

Path Integrals For Stochastic Processes

An Introduction



Horacio S Wio



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Horacio J Wio

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An Introduction

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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.

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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); Wiegel (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.

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Horacio S. Wio
Santander, August 2012

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

1000

Contents

<i>Preface</i>	vii
1. Stochastic Processes: A Short Tour	1
1.1 Stochastic Process	1
1.2 Master Equation	4
1.3 Langevin Equation	5
1.4 Fokker–Planck Equation	7
1.5 Relation Between Langevin and Fokker–Planck Equations	9
2. The Path Integral for a Markov Stochastic Process	13
2.1 The Wiener Integral	13
2.2 The Path Integral for a General Markov Process	16
2.3 The Recovering of the Fokker–Planck Equation	20
2.4 Path Integrals in Phase Space	21
2.5 Generating Functional and Correlations	24
3. Generalized Path Expansion Scheme I	27
3.1 Expansion Around the Reference Path	27
3.2 Fluctuations Around the Reference Path	30
4. Space-Time Transformation I	33
4.1 Introduction	33
4.2 Simple Example	34
4.3 Fluctuation Theorems from Non-equilibrium Onsager–Machlup Theory	39



4.4	Brownian Particle in a Time-Dependent Harmonic Potential	41
4.5	Work Distribution Function	43
5.	Generalized Path Expansion Scheme II	47
5.1	Path Expansion: Further Aspects	47
5.2	Examples	51
5.2.1	Ornstein–Uhlenbeck Problem	51
5.2.2	Simplified Prey–Predator Model	52
6.	Space-Time Transformation II	55
6.1	Introduction	55
6.2	The Diffusion Propagator	56
6.3	Flow Through the Infinite Barrier	60
6.4	Asymptotic Probability Distribution	62
6.5	General Localization Conditions	62
6.6	A Family of Analytical Solutions	63
6.7	Stochastic Resonance in a Monostable Non-Harmonic Time-Dependent Potential	64
7.	Non-Markov Processes: Colored Noise Case	71
7.1	Introduction	71
7.2	Ornstein–Uhlenbeck Case	72
7.3	The Stationary Distribution	77
7.4	The Interpolating Scheme	79
7.4.1	Stationary Distributions	82
8.	Non-Markov Processes: Non-Gaussian Case	85
8.1	Introduction	85
8.2	Non-Gaussian Process η	86
8.3	Effective Markov Approximation	89
9.	Non-Markov Processes: Nonlinear Cases	95
9.1	Introduction	95
9.2	Nonlinear Noise	96
9.2.1	Polynomial Noise	96
9.2.2	Exponential Noise	98
9.3	Kramers Problem	100

10. Fractional Diffusion Process	103
10.1 Short Introduction to Fractional Brownian Motion	103
10.2 Fractional Brownian Motion: A Path Integral Approach . . .	105
10.3 Fractional Brownian Motion: The Kinetic Equation	108
10.4 Fractional Brownian Motion: Some Extensions	109
10.4.1 Case 1	109
10.4.2 Case 2	111
10.5 Fractional Lévy Motion: Path Integral Approach	112
10.5.1 Gaussian Test	114
10.5.2 Kinetic Equation	115
10.6 Fractional Lévy Motion: Final Comments	116
11. Feynman–Kac Formula, the Influence Functional	119
11.1 Feynman–Kac formula	119
11.2 Influence Functional: Elimination of Irrelevant Variables . .	123
11.2.1 Example: Colored Noise	126
11.2.2 Example: Lotka–Volterra Model	127
11.3 Kramers Problem	127
12. Other Diffusion-Like Problems	129
12.1 Diffusion in Shear Flows	129
12.2 Diffusion Controlled Reactions	133
12.2.1 The Model	133
12.2.2 Point of View of Path Integrals	136
12.2.3 Results for the Reaction $A + B \rightarrow B$	138
13. What was Left Out	141
Appendix A Space-Time Transformation: Definitions and Solutions	145
A.1 Definitions	145
A.2 Solutions	146
Appendix B Basics Definitions in Fractional Calculus	147
<i>Bibliography</i>	149
<i>Index</i>	157

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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

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

(1.4)



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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

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

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

a given initial condition. For details we refer the reader to van Kampen (2004); Risken (1983); Horsthemke and Lefever (1984); Gardiner (2009); Wio (1994); Lindenberg and Wio (2003); Wio, Deza and López (2012).

