Renormalized Integrals and a Path Integral Formula for the Heat Kernel on a Manifold

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Contents

Path and functional integrals

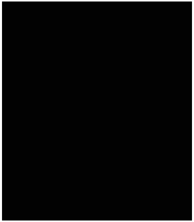
Path and functional integrals are a standard tool in theoretical physics.
But in most cases not mathematically rigorously defined.

Schrödinger equation:

$$i\hbar \frac{\partial u}{\partial t} = Hu$$

where e.g. $H = \Delta - V = \sum_j \frac{\partial^2}{\partial x_j^2} - V$.

Feynman's view on quantum mechanics



Richard Feynman (1918-1988)

Solution of Schrödinger equation given by

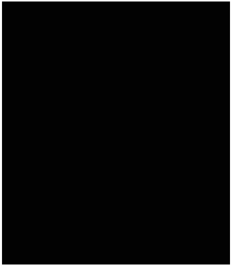
$$u(t,x) = \int_{\mathbb{R}^3} K(t,x,y) u_0(y)\, d^3 y$$

where

$$K(t,x,y) = \int \exp\left(\frac{i}{\hbar}\int_0^t L(\gamma,\dot{\gamma})dt\right)\mathcal{D}\gamma$$

Does it make sense?

Problem: What does $\mathcal{D}\gamma$ mean?



Mark Kac (1914-1984)

Formally replace it by t!
Yields diffusion equation

$$\frac{\partial u}{\partial t} = Hu$$

Heuristic formulas

For operator $H = \Delta - V$ consider the Cauchy problem for the heat equation

$$\begin{cases} \frac{\partial u}{\partial t} = Hu \\ u(x,0) = u_0(x) \end{cases}$$

Brownian motion $\Rightarrow$ heuristic path integral formula:

$$u(t,x) = \frac{1}{Z} \int_{P_x(t)} \exp\left(-\frac{1}{2}\mathrm{E}(\gamma) - \int_0^t V(\gamma(s))\, ds \right) \cdot u_0(\gamma(t))\, \mathcal{D}\gamma.$$

Problems

$$u(t,x) = \frac{1}{Z} \int_{P_x(t)} \exp\left(-\frac{1}{2}\mathrm{E}(\gamma) - \int_0^t V(\gamma(s))\,ds\right) \cdot u_0(\gamma(t))\,\mathcal{D}\gamma.$$

Problems:

- $P_x(t)$ is infinite-dimensional and the measure $\mathcal{D}\gamma$ does not exist.
- Energy $E(\gamma) = \frac{1}{2}\int_0^t |\dot{\gamma}(s)|^2 ds$ is defined only for differentiable paths.
- The normalizing factor $1/Z$ is infinite.

1. Solution: The measure $d\mathbb{W} = \frac{1}{Z}\exp\left(-\frac{1}{2}\mathrm{E}(\gamma)\right)\mathcal{D}\gamma$ does exist.

Feynman-Kac formula

Feynman-Kac Formula:

$$u(t,x) = \int_{P_x(t)} \exp\left(-\int_0^t V(\gamma(s))\,ds\right) \cdot u_0(\gamma(t))\,d\mathbb{W}(\gamma)$$

Problems with this:

- For $V = 0$ this formula is a tautology.
- Kinetic and potential energy are treated differently.
- Does not work for the Schrödinger equation.

2. Solution: Finite-dimensional approximation (later)

Riemannian Manifolds

Replace $\mathbb{R}^n$ by an n-dimensional *Riemannian Manifold*

Notation: $B(x,r) = \{y \in M \mid \mathrm{dist}(x,y) \leq r\}$

$V(x,r) = \mathrm{vol}_n(B(x,r))$

$A(x,r) = \mathrm{vol}_{n-1}(\partial B(x,r))$

Model Manifolds

In polar coordinates the Euclidean metric of $\mathbb{R}^n$ is given by

$$ds^2 = dr^2 + r^2 d\sigma^2$$

Replace this by a more general metric of the form

$$ds^2 = dr^2 + f(r)^2 d\sigma^2$$

where $f : [0, \infty) \to \mathbb{R}$ is
a smooth function s. t.

