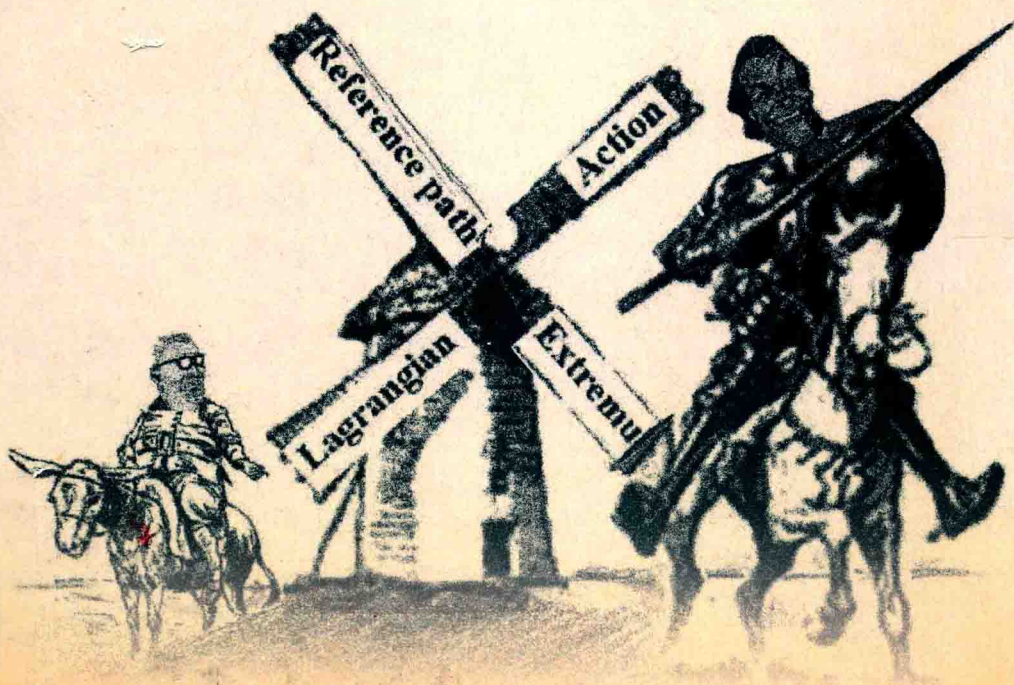


Path Integrals For Stochastic Processes

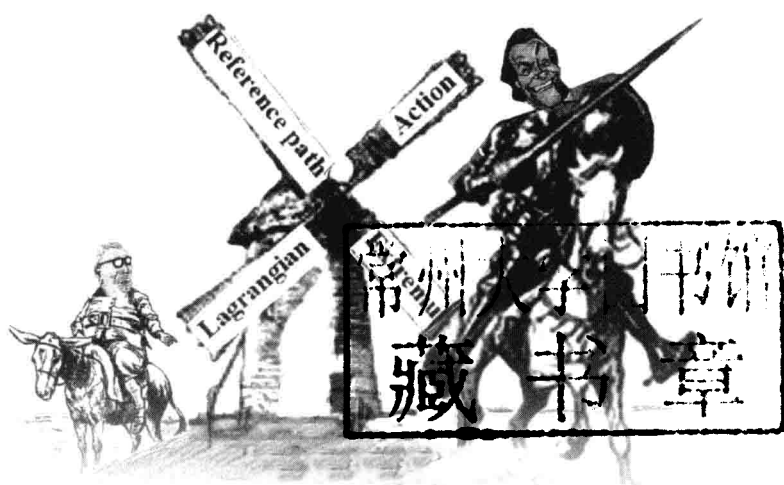
An Introduction



Horacio S Wio

Path Integrals For Stochastic Processes

An Introduction



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An Introduction

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Path Integrals For Stochastic Processes

An Introduction

To the memory of my parents and sister, Welka, Sofia, María Ruth; To my wife María Luz, my sons and daughter Marcelo, Mayra, Nicolás, and my grand children Sofia, Gael, Matilda, Lucas, Ilan, ..., with love.