When an external field is present, we have the pair of equations

$$\begin{aligned}\dot{x} &= v \\ \dot{v} &= \frac{1}{m}F(x) - \gamma v + \xi(t).\end{aligned}\quad (1.22)$$

After differentiating the first one and substituting in the second, it adopts the form

$$\ddot{x} = \frac{1}{m}F(x) - \gamma \dot{x} + \xi(t).\quad (1.23)$$

In the case of large friction (γ very large), through an *adiabatic elimination* ($\ddot{x} \simeq 0$) (Haken (1978); van Kampen (2004); Gardiner (2009); Wio (1994); Wio, Deza and López (2012)), we can rewrite the last equation as

$$\dot{x} = -\frac{\partial}{\partial x} V(x) + \xi(t),\quad (1.24)$$

where $\frac{\partial}{\partial x} V(x) = -F(x)$, and m and γ have been absorbed into the different terms. The last result corresponds to the problem of *diffusion in a field* in the *overdamped* case (van Kampen (2004); Risken (1983); Gardiner (2009); Wio (1994); Lindenberg and Wio (2003)).

1.4 Fokker–Planck Equation

Let us now return to the Master Equation (1.17). We assume that x is a continuous variable, and that its changes correspond to *small jumps* (or variations). In this case it is possible to derive, starting from the Master Equation, a differential equation. The transition probability $W(x | x')$ will decay very fast as a function of $|x - x'|$. We could then write $W(x | x') = W(x', \xi)$, where $\xi = x - x'$ corresponds to the size of the jump. The Master Equation will take the form

$$\begin{aligned}\frac{\partial}{\partial t} P(x, t | x_0, t_0) &= \int W(x - \xi, \xi) P(x - \xi, t | x_0, t_0) d\xi \\ &\quad - P(x, t | x_0, t_0) \int W(x, -\xi) d\xi.\end{aligned}\quad (1.25)$$



Following our assumption of small jumps, and the additional argument that P varies slowly with x , we make a Taylor expansion in ξ that gives

$$\begin{aligned} \frac{\partial}{\partial t} P(x, t | x_0, t_0) = & \int \left[W(x, \xi) P(x, t | x_0, t_0) - \xi \frac{\partial}{\partial x} W(x, \xi) P(x, t | x_0, t_0) \right. \\ & + \xi^2 \frac{\partial^2}{\partial x^2} W(x, \xi) P(x, t | x_0, t_0) - \dots \Big] d\xi \\ & - P(x, t | x_0, t_0) \int W(x, -\xi) d\xi. \end{aligned} \quad (1.26)$$

As the first and the last terms are equal (in the latter changing $-\xi$ by ξ , as well as the integration limits), we get

$$\frac{\partial}{\partial t} P(x, t | x_0, t_0) = \sum_{\nu=1}^{\infty} \frac{(-1)^\nu}{\nu!} \frac{\partial^\nu}{\partial x^\nu} \alpha_\nu(x) P(x, t | x_0, t_0), \quad (1.27)$$

with $\alpha_\nu(x) = \int \xi^\nu W(x, \xi) d\xi$. This result corresponds to the *Kramers–Moyal expansion* of the Master Equation (van Kampen (2004); Risken (1983); Gardiner (2009); Wio (1994); Wio, Deza and López (2012)). Up to this point we have gained nothing. However, there could be situations where, for $\nu > 2$, the α_ν are either zero or very small (even though there are no *a priori* criteria about the relative size of the terms). If this is the case, we have