- $f(0) = 0$
- $f'(0) = 1$
- $f(r) > 0$ for $r > 0$

Sphere

metric of S^n:

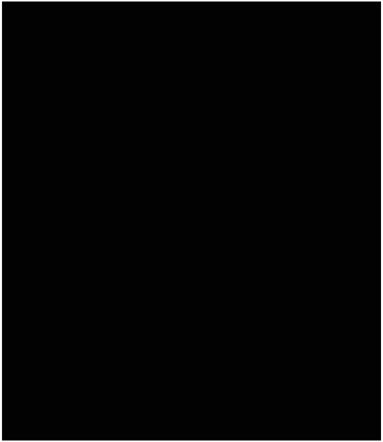
$$ds^2 = dr^2 + \sin(r)^2 d\sigma^2$$

Here f is defined only on $[0, \pi]$

Hyperbolic Space

metric of H^n:

$$ds^2 = dr^2 + \sinh(r)^2 d\sigma^2$$



M. C. Escher
Circle Limit III
(wood-cut, 1958)

Criteria for Stochastic Completeness

Sufficient criteria:

[redacted]

[redacted]

Yau 1976:
$\mathrm{Ric} \geq -C$ for some $C \in \mathbb{R}$

Grigoryan 1986:
$\int^{\infty} \frac{r\,dr}{\log(V(x,r))} = \infty$ for some $x \in M$

Remark: Grigoryan's criterion is applicable if
$V(x,r) \leq \exp(C \cdot r^2)$
Both criteria show: $\mathbb{R}^n$ and H^n are stochastically complete $\forall n$.

Stochastic Completeness of Model Manifolds

Model manifold = $\mathbb{R}^n$ with complete $\mathrm{O}(n)$-invariant metric

Model Manifold stochastically complete $\Leftrightarrow$

$$\int^{\infty} \frac{V(r)}{A(r)} dr = \infty$$

Example for stochastically incomplete (but metrically complete) Model Manifold ($\alpha > 2$)

$$\begin{aligned} V(r) &= \exp(r^{\alpha}), \qquad r \geq 1 \\ A(r) &= V'(r) = \alpha r^{\alpha-1} \exp(r^{\alpha}) \end{aligned}$$

Recurrence of Model Manifolds

Model Manifold recurrent $\Leftrightarrow$

$$\int^{\infty} \frac{1}{A(r)} dr = \infty$$

Example: $M = \mathbb{R}^n$

$A(r) = \omega_{n-1} r^{n-1} \Rightarrow \int^{\infty} \frac{dr}{A(r)} = C \cdot \int^{\infty} \frac{dr}{r^{n-1}}$

Thus $\mathbb{R}^n$ is recurrent $\Leftrightarrow$ $n \leq 2$

Recurrence of General Manifolds

Theorem (Lyons-Sullivan 1984, Grigoryan 1983)

For a general (metrically complete) Riemannian manifold M the following holds: If for some $x \in M$

$$\int^{\infty} \frac{dr}{A(x,r)} = \infty$$

then M is recurrent.

Remark

The converse implication does not hold (counterexamples).

Stochastic Completeness of General Manifolds

Question (Grigoryan 1999)

Given a general (metrically complete) Riemannian manifold M. Does

$$\int^{\infty} \frac{V(x,r)}{A(x,r)} dr = \infty$$

for some $x \in M$ imply that M is stochastically complete?

Stochastic Completeness of General Manifolds

Answer: No!

Theorem (B.-Bessa 2009)

In any dimension $n \geq 2$ there exists a stochastically incomplete, yet metrically complete manifold M such that for some $x \in M$

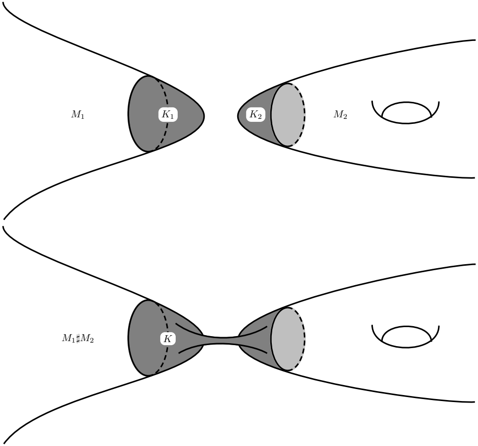
$$\int^{\infty} \frac{V(x,r)}{A(x,r)} dr = \infty$$

holds.