Preface

.....
*caminante no hay camino
se hace camino al andar..*
.....

Antonio Machado

The path-integral technique has proved to be a very powerful tool in various areas of physics, both computationally and conceptually (Feynman (1948); Feynman and Hibbs (1965); Schulman (1981); Langouche *et al.* (1982); Wiegeler (1986); Wio (1990); Kleinert (1990b); Khandekar and Lawande (1986); Khandekar *et al.* (2000)). It often provides an alternative route for the derivation of perturbation expansions as well as an excellent framework for non perturbative analysis. However, with few exceptions till recently, the subject of path-integrals was almost absent from standard textbooks on quantum mechanics and statistical physics (Shankar (1980); Felsager (1985); Das (1994)). As a consequence, students were missing a topic relevant for its application in field theory as well as an alternative approach to standard quantum and statistical mechanics that provides a wealth of approximation methods. However, during the last decades, many authors have tried to overcome this deficiency and have published several papers on this subject with an obvious pedagogical aim. In this way topics such as semiclassical approximations, barrier penetration, description of bound and metastable states and non exponential decay, adiabatic propagators, quantization of constrained Hamiltonians, the density matrix, and the harmonic oscillator with temperature and numerical methods among others, have been discussed within this framework (Holstein (1981a,b, 1982); Holstein and Swift (1982a,b); Mannheim (1983); Holstein (1983); MacK-

eown (1985); Salem and Wio (1986); Sengupta (1986); Ajanapon (1987); Larsen and Ravndal (1988); Donoghue and Holstein (1988); Gerry and Kiefer (1988); Holstein (1988a,b, 1989); Fletcher (1990); Abramson *et al.* (1991a); Cruz (1992)).

What seems to be still missing is an introductory presentation of the path-integral technique within the realm of stochastic processes (Wio (1999)). As a matter of fact, and from a historical point of view, it was in this context that path-integrals were first discussed by Wiener (Wiener (1923, 1924, 1930)), when he introduced a similar approach based on a sum over trajectories—anticipating by two decades Feynman’s work on path integrals (Feynman (1948))—that were later applied by Onsager and Machlup to some Markov out of equilibrium processes in order to describe diffusion-like phenomena (Onsager and Machlup (1953a,b)).

The mathematical theory of stochastic processes has proven to be not only a useful but also a necessary tool when studying physical, chemical and biological systems under the effect of fluctuations (Haken (1978); van Kampen (2004); Risken (1983); Gardiner (2009); Mikhailov (1990); Mikhailov and Loskutov (1992); Wio (1994); Nicolis (1995); Lindenberg and Wio (2003); Wio, Deza and López (2012)). Recent theoretical and experimental studies have shown that there are even situations where fluctuations (or noise) play an essential role triggering new phenomena, solely induced by the presence of noise. A few examples of such situations are: some problems related with self-organization and dissipative structures, noise induced transitions, noise-induced *phase*-transitions, noise sustained patterns, Brownian motors, stochastic resonance in zero-dimensional and in spatially extended systems (Horsthemke and Lefever (1984); Moss (1992); van den Broeck *et al.* (1994); Wiesenfeld and Moss (1995); Walgraef (1997); Mangioni *et al.* (1997, 2000); Jülicher *et al.* (1997); Gammaitoni *et al.* (1998); Reimann (2002); Wio, *et al.* (2002); Lindner *et al.* (2004); Sagues *et al.* (2007); Wio and Deza (2007)).

The aim of this short course is to offer a brief presentation of the path-integral approach to stochastic processes. We will focus on Markov processes, but a few aspects of non-Markov and non-Gaussian processes will also be discussed. Before starting our presentation, I would like to list a few more books, proceedings and review articles that, in addition to those indicated before, are a useful complementary reference material to this short introductory course and to the path integral approach in general (Khandekar and Lawande (1975, 1986); Papadopoulos and Devreese (1978); Marinov (1980); Brink (1985); Fox (1986); Sa-yakanit *et al.* (1989); Hänggi

et al. (1990); Grosche and Steiner (1998); Cerdeira *et al.* (1992); Dykman and Lindenberg (1994); Wio (1999); Mazzucchi (2009)).