$$\begin{aligned} \frac{\partial}{\partial t} P(x, t | x_0, t_0) = & - \frac{\partial}{\partial x} \alpha_1(x) P(x, t | x_0, t_0) \\ & + \frac{1}{2} \frac{\partial^2}{\partial x^2} \alpha_2(x) P(x, t | x_0, t_0), \end{aligned} \quad (1.28)$$

which corresponds to the *Fokker–Planck equation* (van Kampen (2004); Risken (1983); Gardiner (2009); Wio (1994); Lindenberg and Wio (2003); Wio, Deza and López (2012)).

Let us look at a couple of examples. For the Wiener–Levy process we find that $\alpha_1(x) = 0$ and $\alpha_2(x) = 1$, then

$$\frac{\partial}{\partial t} P(x, t | x_0, t_0) = \frac{\partial^2}{\partial x^2} P(x, t | x_0, t_0),$$

while for the case of the Ornstein–Uhlenbeck process we find $\alpha_1(x) = x$, $\alpha_2(x) = D$, and we get

$$\frac{\partial}{\partial t} P(x, t | x_0, t_0) = - \frac{\partial}{\partial x} x P(x, t | x_0, t_0) + \frac{\partial^2}{\partial x^2} P(x, t | x_0, t_0).$$



Equation (1.28) corresponds to a *nonlinear* Fokker–Planck equation (due to the dependence of $\alpha_1(x)$ and $\alpha_2(x)$ on x), which is the result of poorly grounded assumptions (i.e., the criteria to decide where to cut the expansion, etc). Even worse, it is **not a systematic** approximation to the Master Equation. However, there is a procedure due to van Kampen that does make it possible to build up such a systematic procedure, but we will not discuss it here and instead refer the reader to van Kampen (2004); Gardiner (2009); Wio (1994); Wio, Deza and López (2012).

Consider the long time limit, where we expect that the system will reach a stationary behavior (that is: $\partial_t P(x, t | x_0, t_0) = 0$). In such a case we will have that

$$0 = - \frac{d}{dx} \alpha_1(x) P_{st}(x) + \frac{D}{2} \frac{d^2}{dx^2} P_{st}(x), \quad (1.29)$$

where in order to simplify we have taken $\alpha_2(x) = \text{const.} = D$. The stationary distribution turns out to be

$$P_{st}(x) \simeq \mathcal{N} e^{-\int dx' \alpha_1(x')/D}. \quad (1.30)$$

The exponent in the last equation allows us to define the (*non equilibrium*) *potential* $U(x)$ through

$$U(x) = - \int dx' \alpha_1(x'). \quad (1.31)$$

1.5 Relation Between Langevin and Fokker–Planck Equations

Here we give a brief and more or less formal (but not completely rigorous from a mathematical point of view) presentation of the relation between *stochastic differential equations* (SDE) of the *Langevin type* (LE), and *Fokker–Planck equations* (FPE). We start considering a general form for the one-dimensional SDE as indicated in (1.2):

$$\dot{x}(t) = \frac{dx(t)}{dt} = f(x(t), t) + g(x(t), t) \xi(t) \quad (1.32)$$

where $\xi(t)$ is a *white noise* with

$$\langle \xi(t) \rangle = 0 \quad \text{and} \quad \langle \xi(t) \xi(t') \rangle = \delta(t - t')$$

as in (1.19) and (1.20), with $D = 1$. We made the usual assumption that the process is Gaussian. However, $\xi(t)$ is not a well defined stochastic process. In a loose way, it could be considered as the derivative of the well

defined *Wiener process*, but such a derivative does not really exist (van Kampen (2004); Gardiner (2009)). We now integrate (1.32) over a short time interval δt

$$x(t + \delta t) - x(t) = f(x(t), t) \delta t + g(x(t), t) \xi(t) \delta t. \quad (1.33)$$

It is worth commenting here that in writing the above equation we have adopted the so called *Ito* prescription. The two most usual prescriptions are the Ito and the Stratonovich ones (Gardiner (2009)). The first corresponds to evaluating $g(x(t), t) \xi(t)$ at the beginning of the interval $[t, t + \delta t]$, while the second corresponds to evaluating it in the middle of that interval (i.e. $t^* = t + \delta t/2$). This is a point we will briefly comment in the next chapter.