Remark

The converse implication does not hold either (counterexamples).

Connected Sum



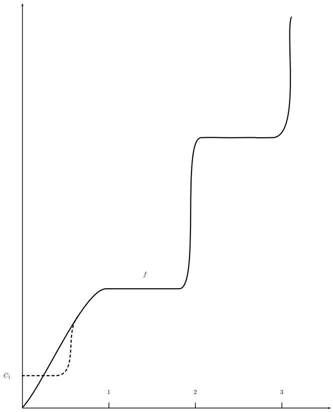
$M_1 \sharp M_2$ is stochastically complete

$\Leftrightarrow$

M_1 and M_2 are stochastically complete.

Idea of Proof

- Choose stochastically incomplete model manifold M_1
- Then $M = M_1 \sharp M_2$ will be stochastically incomplete as well
- Choose model manifold M_2 with function f such that the volume growth gets “fixed”



Renormalized integrals

Aim: Replace measure theoretic integrals by a more general concept of integral.

Let $\mathcal{J}$ be a directed system, i.e., $\mathcal{J}$ is a set equipped with a relation $\preceq$ such that the following holds:

- Reflexivity: $\mathcal{T} \preceq \mathcal{T}$
- Transitivity: $\mathcal{T} \preceq \mathcal{S}$ & $\mathcal{S} \preceq \mathcal{U} \;\Rightarrow\; \mathcal{T} \preceq \mathcal{U}$
- Antisymmetry: $\mathcal{T} \preceq \mathcal{S}$ & $\mathcal{S} \preceq \mathcal{T} \;\Rightarrow\; \mathcal{T} = \mathcal{S}$
- $\forall \mathcal{T}, \mathcal{S} \in \mathcal{J} \; \exists \mathcal{U} \in \mathcal{J} : \quad \mathcal{T} \preceq \mathcal{U}$ & $\mathcal{S} \preceq \mathcal{U}$

Renormalized integrals

Definitions

- measure space family = family of measure spaces $\Omega = \{(\Omega_{\mathcal{T}}, \mu_{\mathcal{T}})\}_{\mathcal{T}\in\mathcal{J}}$ parameterized by $\mathcal{J}$.
- measurable function on Ω = family $f = \{f_{\mathcal{T}}\}_{\mathcal{T}\in\mathcal{J}}$ of measurable functions $f_{\mathcal{T}} : \Omega_{\mathcal{T}} \to X$.
- f is called integrable if $f_{\mathcal{T}}$ is eventually integrable and the limit exists:

$$\fint_{\Omega} f(x)\mathcal{D}x := \varinjlim_{\mathcal{T}\in\mathcal{J}} \int_{\Omega_{\mathcal{T}}} f_{\mathcal{T}}(x)\, d\mu_{\mathcal{T}}(x)$$

- $\fint_{\Omega} f(x)\mathcal{D}x$ = renormalized integral of f over Ω.

By abuse of notation, write $f : \Omega \to X$ and think of f as a function on the virtual space Ω.

Renormalized integrals, examples

Improper integrals

$\mathcal{J} = \{\text{compact intervals } I \subset \mathbb{R}\}$, "$\preceq$" = "$\subset$", $\Omega_I = I$, $\mu_I = dx$

For measurable function $f : \mathbb{R} \to \mathbb{R}$ put $f_I := f|_I$. Then

$$\fint_\Omega f(x)\,\mathcal{D}x = \int_{-\infty}^{\infty} f(x)\,dx$$

Improper integrals, renormalized

$\mathcal{J} = \{\text{compact intervals } I \subset \mathbb{R}\}$, "$\preceq$" = "$\subset$", $\Omega_I = I$, $\mu_I = \frac{dx}{\text{length}(I)}$

E.g., for $\alpha > -1$ and $f(x) = (|x| + 1)^\alpha$:

$$\fint_\Omega (|x| + 1)^\alpha\,\mathcal{D}x = \begin{cases} 0, & \alpha < 0 \\ 1, & \alpha = 0 \\ \infty, & \alpha > 0 \end{cases}$$