These notes are based on courses on path integrals taught at the Instituto Balseiro (Universidad Nacional de Cuyo) and the Physics Department (Universidad Nacional de Mar del Plata), in Argentina; at the Universitat de les Illes Balears and Universidad de Cantabria in Spain, and summer courses at San Luis, Argentina and St. Etienne de Tinée, France.

The material is organized as follows. For the sake of completeness, we start making a brief review of stochastic processes. After that, we present a derivation of the path integral representation for the propagator of Markov processes. We describe next the path expansion method as adapted to the present stochastic case. After that, we present a simple example of a space-time transformation within the path integral framework. The results of this transformation are exploited to proceed a little further on the path expansion method. We also discuss some results for non-Markov and non-Gaussian processes. Next we present a few aspects related to fractional Brownian motion. We then analyze the usefulness of the Feynman-Kac formula, and always within the stochastic framework, how to use an influence functional like procedure to eliminate irrelevant variables. Afterwards, we discuss a few more applications to different diffusive-like problems. The last chapter is devoted to comment on some aspects that have not been touched upon in these notes.

I wish to express my thanks to G. Abramson, C. Batista, C.B. Briozzo, C.E. Budde, F. Castro, P. Colet, R.R. Deza, G. Drazer, M.A. Fuentes, J. Giampaoli, P. Hänggi, G. Izús, M.N. Kuperman, K. Lindenberg, S. Mangioni, L. Pesquera, J.A. Revelli, M.A. Rodriguez, L.D. Salem, A. Sánchez, M. San Miguel, L. Schulman, U. Smilanski, D. Strier, E. Tirapegui, R. Toral, D.H. Zanette, for fruitful discussions and/or collaborations on the path-integral approach to stochastic processes. I also thank the many students who have endured with stoicism the courses on path-integrals that I have taught. Last but not least, I thank V. Grunfeld for the critical reading of an earlier version of the manuscript.

Horacio S. Wio
Santander, August 2012

*Along this road
Goes no one,
This autumn eve
Matsuo Bashô*

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Chapter 1

Stochastic Processes: A Short Tour

1.1 Stochastic Process

We start this section by writing the evolution equation for a one dimensional dynamical system (Haken (1978); Wio (1994); Nicolis (1995); Wio (1997))

$$\frac{dx}{dt} = F(x, \zeta), \quad (1.1)$$

where x corresponds to the state variable while ζ is a control parameter. Such a parameter could be, for instance, the temperature, an external field, a reactant's controlled flux, etc, indicating the form in which the system is coupled to its surroundings. Experience tells us that it is usually impossible to keep the value of such parameters fixed, and consequently that fluctuations become relevant. Hence, the original *deterministic* equation will acquire a random or *stochastic* character.

Among the many reasons justifying the growing interest in the study of fluctuations we can point out that they present a serious impediment to accurate measurements in very sensitive experiments, demanding some very specific techniques in order to reduce their effects, and that the fluctuations might be used as an additional source of information about the system. But maybe the most important aspect is that fluctuations can produce macroscopic effects contributing to the appearance of some form of *noise-induced order* like *space-temporal patterns* or *dissipative structures* (Horsthemke and Lefever (1984); Nicolis (1995); Wio (1994); Walgraef (1997); Wio (1997); Gammaitoni *et al.* (1998); Reimann (2002); Wio, *et al.* (2002); Lindner *et al.* (2004); Sagues *et al.* (2007); Wio and Deza (2007); Wio, Deza and López (2012)).

The general character of the evolution equations of dynamical systems makes it clear why stochastic methods have become so important in dif-

ferent branches of physics, chemistry, biology, technology, population dynamics, economy, and sociology. In spite of the large number of different problems that arise in all these fields, there are some common principles and methods that are included in a global framework: *the theory of stochastic processes*. Here we will only briefly review the few aspects relevant for our present needs. For deeper study we refer to van Kampen (2004); Risken (1983); Horsthemke and Lefever (1984); Gardiner (2009); Wio (1994); Lindenberg and Wio (2003); Wio, Deza and López (2012).