As $x(t)$ is a Markov process, it is well defined if we are able to determine its probability distribution $P_1(x, t)$ as well as its conditional probability distribution $P(x, t | x', t')(t > t')$. In order to obtain an equation for the latter quantity, we define now a *conditional average*, corresponding to the average of a function of the stochastic variable x (say $F(x)$), given that x has the value y at $t' < t$:

$$\langle F(x(t)) | x(t') = y \rangle = \ll F(x(t)) \gg = \int dx' F(x') P(x', t | y, t'). \quad (1.34)$$

Due to the property $P(x, t | x', t) = \delta(x - x')$, we have

$$\langle F(x(t)) | x(t) = y \rangle = F(y). \quad (1.35)$$

We use now this definition in order to obtain the first few *conditional moments* of $x(t)$.

$$\begin{aligned} \ll \Delta x(t) \gg &= \langle x(t + \delta t) | x(t) = x \rangle = \\ &= \ll f(x(t), t) \delta t \gg + \ll g(x(t), t) \xi(t) \delta t \gg. \end{aligned} \quad (1.36)$$

The result shown in (1.35) indicates that $\ll f(x(t), t) \delta t \gg = f(x(t), t) \delta t$, and also that $\ll g(x(t), t) \xi(t) \delta t \gg = g(x(t), t) \ll \xi(t) \gg \delta t = 0$, resulting in

$$\ll \Delta x(t) \gg = f(x(t), t) \delta t. \quad (1.37)$$

For the second moment we need to resort to properties of the Wiener process; i.e. using that $\xi(t) \delta t = \int_t^{t+\delta t} dt \xi(t') = d\Delta W(t)$, where $W(t)$ is the Wiener process, and $\langle [\xi(t) \delta t]^2 \rangle \simeq \langle \Delta W(t)^2 \rangle = \Delta t$; to obtain

$$\ll \Delta x(t)^2 \gg = g(x(t), t)^2 \delta t + O(\delta t^2). \quad (1.38)$$



Let us now consider an arbitrary function $R(x)$, and evaluate its conditional average. Using the Chapman–Kolmogorov equation

$$\int dx R(x) P(x, t + \delta t | y, s) = \int dz P(z, t | y, s) \int dx R(x) P(x, t + \delta t | z, t), \quad (1.39)$$

We can expand $R(x)$ in a Taylor series around z , since for $\delta t \simeq 0$ we know that $P(x, t + \delta t | z, t) \simeq \delta(x - z)$, and that only a neighborhood of z will be relevant. If we also remember the normalization condition for $P(z, t | y, s)$, integrate by parts and use (1.37) and (1.38) we obtain an equation that, after arranging terms and taking the limit $\delta t \rightarrow 0$, gives

$$\begin{aligned} \int dx R(x) \left(\frac{\partial}{\partial t} P(x, t | y, s) - \left(-\frac{\partial}{\partial x} [f(x, t) P(x, t | y, s)] \right. \right. \\ \left. \left. + \frac{1}{2} \frac{\partial^2}{\partial x^2} [g(x, t)^2 P(x, t | y, s)] \right) \right) = 0 \end{aligned} \quad (1.40)$$

Due to the arbitrariness of the function $R(x)$, we arrive at the condition

$$\begin{aligned} \frac{\partial}{\partial t} P(x, t | y, s) = -\frac{\partial}{\partial x} [f(x, t) P(x, t | y, s)] \\ + \frac{1}{2} \frac{\partial^2}{\partial x^2} [g(x, t)^2 P(x, t | y, s)], \end{aligned} \quad (1.41)$$

which is the desired Fokker–Planck equation for $P(x, t | y, s)$, the transition probability associated with the stochastic process driven by the SDE (1.32).

