



Physics Department "E. Fermi"
University of Pisa

Brownian motion on d-dimensional Riemannian Manifolds

Formalism and applications



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Introduction

Brownian motion

Fokker-Planck and QM formalism

- QM formalism

- Fokker-Planck hamiltonian

- Path integral approach

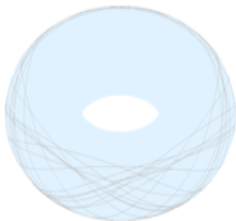
Brownian motion on a Manifold

- Frames and metric tensor

- Fokker-Planck on a Manifold

- Brownian motion on a Manifold

Conclusions



Introduction



Introduction

Reasons for this work



Following the approach of Zinn-Justin and Linda Reichl, we explore here the connections between Schrödinger and Fokker-Planck equations, leading to the path integral formalism and its application to Riemannian Manifolds.

We start from general properties of the time evolution operator to define the Fokker-Planck hamiltonian and obtain a path-integral representation of the general problem. Next, we import these concepts on Riemannian Manifolds and describe the path integral expression of the Brownian motion.

This work also serve as an introduction to some basic concepts discussed during the course and to the treatment of Stochastic Field Theory and Supersymmetry.

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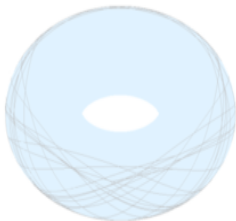
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Brownian motion



Brownian motion

History



Brownian motion was first investigated by Robert Brown in 1827 who, observing small pollen grains suspended in water, noticed that they were in a very animated and irregular state of motion.

In 1905 Einstein published an explanation to the problem that has to be regarded as the beginning of stochastic modelling of natural phenomena.

He started from what we call today the Chapman-Kolmogorov Equation (1) - the central dynamical equation to all Markov processes - and obtained a diffusion equation, describing the probability distribution of the position of a pollen grain at a given time.

$$P(x, t|x_0, t_0) = \int P(x, t|y, t')P(y, t'|x_0, t_0)dy \quad (1)$$

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Today we use the differential Chapman-Kolmogorov Equation to describe Markov processes. Its continuous part - the Fokker-Planck Equation - without the drift coefficient defines the Wiener process. The Brownian motion is a Wiener process.

The corresponding Fokker-Planck Equation is

$$\partial_t P(\omega, t | \omega_0, t_0) = \frac{1}{2} \partial_\omega^2 P(\omega, t | \omega_0, t_0)$$

The solution is then

$$P(\omega, t | \omega_0, t_0) = \frac{1}{\sqrt{2\pi\Delta t}} \exp\left\{-\frac{(\omega - \omega_0)^2}{2\Delta t}\right\} \quad (2)$$

It is a Gaussian distribution centered in ω_0 and with variance Δt .



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Brownian motion

Langevin equation and correlations



The dynamics is described by a Langevin equation, in which the ξ is well defined if ω is a differentiable stochastic process.

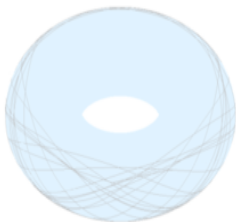
$$\dot{q}(t) = -f(q, t) + \xi(t) \quad \text{where } \xi = \frac{d\omega}{dt} \quad (3)$$

Unfortunately this is not the case of Wiener processes, but being careful about the definition, and recalling the relation

$$\langle O(\omega(t)) \rangle = \int O(\omega) P(\omega, t) d\omega$$

from equation 2 we observe

$$\frac{d}{dt} \langle q(t) \rangle = -f(q, t) \quad \langle \xi \rangle = 0 \quad \langle \xi(t) \xi(t') \rangle = \delta(t - t')$$



Fokker-Planck and QM formalism



SDE and Fokker-Planck Equation

Forward Fokker-Planck



Equation 3 is more correctly expressed as a stochastic differential equation. Switching to several dimensions, the motion of the particle is described by

$$dq_i = -f_i(q)dt + g_{ij}(q)d\omega_j \quad (4)$$

The SDE above is associated to the Fokker-Planck Equation

$$\partial_t P(q, t|q_0, t_0) = \hat{\mathcal{L}}P(q, t|q_0, t_0) \quad (5)$$

in which $\hat{\mathcal{L}}$ is the differential operator defined as

$$\hat{\mathcal{L}} \equiv \sum_i \partial_{q_i} f_i(q) + \frac{1}{2} \sum_{i,j} \partial_{q_i} \partial_{q_j} [g(q)g^T(q)]_{ij} \quad (6)$$

The general idea is that, once the solution to the equation 5 is known, the statistical properties of the process are completely defined.

