop is of the form $\delta(0) \times \int$(external edges) $\times$ Trace(product of a^{-1}s and $-\partial^n a$s)$d\tau$.

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- By assumption, $\det a(q) = 1$. So $\log\det a(q) = 0$. So:

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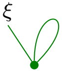

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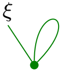

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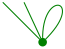
$= -$divergent part of  $+$ 

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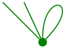
$= -$divergent part of  $+$ 

- In general, the nth derivative is, counting symmetry factors, the divergent part of the sum of all loops with n external edges. □

Back to Definitions: The Determinant

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Back to Definitions: The Determinant

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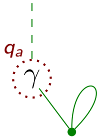

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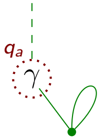

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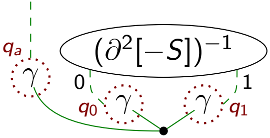

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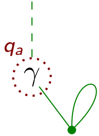

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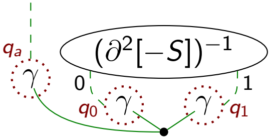

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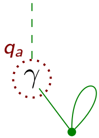

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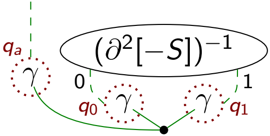

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Coordinate Independence

Problem

Our definition of the formal path integral depends on a choice of local coordinates.

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Solution

Theorem

When there are no UV divergences (or, rather, when the determinant is defined so that it has the correct derivatives), the value of the formal path integral is unchanged under volume-preserving changes of coordinates.

In particular, if two volume-compatible coordinate patches overlap and a classical nondegenerate path is contained in the intersection, then to compute the integral near that path you may work in either patch: the definitions agree. ▸ Skip Proof

Proof of Coordinate Independence

Proof

- It suffices to consider smooth maps $f : \mathbb{R}^n \to \mathbb{R}^n$ with $f(0) = 0$ and $f^{(1)}(0) = 1$, as there is good behavior under affine changes of variables.

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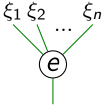
- But these are linear conditions on $\frac{\partial^2 f}{(\partial q)^2}$, and any function satisfying them integrates to a locally-volume-preserving map. So any two locally-volume-preserving maps are homotopic through such maps.
- So we restrict our attention to maps $f(q) = q + e(q)$, and work $o(e)$. By assumption, $\frac{\partial e}{\partial q} \in \mathfrak{sl}(n)$ for each q.

Proof of Coordinate Independence

- Expand $e(q)$ in Taylor series around $q = \gamma(\tau)$, thereby defining:



$$= \sum_{j_1,\dots,j_n} \frac{\partial^n e(q)}{\partial q^{j_1} \cdots \partial q^{j_n}} \bigg|_{q=\gamma(\tau)} \xi_1(\tau)^{j_1} \cdots \xi_n(\tau)^{j_n}$$

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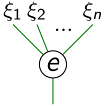

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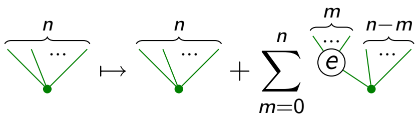
- Then under $q \mapsto q + e(q)$, we have up to $o(e)$:

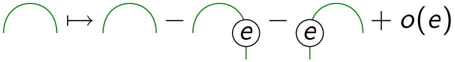


$+$ permutations

When $\xi_k(0) = \xi_k(t) = 0$ for all k, the $m = n$ summand is 0.

Proof of Coordinate Independence

- We also have:



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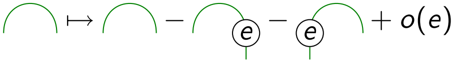

- Assuming $\det \mathcal{A}^{(2)}$ is defined correctly (i.e. no UV divergences), we have:

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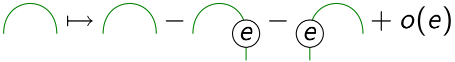

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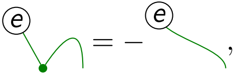
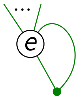
- Some cancellations are immediate in the sum:



$\pm \textcircled{e}$ from edge, vertex

Proof of Coordinate Independence

- The only diagrams that don't cancel immediately include components of the form:



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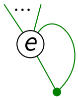

But these diagrams vanish because Trace $\frac{\partial e}{\partial q} = 0$ for all q. $\square$

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What about paths that are not contained in a coordinate patch?