We interrupted this brief overview on stochastic processes at this point, and start to discuss their path integral representation.

.. .. .

Chapter 2

The Path Integral for a Markov Stochastic Process

2.1 The Wiener Integral

Here we focus on one-dimensional Markovian processes describable through Langevin or Fokker–Planck equations as discussed in the previous chapter. The most general form of the Langevin equation we will consider is (see (1.32))

$$\dot{q} = f(q, t) + g(q, t)\xi(t) \quad (2.1)$$

where $f(q, t)$ and $g(q, t)$ are known (smooth) functions, and $\xi(t)$ is a Gaussian white noise with zero mean and δ -correlated. The form of the FPE, which could be related with such a Langevin equation is (in the Ito prescription) given by (1.41). As has been discussed in the last section, $P(q, t | q', t')$ fulfills the Chapman–Kolmogorov equation ($t_1 < t_2 < t_3$)

$$P(q_3, t_3 | q_1, t_1) = \int_{-\infty}^{\infty} dq_2 P(q_3, t_3 | q_2, t_2) P(q_2, t_2 | q_1, t_1). \quad (2.2)$$

Such an equation allows, by making a partition of the time interval in N steps: $t_0 < t_1 < \dots < t_f$, with $t_j = t_o + j(t_f - t_o)/N$, to obtain a path-dependent representation of the propagator. With the given partition, we reiterate (2.2) n -times and write

$$P(q_f, t_f | q_0, t_0) = \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} dq_1 dq_2 \dots dq_{N-1} P(q_f, t_f | q_{N-1}, t_{N-1}) \dots \\ \dots P(q_2, t_2 | q_1, t_1) P(q_1, t_1 | q_o, t_o). \quad (2.3)$$

The last expression can be interpreted as an integration over all possible paths that the process could follow (corresponding to the different values of the sequence: $q_0, q_1, q_2, \dots, q_N = q_f$). In the last expression we need the

form of the *short time propagator* $P(q_{j+1}, t_{j+1} | q_j, t_j)$ in order to find the more conventional representation of the integration over paths. However we follow an alternative way.

Now, the probability that at a given time t , the process takes a value between a and b is given by

$$\int_a^b dq P(q, t | q_0, t_0) \quad (2.4)$$

Likewise, the probability that the process, starting at $q = q_0$ at $t = t_0$, has a value between a_1 and b_1 at t_1 , between a_2 and b_2 at $t_2, \dots$, between a_{N-1} and b_{N-1} at t_{N-1} (with $a_j < b_j$ and $t_j < t_{j+1}$), and reaching q_N at t_N , will be given by

$$\int_{a_1}^{b_1} \int_{a_2}^{b_2} \dots \int_{a_{N-1}}^{b_{N-1}} dq_1 dq_2 \dots dq_{N-1} P(q_N, t_N | q_{N-1}, t_{N-1}) \dots P(q_2, t_2 | q_1, t_1) P(q_1, t_1 | q_0, t_0). \quad (2.5)$$

If we increase the number of time slices within the time partition where the intervals (a_j, b_j) are specified, and at the same time take the limit $b_j - a_j \rightarrow 0$, the trajectory is defined with higher and higher precision. Clearly, a requisite is that the trajectories be continuous. This happens in particular for the Wiener process (van Kampen (2004); Gardiner (2009)). With all this in mind (2.3) can be interpreted as an integration over all the possible paths that the process could follow (corresponding to the different values of the sequence $q_0, q_1, q_2, \dots, q_{N-1}, q_f$). For the Wiener process we have that

$$P(W_2, t_2 | W_1, t_1) = \frac{1}{\sqrt{2\pi D (t_2 - t_1)}} \exp \left[-\frac{1}{2D(t_2 - t_1)} [W_2 - W_1]^2 \right]. \quad (2.6)$$