In order to include the presence of fluctuations into our description, we write $\zeta = \zeta_0 + \xi(t)$, where ζ_0 is a constant value and $\xi(t)$ is the random or fluctuating contribution to the parameter ζ . The simplest (or lowest order) form that equation (1.1) can adopt is

$$\frac{dx}{dt} = \dot{x} = F(x, \zeta_0) + g(x, \zeta_0)\xi(t), \quad (1.2)$$

The original deterministic differential equation has been transformed into a *stochastic differential equation* (SDE), where $\xi(t)$ is called a *noise* term or stochastic process.

Any stochastic process $x(t)$ is completely specified if we know the complete hierarchy of probability densities. We write

$$P_n(x_1, t_1; x_2, t_2; \dots; x_n, t_n) dx_1 dx_2 \dots dx_n, \quad (1.3)$$

for the probability that $x(t_1)$ is within the interval $(x_1, x_1 + dx_1)$, $x(t_2)$ in $(x_2, x_2 + dx_2)$, and so on. These P_n may be defined for $n = 1, 2, \dots$, and only for different times. This hierarchy fulfills some properties

$$i) P_n \geq 0$$

$$ii) P_n \text{ is invariant under permutations of pairs } (x_i, t_i) \text{ and } (x_j, t_j)$$

$$iii) \int P_n dx_n = P_{n-1}, \text{ and } \int P_1 dx_1 = 1.$$

Another important quantity is the *conditional probability density* $P_{n/m}$ that corresponds to the probability of having the value x_1 at time t_1 , x_2 at t_2, \dots, x_n at t_n ; given that we have $x(t_{n+1}) = x_{n+1}, x(t_{n+2}) = x_{n+2}, x(t_{n+3}) = x_{n+3}, \dots, x(t_{n+m}) = x_{n+m}$. Its definition is

$$\begin{aligned} P_{n/m}(x_1, t_1; \dots; x_n, t_n | x_{n+1}, t_{n+1}; \dots; x_{n+m}, t_{n+m}) &= \\ &= \frac{P_{n+m}(x_1, t_1; \dots; x_n, t_n; x_{n+1}, t_{n+1}; \dots; x_{n+m}, t_{n+m})}{P_m(x_{n+1}, t_{n+1}; \dots; x_{n+m}, t_{n+m})} \end{aligned} \quad (1.4)$$

Among the many possible classes of stochastic processes, there is one that plays a central role: *Markov Processes* (van Kampen (2004); Risken (1983); Gardiner (2009); Wio (1994); Lindenberg and Wio (2003)). For a stochastic process $x(t)$,

$$P(x_2, t_2 | x_1, t_1)$$

is the *conditional* or *transition* probability that $x(t_2)$ takes the value x_2 , knowing that $x(t_1)$ has taken the value x_1 . From this definition and (1.4) results the following identity for the *joint probability* $P_2(x_1, t_1; x_2, t_2)$ (Bayes' rule)

$$P_2(x_1, t_1; x_2, t_2) = P(x_2, t_2 | x_1, t_1) P_1(x_1, t_1). \quad (1.5)$$

A process $x(t)$ is called *Markovian* if for every set of successive times $t_1 < t_2 < \dots < t_n$, the following condition holds

$$\begin{aligned} P_n(x_1, t_1, \dots, x_n, t_n) &= P_1(x_1, t_1) P_{n-1}(x_2, t_2, \dots, x_n, t_n | x_1, t_1) \\ &= P_1(x_1, t_1) P(x_n, t_n | x_{n-1}, t_{n-1}) \dots P(x_2, t_2 | x_1, t_1), \end{aligned} \quad (1.6)$$