Renormalized integrals, examples

Cauchy's Principal Value

$\mathcal{J} = (0,1)$, "$\preceq$" = "$\geq$", $\Omega_T = [-1,-T] \cup [T,1]$, $\mu_T = dx$.
For $f : [-1,1] \to \mathbb{R}$ put $f_T := f|_{\Omega_T}$.

$$\fint_\Omega f(x)\,\mathcal{D}x = \lim_{T \searrow 0} \left[\int_{-1}^{-T} f(x)\,dx + \int_T^1 f(x)\,dx \right] = \mathrm{CH} \int_{-1}^1 f(x)\,dx$$

Renormalized integrals, examples

Fredholm Determinant

$\mathcal{H}$ = separable real Hilbert space,
$\mathcal{J} = \{\text{finite-dim. subspaces } H \subset \mathcal{H}\}$, "$\preceq$" $=$ "$\subset$", $\Omega_H = H$,
$\mu_H = \pi^{-n/2} d^n x$ where $n = \dim(H)$.
Let $L = \mathrm{Id} + A$ be a bounded positive self-adjoint operator where A is of trace class. Then the determinant is defined and satisfies

$$\det(L) = \prod_{j=1}^{\infty}(1 + \lambda_j)$$

Then

$$⨍_{\Omega} \exp(-Lx, x)\mathcal{D}x = \det(L)^{-1/2}$$

Path integrals on manifolds

Consider partitions $\mathcal{P} = (0 = s_0 < s_1 < \cdots < s_r = 1)$ of the unit interval.

The set of partitions $\mathcal{P}$ forms a directed system where $\mathcal{P} \preceq \mathcal{P}'$ if $\mathcal{P}'$ is a subdivision of $\mathcal{P}$.

Let M be a Riemannian manifold.

A piecewise smooth curve in M is a pair $(\mathcal{P}, \gamma)$ where $\mathcal{P}$ is a partition and $\gamma : [0,1] \to M$ is a continuous curve with $\gamma|_{[s_{j-1}, s_j]}$ smooth.

A geodesic polygon is a piecewise smooth curve $(\mathcal{P}, \gamma)$ if $\gamma(s_j)$ is not in the cut-locus of $\gamma(s_{j-1})$ and $\gamma|_{[s_{j-1}, s_j]}$ is the unique shortest geodesic joining its endpoints.

Put

$$\mathfrak{P}(\mathcal{P}, M)_x^y := \{(\mathcal{P}, \gamma) \mid \text{geodesic polygon s.t. } \gamma(0) = x \text{ and } \gamma(1) = y\}$$

Path integrals on manifolds

The map

$$\mathfrak{P}(\mathcal{P}, M)_x^y \to M \times \ldots \times M, \quad (\mathcal{P}, \gamma) \mapsto (\gamma(s_1), \ldots, \gamma(s_{r-1}))$$

is injective and surjective up to a null set.
Riemannian volume measure on $M \times \ldots \times M$ induces measure $\mathcal{D}\gamma$ on $\mathfrak{P}(\mathcal{P}, M)_x^y$.
Define the renormalization constant

$$Z(\mathcal{P}, t) := t^{rm/2} \prod_{j=1}^{r} (4\pi(s_j - s_{j-1}))^{m/2}$$

where $m = \dim(M)$.
We obtain a measure space family

$$\{(\mathfrak{P}(\mathcal{P}, M)_x^y, Z(\mathcal{P}, \dim(M), t)^{-1} \cdot \mathcal{D}\gamma)\}_{\mathcal{P}}$$

Heat equation on manifolds

- M = compact m-dimensional Riemannian manifold without boundary
- $E \to M$ = Hermitian vector bundle
- $H = \Delta^E - V$ = self-adjoint generalized Laplace operator acting on sections of E. Locally, H has the form

$$H = \sum_{j,k=1}^{m} g^{jk} \frac{\partial^2}{\partial x^j \partial x^k} + \text{lower order terms.}$$