Cfr. section 4.3 of [2]

SDE and Fokker-Planck Equation

Backward Fokker-Planck



We define also the backward Fokker-Planck operator as the adjoint of the operator¹ in equation 6, respect to the standard L^2 inner product

$$\langle f, g \rangle = \int f(x)g(x)dx \quad \langle \hat{\mathcal{L}}^\dagger f, g \rangle = \langle f, \hat{\mathcal{L}} g \rangle$$

We obtain

$$\hat{\mathcal{L}}^\dagger \equiv - \sum_i f_i(q) \partial_{q_i} + \frac{1}{2} \sum_{i,j} [g(q)g^T(q)]_{ij} \partial_{q_i} \partial_{q_j} \quad (7)$$

We observe that, in general, the FP operator is not self-adjoint.

¹More formally, the forward operator has to be considered as the adjoint of the backward.



Let $U(t, t')$, with $t > t'$, be a bounded operator in Hilbert space, which describes an evolution between two times t and t' and satisfies a Markov property, so

$$\mathcal{A}_{q q_0} = \langle q | U(t, t_0) | q_0 \rangle \quad U(t, t') U(t', t_0) = U(t, t_0) \quad t \geq t' \geq t_0 \quad (8)$$

When the QM hamiltonian is time-independent, it is the generator of time translations and the time evolution operator in euclidean time can be written as

$$U(t, t') = \exp\{-(t - t')\mathcal{H}/\hbar\} \quad \text{with} \quad U(t, t) = 1 \quad (9)$$

If \mathcal{H} is anti-hermitian - i.e. $\mathcal{H} = i\tilde{\mathcal{H}}$ - then $\tilde{\mathcal{H}}$ is a quantum hamiltonian. Otherwise, if it is hermitian, we're in the domain of statistical physics.



Using the general formulation of equations 8 and 9 and assuming that the space of solutions is a Hilbert space, we can rewrite the probability as

$$P(q, t | q_o, t_o) = \langle q | P(t, t_o) | q_o \rangle \quad P(t, t') = \exp\{-(t - t')\mathcal{H}\} \quad (10)$$

in which \mathcal{H} is defined as the Fokker-Planck hamiltonian.

Integrating equation 4 for small enough time steps

$$q_i(t + \Delta t) = q_i(t) - f_i(q)\Delta t + g_{ij}(q)\Delta\omega_j$$

and comparing its Fourier transform with equation 9, we find

$$P(p, t + \Delta t | q_o, t) = \langle e^{-ipq} \rangle = e^{-ip[q_o - f(q)\Delta t]} \langle e^{-ip_i g_{ij}(q)\Delta\omega_j} \rangle$$

Note that $\Delta\omega$ goes like $\sqrt{\Delta t}$.



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Note that $\Delta\omega$ goes like $\sqrt{\Delta t}$.



Assuming $g_{ij}(q, t) = \sigma \delta_{ij}$ and recalling equations 2 in the calculation, we have

$$P(p, t + \Delta t | q_0, t) = e^{-ipq_0} e^{-\Delta t [\frac{1}{2} \sigma^2 p^2 - ipf(q)]} = e^{-ipq_0} e^{-\Delta t \mathcal{H}(p|q_0)}$$

from which we get two important results:

- The shape of the propagator for small time steps that will be useful in the path integral formulation

$$P(q, t + \Delta t | q_0, t) = (2\pi\sigma^2\Delta t)^{-d/2} e^{-\frac{1}{2\sigma^2\Delta t}(q - q_0 + f(q)\Delta t)^2} \quad (11)$$

- The shape of the Fokker-Planck hamiltonian which corresponds to minus the operator in equation 6!