From this definition, it follows that a Markov process is completely determined if we know $P_1(x_1, t_1)$ and $P(x_2, t_2 | x_1, t_1)$. It is easy to find a relevant condition to be fulfilled for Markov processes: specifying the previous equation for the case $n = 3$ and integrating over x_2 , we obtain

$$\begin{aligned} \int dx_2 P_3(x_1, t_1, x_2, t_2, x_3, t_3) &= P_2(x_1, t_1, x_3, t_3) \\ &= P_1(x_1, t_1) P(x_3, t_3 | x_1, t_1) \\ &= \int dx_2 P_1(x_1, t_1) P(x_3, t_3 | x_2, t_2) P(x_2, t_2 | x_1, t_1). \end{aligned} \quad (1.7)$$

For $t_1 < t_2 < t_3$ we find the identity

$$P(x_3, t_3 | x_1, t_1) = \int dx_2 P(x_3, t_3 | x_2, t_2) P(x_2, t_2 | x_1, t_1), \quad (1.8)$$

which is the *Chapman-Kolmogorov Equation* for Markov processes. Every pair of non-negative functions $P_1(x_1, t_1)$ and $P(x_2, t_2 | x_1, t_1)$, adequately normalized and satisfying not only (1.8) but also

$$P_1(x_2, t_2) = \int dx_1 P_1(x_1, t_1) P(x_2, t_2 | x_1, t_1), \quad (1.9)$$

defines a Markov process. Some typical (useful) examples of Markov processes are: the *Wiener-Levy*, the *Ornstein-Uhlenbeck* and the *Poisson* processes (van Kampen (2004); Gardiner (2009)).

Before introducing the master equation, let us briefly discuss about changing variables. Assume we have the following relation between stochastic variables y and x

$$y = f(x). \quad (1.10)$$

A familiar example could be the use of a logarithmic scale $y = \log x$. In general, the ranges of both variables will differ. The probability that y has a value between y and $y + \Delta y$ is given by

$$P(y)\Delta y = \int_{y < f(x) < y + \Delta y} dx P(x), \quad (1.11)$$

where the integral extends over all intervals of the range of x where the inequality is fulfilled. We can write equivalently

$$P(y) = \int dx \delta[f(x) - y] P(x). \quad (1.12)$$

If we have a one-to-one relation among the variables (the dimensions of x and y are the same) it is possible to invert (1.10) obtaining

$$P(y) = \mathcal{J} P(x), \quad (1.13)$$

with \mathcal{J} the absolute value of the Jacobian's determinant.

1.2 Master Equation

The Chapman–Kolmogorov equation (which is only a property of the solutions for Markov processes) can be recast into a useful form. Going back to (1.8), we take $t_3 = t_2 + \delta t$ and consider the limit $\delta t \rightarrow 0$. It is clear that we have $P(x_3, t_3 | x_2, t_2) = \delta(x_3 - x_2)$, and it is intuitive to assume that, if $t_3 - t_2 \simeq \delta t$ (very small), the probability that a transition happens must be proportional to δt . Accordingly we adopt

$$\begin{aligned} P(x_3, t_2 + \delta t | x_2, t_2) &= \delta(x_3 - x_2) [1 - A(x_2) \delta t] \\ &\quad + \delta t W(x_3 | x_2) + O(\delta t^2), \end{aligned} \quad (1.14)$$

where $W(x_3 | x_2)$ is the *transition probability per unit time* from x_2 to x_3 (which in general could also be a function of t_2). The probability normalization tells us that

$$A(x_2) = \int W(x_3 | x_2) dx_3.$$

Substitution of the form for $P(x_3, t_2 + \delta t \mid x_2, t_2)$ into (1.8) gives

$$\begin{aligned}
 P(x_3, t_2 + \delta t \mid x_1, t_1) &= \int P(x_3, t_2 + \delta t \mid x_2, t_2) P(x_2, t_2 \mid x_1, t_1) dx_2 \\
 &= [1 - A(x_3) \delta t] P(x_3, t_2 \mid x_1, t_1) + \delta t \int W(x_3 \mid x_2) P(x_2, t_2 \mid x_1, t_1) dx_2 \\
 &= P(x_3, t_2 \mid x_1, t_1) - \delta t \int W(x_2 \mid x_3) P(x_3, t_2 \mid x_1, t_1) dx_2 \\
 &\quad + \delta t \int W(x_3 \mid x_2) P(x_2, t_2 \mid x_1, t_1) dx_2. \quad (1.15)
 \end{aligned}$$