For $N \rightarrow \infty$, we can define a *measure* in the path-space known as the *Wiener measure* (Schulman (1981); Wio (1990)). By substituting (2.6) into (2.5) we get

$$\prod_{j=1}^N \left(\frac{dW_j}{\sqrt{4\pi\epsilon D}} \right) \exp \left[-\frac{1}{4D\epsilon} \sum_j (W_j - W_{j-1})^2 \right], \quad (2.7)$$

which is the desired probability of following a given path. Figure 2.1 depicts a “practical” example of such a trajectory, while Fig. 2.2 indicates alternative trajectories.

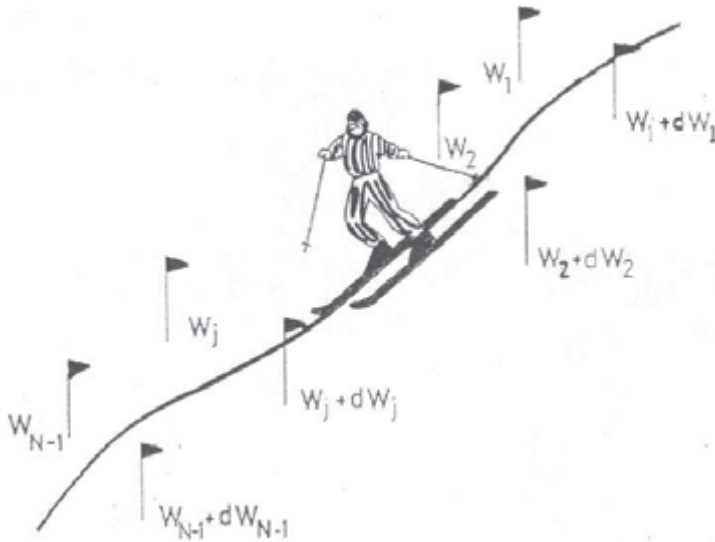


Fig. 2.1 A practical realization of a typical trajectory.

When $\epsilon \rightarrow 0$ and $N \rightarrow \infty$, we can write the exponential in (2.7) in the continuous limit as

$$e^{-\frac{1}{4D} \int_{t_0}^t d\tau \left(\frac{dW}{d\tau}\right)^2}. \quad (2.8)$$

If we integrate the expression in (2.5) over all the intermediate points (which is equivalent to a sum over all the possible paths), as all the integrands are Gaussian, and the convolution of two Gaussian is again a Gaussian, we recover the result of (2.8) for the probability density of the Wiener process. Hence, we have expressed the probability density as a **Wiener** path integral (Schulman (1981); Langouche *et al.* (1982))

$$P(W, t | W_0, t_0) = \int \mathcal{D}[W(\tau)] e^{-\frac{1}{4D} \int_{t_0}^t d\tau \left(\frac{dW}{d\tau}\right)^2}, \quad (2.9)$$

where the expression inside the integral represents the continuous version of the integral of (2.5), over all possible values of the intermediate points $\{W_j\}$.