$$\hat{\mathcal{H}} = \frac{1}{2} \sigma^2 \hat{p}^2 - i \hat{p} \cdot f(q) = -\frac{1}{2} \sigma^2 \nabla_q^2 - \nabla_q \cdot f(q) = -\hat{\mathcal{L}} \quad (12)$$



We can calculate the expression of $f(q)$ that guaranties the existence of a stationary solution like $P_o(q) = \exp\{-\Delta V/\sigma^2\}$. We find

$$\begin{aligned}(\sigma^2 \nabla - \nabla V(q)) \cdot (f(q) - \frac{1}{2} \nabla V(q)) &= 0 \\ \rightarrow f(q) &= \frac{1}{2} \nabla_q V(q) + g(q) \exp\{\Delta V/\sigma^2\} \quad \text{with} \quad \nabla \cdot g(q) = 0\end{aligned}$$

Looking at equation 12, we also see that this condition leads to a hermitian hamiltonian² and real eigenvalues are expected.

On the other hand, if a stationary state doesn't exists or it hasn't a finite norm, it is possible to demonstrate that all eigenvalues of \mathcal{H} have strictly positive real parts and only runaway solution are possible - i.e. the probability of finding $q(t)$ inside a ball of finite radius goes to zero ³.

²Via the transformation in section 10.2 of [4] we obtain an hermitian hamiltonian.

³This is the case with Brownian motion on non-compact manifolds.



Taking in mind that $\hat{\mathcal{L}}$ is not generally hermitian, the methods of QM can now be applied. If the equilibrium distribution exists, then

$$P_o(x) \equiv \lim_{t \rightarrow \infty} P(x, t; \dots)$$

Recalling the shape of the operator $\hat{\mathcal{L}}^\dagger$ in equation 7, we can define the action of \mathcal{H} on right and left state vectors as

$$\hat{\mathcal{H}}P_o(q) = \int dq' \langle q | \mathcal{H} | q' \rangle \langle q' | o \rangle = \langle q | \mathcal{H} | o \rangle = 0 \quad \text{with} \quad \langle q | o \rangle = P_o(q)$$

$$\hat{\mathcal{H}}^\dagger \mathbf{1} = \int dq' \langle o | q' \rangle \langle q' | \mathcal{H} | q \rangle = \langle o | \mathcal{H} | q \rangle = 0 \quad \text{with} \quad \langle o | q \rangle = 1$$

$$\text{and} \quad \langle o | o \rangle = \int dq' P_o(q') < \infty$$



Suppose $\{|\lambda\rangle\}$ is an orthogonal basis in which \mathcal{H} is diagonal. Next, we can define the "wave functions" as $P_\lambda(x) \equiv \langle x|\lambda\rangle$ and $Q_\lambda(x) \equiv \langle \lambda|x\rangle$. So, completeness relations of the Hilbert space are

$$\begin{aligned}\langle x|e^{-\Delta t\mathcal{H}}|x_0\rangle &= \sum_{\lambda} \langle x|\lambda\rangle e^{-\Delta t\lambda} \langle \lambda|x_0\rangle = \sum_{\lambda} P_{\lambda}(x)e^{-\Delta t\lambda}Q_{\lambda}(x_0) \\ &\xrightarrow{\Delta t \rightarrow 0} \sum_{\lambda} P_{\lambda}(x)Q_{\lambda}(x_0) = \delta(x - x_0)\end{aligned}$$

$$\begin{aligned}-\lambda'\langle Q_{\lambda'}, P_{\lambda}\rangle &= \langle \hat{\mathcal{L}}^\dagger Q_{\lambda'}, P_{\lambda}\rangle = \langle Q_{\lambda'}, \hat{\mathcal{L}} P_{\lambda}\rangle = -\lambda\langle Q_{\lambda'}, P_{\lambda}\rangle \\ &\implies \int P_{\lambda}(x)Q_{\lambda'}(x)dx = \delta_{\lambda,\lambda'}\end{aligned}$$

Attention is needed on the boundary conditions of the FP Equation.