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$$U_{12}(t_1 + t_2, q_1, q_2) = \int_{q \text{ near } \gamma_{12}(t_1)} U_1(t_1, q_1, q)\, U_2(t_2, q, q_2)\, dq$$

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The theorem requires all the choices so far: $\eta(\gamma)$, $\dim\{\text{paths}\}$, ...

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Proof

The formal path integral is non-zero as a distribution only if the corresponding classical path has momentum $= 0$ at an endpoint. $\square$

What We Have Done

- We have defined the formal path integral

$$U(t, q_0, q_1) = \int_{\substack{\text{paths } \varphi:[0,t]\to\mathcal{N} \\ \varphi(0)=q_0,\, \varphi(t)=q_1}} \exp\left(\frac{i}{\hbar}\mathcal{A}(\varphi)\right) d\varphi$$

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- For each classical path γ, $U_\gamma = (2\pi i\hbar)^{-\dim\mathcal{N}/2}(-i)^{\eta(\gamma)}\times$ $\times \exp\big((i\hbar)^{-1}(\text{classical action})\big) \times \big(\text{formal power series in } i\hbar\big)$.

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- U_γ satisfies the correct Fubini theorem / semigroup law.

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The Lagrangian $L(v,q) = \frac{1}{2}\sum_{ij} a_{ij}(q)\, v^i v^j + \sum_i b_i(q)\, v^i + c(q)$ defines a Schrödinger operator. In local coordinates such that $\det a(q) = 1$:

$$\hat{H}_q = \sum_{jk} \left(i\hbar \frac{\partial}{\partial q^j} + b_j(q) \right) \frac{(a^{-1})^{jk}}{2} \left(i\hbar \frac{\partial}{\partial q^k} + b_k(q) \right) - c(q)$$

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Theorem

For each classical nondegenerate path γ, $U_\gamma(t, q_0, q_1)$ satisfies Schrödinger's equation:

$$i\hbar \frac{\partial}{\partial t} U_\gamma(t, q_0, q_1) = \hat{H}_{q_1}\left[U(t, q_0, q_1)\right]$$

The Initial Value Problem

- The semigroup law and Schrödinger's equation almost imply that $\psi \mapsto \int_{\mathcal{N}} U(t, q_0, -)\, \psi(q_0)\, dq_0$ is the $\mathbb{R}$ action on $\mathrm{L}^2(\mathcal{N})$ describing the quantum-mechanical time evolution.

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Theorem

Let $\mathcal{O}$ be a convex open neighborhood of $(\mathcal{N}, a)$ with compact closure. Then there exists ϵ so that as distributions:

$$\lim_{t\to 0} \sum_{\substack{\gamma \text{ classical and nondegenerate} \\ \text{with boundary values } (t, q_0, q_1) \\ \text{varying in } (0,\epsilon)\times\mathcal{O}\times\mathcal{O}}} U_\gamma(t, q_0, q_1) = \delta(q_0, q_1)$$

In a Riemannian manifold, a neighborhood $\mathcal{O}$ is convex if any two points in $\mathcal{O}$ can be connected by a unique geodesic in $\mathcal{O}$.

Things I Would Like To Have Answers To

- When the measure is incompatible with the metric, there are UV divergences: e.g. $\mathcal{N} = \mathbb{R}_{>0}$, $L(v, q) = \frac{v^2}{2q^2}$. Are the divergences connected to the failure of $\hat{H}$ to be Hermitian? What else might they measure?

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- What is the correct (divergent) replacement for the determinant, so that Schrödinger equation, Fubini/semigroup law, coordinate-independence, etc., are still formally true?
- Most of the techniques used here work provided the matrix $\partial^2 L/\partial v^2$ is never degenerate. Is there a formal path integral that works in the degenerate case?

- These slides are at:
  `http://math.berkeley.edu/~theojf/QMtalk.pdf`
- For the case of quantum mechanics on $\mathbb{R}^n$, including the Schrödinger equation initial value problem, see:
  `http://math.berkeley.edu/~theojf/QM1.pdf`
- A second paper with the rest of the material should appear soon.