- $k^H(t, x, y)$ = heat kernel of H, i.e.,

$$u(t,x) = \int_M k^H(t,x,y)\, u_0(y)\, dy$$

solves

$$\begin{cases} \frac{\partial u}{\partial t} = Hu \\ u(x,0) = u_0(x) \end{cases}$$

Path integral formula for the heat kernel

Theorem (B., 2011)

$$k^H(t,y,x) =$$

$$⨍_{\mathfrak{P}(M)_x^y} \exp\left[-\frac{\mathrm{E}[\gamma]}{2t} + t\int_0^1 \left(\frac{1}{3}\mathrm{scal}(\gamma(s)) - V(\gamma(s))\right) ds\right] \mathcal{D}\gamma.$$

Application: Comparison results (Hess-Schrader-Uhlenbrock inequality)
Hope: Applicable to Schrödinger equation

Earlier results

Andersson-Driver (1999)

Path integral formula for solution to heat equation for scalar operators (not for heat kernel itself)

B.-Pfäffle (2008)

Path integral formula for solution to heat equation in the present setup (not for heat kernel itself)

Idea of the proof

- Start with tautological path integral formula

$$k^H(t,y,x) = \int_{\mathfrak{P}(M)_x^y} Z(\mathcal{P}, \dim(M), t)\, K_t^H(\mathcal{P},\gamma)\; \mathcal{D}\gamma.$$

  where $K_t^H(\mathcal{P},\gamma) = k^H(t(s_r - s_{r-1}), \gamma(s_r), \gamma(s_{r-1})) \circ \cdots \circ k^H(t(s_1 - s_0), \gamma(s_1), \gamma(s_0))$

- Modify integrand in the path integral without changing the value of the integral.
- Start modification using *short time heat asymptotics*:

$$k^H(t,y,x) \sim (4\pi t)^{-m/2} \exp\left(-\frac{d(x,y)^2}{4t}\right) \sum_{j=0}^{\infty} a_j(x,y) t^j$$

Gaussian integrals

Quantum field theory: Integrals over spaces of fields (e.g. functions on a manifold)
Aim: Make

$$\int \exp(-S(\phi))\mathcal{D}\phi$$

rigorous, where $S(\phi) = \frac{1}{2}(L\phi, \phi)$ with L self-adjoint and positive.
Recall that for suitable bounded L:

$$\int \exp(-S(\phi))\mathcal{D}\phi = \det(L)^{-1/2}$$

Determinants

Question: What is $\det(L)$?
Zeta function:

$$\zeta_L(s) := \sum_{\lambda \in \mathrm{spec}(L)} \lambda^{-s}$$

$$\det(L) := \exp(-\zeta'(0))$$

Determinant of the Dirac operator

Let D be the Dirac operator on M.
The spectrum of D is unbounded from above and from below.
For simplicity assume that $0 \notin \mathrm{spec}(D)$.
Then:

$$\det(D) := \exp\left(\frac{i\pi}{2}(\zeta_{D^2}(0) - \eta_D(0))\right) \cdot \exp\left(-\frac{\zeta'_{D^2}(0)}{2}\right)$$

where

$$\eta_D(s) = \sum_{\lambda \in \mathrm{spec}(D)} \frac{\mathrm{sgn}\lambda}{|\lambda|^s}$$

Determinant of the Dirac operator on S^n

Theorem (Branson 1993, B.-Schopka 2003)

$$\log \det(D^2; S^n) = \sum_{k=0}^{n-1} \big(A(k,n) \cdot \zeta_R'(-k) + B(k,n) \cdot \zeta_R(-k)\big) + C(n)$$

$$\det(D; S^n) = \exp(i\pi K(n)) \sqrt{\det(D^2; S^n)}$$

with $K(n) = 0$*, if* n *is odd.*

Determinant of the Dirac operator on S^n

n	$\det(D)$
3	0.803354268824629
5	1.090359845142337
7	0.963796369884191
9	1.016473922384390
11	0.992614518464762
13	1.003422630166412
15	0.998408322304586
17	1.000749343263366
19	0.999645452552308
21	1.000168795852563

Conjecture:
$\lim_{n\to\infty} \det(D; S^n) = 1$

Proved by N. M. Møller (2007)