We can take advantage of the Heisenberg picture to write down the time evolution of observables and the generating functional of the correlation functions on the ground state as

$$\mathcal{O}(q) = \langle 0 | \hat{\mathcal{O}}(q) | q \rangle$$

$$\hat{\mathcal{O}}(q(t)) = e^{\mathcal{H}t} \hat{\mathcal{O}}(q) e^{-\mathcal{H}t}$$

$$\langle \mathcal{O}(q(t)) \rangle = \langle 0 | \hat{\mathcal{O}}(q(t)) e^{\mathcal{H}t_0} | q_0 \rangle \quad \frac{d}{dt} \hat{\mathcal{O}}(q(t)) e^{\mathcal{H}t_0} = [\mathcal{H}, \hat{\mathcal{O}}(q(t)) e^{\mathcal{H}t_0}]$$

$$Z^n(t_1, t_2, \dots, t_n) = \langle q(t_1) q(t_2) \dots q(t_n) \rangle = \langle 0 | \hat{q}(t_1) \hat{q}(t_2) \dots \hat{q}(t_n) e^{\mathcal{H}t_0} | q_0 \rangle$$

Notice that $e^{\mathcal{H}t_0} | q_0 \rangle$ is the anti-evolution of the Heisenberg state $| q_0 \rangle$ and for $t_0 \rightarrow -\infty$ we have $e^{\mathcal{H}t_0} | q_0 \rangle \rightarrow | 0 \rangle$.

Main applications are the eigenvalues calculation and some problems in chapter 10 of [4].

Path integral representation

Calculation



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We can write a path integral expression for the probability density function, using the Markov property of equation 1 and the shape of the propagator in equation 11. Setting $x = x_{N+1}$, we have

$$\begin{aligned} P(x, t | x_0, t_0) &= \int P(x, t | y, t') P(y, t' | x_0, t_0) dy = \\ &= \int \prod_{i=1}^N [dx_i] \prod_{i=0}^N \left[\frac{1}{(2\pi\sigma^2\Delta t)^{d/2}} \exp \left\{ -\frac{\Delta t}{2\sigma^2} \left(\frac{x_{i+1} - x_i}{\Delta t} + f(x_i) \right)^2 \right\} \right] = \\ &= \int_{x(t_0)}^{x(t)} \mathcal{D}_N[x] \exp \left\{ -\frac{\Delta t}{2\sigma^2} \sum_{i=0}^N \left(\frac{x_{i+1} - x_i}{\Delta t} + f(x_i) \right)^2 \right\} \end{aligned}$$

In the continuum limit, working with terms of the order $\sqrt{\Delta t}$, we obtain

$$P(x, t | x_0, t_0) = \int_{x(t_0)}^{x(t)} \mathcal{D}[x] e^{-S[x]/\sigma^2} \quad (13)$$

in which

$$\mathcal{D}[x] = \lim_{N \rightarrow \infty} \frac{\prod_{i=1}^N dx_i}{(2\pi\sigma^2\Delta t)^{\frac{d}{2}(N+1)}} \quad S[x] = \int_{t_0}^t \frac{1}{2} (\dot{x} + f(x))^2 dt$$

according to equation 12, the real time momentum and hamiltonian are

$$p = (\dot{x} + f(x)) \sim \sigma \frac{\Delta\omega}{\Delta t} \quad \mathcal{H}(p|q) = \frac{1}{2}p^2 - p \cdot f(x)$$

From which Hamilton's equations are easily derived.

Path integral representation

Quantization



The previous results gives a nice toolkit to deal with stochastic processes and an Ito interpretation of the starting SDE.

If we are interested in physical processes, we have to symmetrize our SDE up to order Δt and use the Stratonovich integration rules.⁴

With symmetric quantization, any classical hamiltonian is associated with a hermitian quantum hamiltonian. The Wigner's rule shares this property.⁵ The dynamical action is then obtained trough a coordinate transformation

$$f(x_i) = f((x_{i+1} + x_i)/2) - \frac{1}{2}(x_{i+1} - x_i) \nabla f(x)$$

$$J = \det \left[\partial_x (x_{i+1} - x_i - \frac{1}{2} \Delta t (x_{i+1} - x_i) \cdot \nabla f_i) \right]^{-1} = e^{-\frac{1}{2} \Delta t \nabla \cdot f_i}$$

$$S[x] = \int_{t_0}^t \frac{1}{2} [(\dot{x} + f(x))^2 - \sigma^2 \nabla \cdot f(x)] dt$$

⁴Cfr. [3] for insights into this issue.