After rearranging and taking the limit $\delta t \rightarrow 0$ we get

$$\frac{P(x_3, t_2 + \delta t \mid x_1, t_1) - P(x_3, t_2 \mid x_1, t_1)}{\delta t} \approx \frac{\partial}{\partial t} P(x, t \mid x_0, t_0), \quad (1.16)$$

finally yielding

$$\frac{\partial}{\partial t} P(x, t \mid x_0, t_0) = \int \left(W(x \mid x') P(x', t \mid x_0, t_0) - W(x' \mid x) P(x, t \mid x_0, t_0) \right) dx', \quad (1.17)$$

which corresponds to the *Master Equation* (van Kampen (2004); Gardiner (2009); Wio (1994); Lindenberg and Wio (2003); Wio, Deza and López (2012)).

The master equation is a differential form of the Chapman–Kolmogorov equation. It is an equation for the transition probability $P(x, t \mid x_0, t_0)$, and more adequate for mathematical manipulations than the Chapman–Kolmogorov equation, and it has a direct physical interpretation as a balance equation. At the same time, $W(x \mid x') \delta t$ is the transition probability during a very short time (δt). It could be evaluated by approximate methods, for instance by time dependent perturbation theory (i.e. : the *Fermi golden rule*), (van Kampen (2004); Gardiner (2009); Wio (1994)).

1.3 Langevin Equation

Brownian motion is the oldest and best known physical example of a Markov process. This phenomenon corresponds to the motion of a heavy test particle, immersed in a fluid composed of light particles in random motion. Due to the (random) collisions of the light particles against the test particle, the velocity of the latter varies in a (wide) sequence of small, uncorrelated jumps. However, similar ideas can (and have) been applied to a large variety of systems (van Kampen (2004); Gardiner (2009); Brink (1985); Wio

(1994); Lindenberg and Wio (2003); Wio, Deza and López (2012)). To simplify the presentation we restrict the description to a one dimensional system.

We will give a simple quantitative picture of Brownian motion. We start by writing Newton's equation as

$$m \dot{v} = F(t) + f(t), \quad (1.18)$$

where m is the mass of the Brownian particle, v its velocity, $F(t)$ the force due to some external field (i.e. gravitational, electrical for charged particles, etc), and $f(t)$ is the force produced by the collisions of fluid particles against the test particle. Due to the rapid fluctuations in v , we have two effects. On one hand a *systematic* one, i.e., a kind of *friction* that tends to slow down the particle, while on the other hand, a *random* contribution from the random hits of the fluid particle. If the mass of the test particle is much larger than the mass of the fluid particles (implying that the fluid *relaxes* faster than the test particle, allowing us to assume that it is always in equilibrium), we can write

$$\frac{1}{m}f(t) = -\gamma v + \xi(t). \quad (1.19)$$

In the r.h.s., γ is the friction coefficient, and the minus sign in the first term indicates that this contribution should oppose the motion (as a well behaved friction term). The second term corresponds to the stochastic or random contribution, since we have separated the systematic contribution in the first term, and this random contribution averages to zero: $\langle \xi(t) \rangle = 0$ (where the average is over an *ensemble* of noninteracting Brownian particles). In order to define the so called *Langevin force* (or *white noise*) it is required that

$$\langle \xi(t)\xi(t') \rangle = D \delta(t - t'). \quad (1.20)$$

We will not consider higher order moments, but it is clear that to fully characterize the fluctuating force, we need the whole hierarchy of moments (van Kampen (2004); Gardiner (2009)).

With the above indicated arguments, and without an external field, (1.18) adopts the form

$$\dot{v} = -\gamma v + \xi(t), \quad (1.21)$$

which is known as the *Langevin equation*. This is the simplest example of a SDE (that is, a differential equation whose coefficients are random functions with known stochastic properties). Hence $v(t)$ is a stochastic process, with