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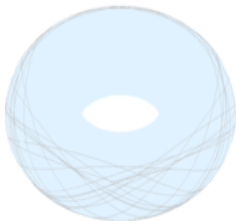
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Brownian motion on a Manifold



In General Relativity, the concept of distance on a manifold \mathcal{M} is related to the definition of the metric tensor g , which defines an inner product between vectors of the tangent space.

For $v, w \in T(\mathcal{M})$, we have $v = v^\mu \partial_\mu$ and $g(v, w) = g_{\mu\nu} v^\mu w^\nu$.

A vielbein is a set of linearly independent vector fields that gives a locally flat metric tensor.

$$\begin{aligned} e_a &= e_a^\mu \partial_\mu & e^a(e_b) &= e^a_\mu e^\mu_b = \delta^a_b \\ g(e_a, e_b) &= g_{\mu\nu} e_a^\mu e_b^\nu = \delta_{ab} \rightarrow g^{\mu\nu} = e_a^\mu e_a^\nu \\ g &= \det\{g_{\mu\nu}\} = \det\{e_a^\mu\} \det\{e^a_\nu\} = e^2 \end{aligned} \quad (14)$$

Our coordinate can be written in terms of the vielbein as $x = x^\mu \partial_\mu = x^a e_a$.

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Our coordinate can be written in terms of the vielbein as $x = x^\mu \partial_\mu = x^a e_a$.



The generalized Langevin equation can be written as

$$dx^\mu = -f^\mu(x)dt + \sigma e^\mu_a(x)d\omega^a$$

which integrated for small step size becomes

$$x^\mu(t + \Delta t) = x^\mu(t) - f^\mu(x)\Delta t + \sigma e^\mu_a(x)\Delta\omega^a$$

and using the Stratonovich integration we obtain an order Δt equation

$$x^\mu(t + \Delta t) - x^\mu(t) = -f^\mu(x)\Delta t + \frac{1}{2}\sigma^2 e^\nu_a(x)\partial_\nu e^\mu_a(x)\Delta t + \sigma e^\mu_a(x)\Delta\omega^a$$

Note that increments are identically distributed in every tangent space, defined on a flat metric and projected on \mathcal{M} thanks to \hat{e}_a .

Recalling the procedure adopted for equation 10, we can derive expressions for the FP equation, hamiltonian and propagator.⁶

Defining

$$h^\mu \equiv f^\mu - \frac{1}{2}\sigma^2 e^\nu{}_a \partial_\nu e^\mu{}_a \quad d^\mu \equiv x^\mu - x_0^\mu + h^\mu(x_0)\Delta t$$

and recalling equations 14, we have

$$\partial_t P(x, t|x_0, t_0) = \partial_\mu (h^\mu + \frac{1}{2}\sigma^2 \partial_\nu g^{\mu\nu}) P(x, t|x_0, t_0)$$

$$\hat{\mathcal{H}} = \frac{1}{2}\sigma^2 g^{\mu\nu} \hat{p}_\mu \hat{p}_\nu - i\hat{p}_\mu \cdot h^\mu$$

$$P(x, t + \Delta t|x_0, t) = \frac{\sqrt{g(x_0)}}{(2\pi\sigma^2\Delta t)^{\frac{d}{2}}} \exp\left\{-\frac{1}{2\sigma^2\Delta t} g_{\mu\nu}(x_0) d^\mu d^\nu\right\}$$

⁶Recall equations 11 and 12.

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Brownian motion on a Manifold

Free Brownian motion and path integral



Setting $f^\mu(x) = -\frac{1}{2}\sigma^2 e^\mu_a \nabla_\nu e^\nu_a$, or equivalently $h^\mu = \frac{1}{2}\sigma^2 g^{\alpha\beta} \Gamma_{\alpha}{}^\mu{}_\beta$, we obtain the equations of the free Brownian motion on a Manifold. Observing that P is a scalar density, the most general covariant equation becomes

$$\partial_t D = \frac{\sigma^2}{2\sqrt{g}} \partial_\mu \sqrt{g} g^{\mu\nu} \partial_\nu D = \frac{\sigma^2}{2} \nabla_{LB}^2 D \quad (15)$$

in which $\sqrt{g}D = P(x, t|x_0, t_0)$ and ∇_{LB}^2 is the Laplace-Beltrami operator.

Recalling equation 13, in the path integral representation we have

$$D(x, t|x_0, t_0) = \int_{x(t_0)}^{x(t)} \mathcal{D}[x] e^{-S[x]/\sigma^2}$$

in which

$$\mathcal{D}[x] = \lim_{N \rightarrow \infty} \frac{\prod_{i=1}^N dx_i \sqrt{g(x)}}{(2\pi\sigma^2\Delta t)^{\frac{d}{2}(N+1)}} \quad S[x] = \int_{t_0}^t \frac{1}{2} \dot{d}^\mu g_{\mu\nu} \dot{d}^\nu dt$$

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Free Brownian motion and path integral



Setting $f^\mu(x) = -\frac{1}{2}\sigma^2 e^\mu{}_a \nabla_\nu e^\nu{}_a$, or equivalently $h^\mu = \frac{1}{2}\sigma^2 g^{\alpha\beta} \Gamma_{\alpha}{}^\mu{}_\beta$, we obtain the equations of the free Brownian motion on a Manifold. Observing that P is a scalar density, the most general covariant equation becomes

$$\partial_t D = \frac{\sigma^2}{2\sqrt{g}} \partial_\mu \sqrt{g} g^{\mu\nu} \partial_\nu D = \frac{\sigma^2}{2} \nabla_{LB}^2 D \quad (15)$$

in which $\sqrt{g}D = P(x, t|x_0, t_0)$ and ∇_{LB}^2 is the Laplace-Beltrami operator. Recalling equation 13, in the path integral representation we have

$$D(x, t|x_0, t_0) = \int_{x(t_0)}^{x(t)} \mathcal{D}[x] e^{-S[x]/\sigma^2}$$

in which

$$\mathcal{D}[x] = \lim_{N \rightarrow \infty} \frac{\prod_{i=1}^N dx_i \sqrt{g(x)}}{(2\pi\sigma^2 \Delta t)^{\frac{d}{2}(N+1)}} \quad S[x] = \int_{t_0}^t \frac{1}{2} \dot{x}^\mu g_{\mu\nu} \dot{x}^\nu dt$$

Brownian motion on a Manifold

Applications



For a given metric, this formalism allows to integrate Hamilton's equations of motion to find the optimal path and evaluate averaged observables.

The main differences between Brownian motion on Euclidean space and complex Manifolds is the presence of a drift term in the Langevin equation that represents the geodesic flow, while σ generates deviation from it.

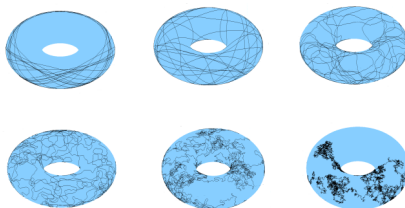
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Kinetic Brownian motion on the flat torus for $\sigma = 10^{-2}, 10^{-1}, 1, 2, 4, 10$.

"It interpolates between geodesic flow and pure Brownian motion." [1]



Some applications are:

- ▶ description of diffusion processes on molecular surfaces
- ▶ estimation of the MFPT in complex geometries
- ▶ analysis of the existence of harmonic solution of LB
- ▶ solution of the coverage and heat kernel problem
- ▶ stochastic quantization and SUSY⁷

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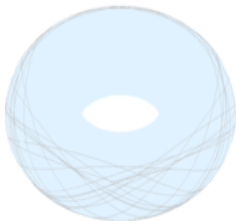
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Conclusions



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- ▶ **A covariant approach and the path integral representation of stochastic processes**

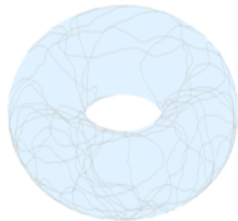
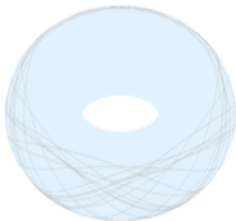
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Thank you for your attention!