2.2 The Path Integral for a General Markov Process

Let us go now back to the general SDE in (2.1). We start by writing the discrete version of the Langevin equation given by (1.33) (in order to simplify the notation we adopt $g(q, t) = 1$ and $f(q, t)$ to be independent of t)

$$q_{j+1} - q_j \simeq \{\alpha f(q_{j+1}) + (1 - \alpha) f(q_j)\} \epsilon + [W_{j+1} - W_j], \quad (2.10)$$

where $\epsilon = t_{j+1} - t_j = (t_f - t_o)/N$, and $W_j = W(t_j)$ is the Wiener process (just formally, $dW(t) \simeq \xi(t) dt$). The parameter α ($0 \leq \alpha \leq 1$) is arbitrary, the most usual choices being $\alpha = 0, 1/2$ and 1 , corresponding to the pre-point, midpoint and endpoint discretization, respectively. The first two are related to the so called Ito and Stratonovich schemes, respectively (Gardiner (2009)). Clearly, for the case of additive noise, there is no problem. However, for the case of multiplicative noise, that is when we have a general function for $g(q, t)$, the discretization procedure becomes a more delicate issue.

In addition to the above indicated discretization scheme, there are many others that yield the same continuous limit. For instance, instead of the form adopted before

$$\int_{t_j}^{t_{j+1}=t_j+\epsilon} f(q) ds \approx \{\alpha f(q_{j+1}) + (1 - \alpha) f(q_j)\} \epsilon$$

we can also use

$$\int_{t_j}^{t_{j+1}=t_j+\epsilon} f(q) ds \approx f(\alpha q_{j+1} + (1 - \alpha) q_j) \epsilon.$$

The last is the one to be used when discussing the recovering of the Fokker-Planck equation.

We don't want to deep into this aspect here, but just call the attention, and alert the reader about the existence of several possible discretization procedures for the path integral representation of the transition probability. And this is valid in both, configuration and phase space representations. A detailed discussion on the different discretization procedures, the equivalence and/or relations among them, as well as its relation in the quantum case to operator ordering, could be found in Langouche *et al.* (1982). We will not go into the usual difficulties related to this problem, but will keep

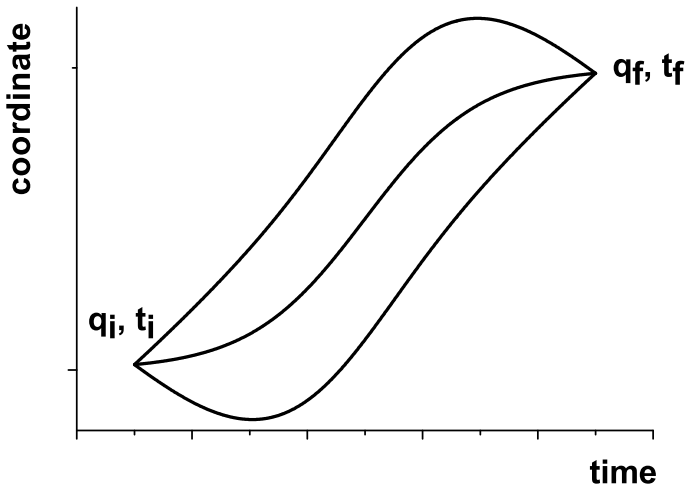


Fig. 2.2 A few possible trajectories starting at (q_i, t_i) and reaching (q_f, t_f) .

this parameter in order to show the dependence of the final *Lagrangian* on it.

According to the previous results, the probability that

$$W(t_0) = 0; W_1 < W(t_1) < W_1 + dW_1; \dots; W_N < W(t_N) < W_N + dW_N$$

is given by

$$P(\{W_j\}) \Delta\{W_j\} = \prod_{j=1}^N \left(\frac{dW_j}{\sqrt{4\pi\epsilon D}} \right) \exp \left[-\frac{1}{4D\epsilon} \sum_j (W_j - W_{j-1})^2 \right]. \quad (2.11)$$

As our interest is to have the corresponding probability in q -space, we need to transform the probability given in the last equation. As is well known, to do this we need the Jacobian of the transformation connecting both sets of stochastic variables $(\{W_j\} \rightarrow \{q_j\})$. To find it we write (2.10) as

$$W_j = q_j - q_{j-1} - \{\alpha f(q_j) + (1 - \alpha) f(q_{j-1})\} \epsilon + W_{j-1}. \quad (2.12)$$

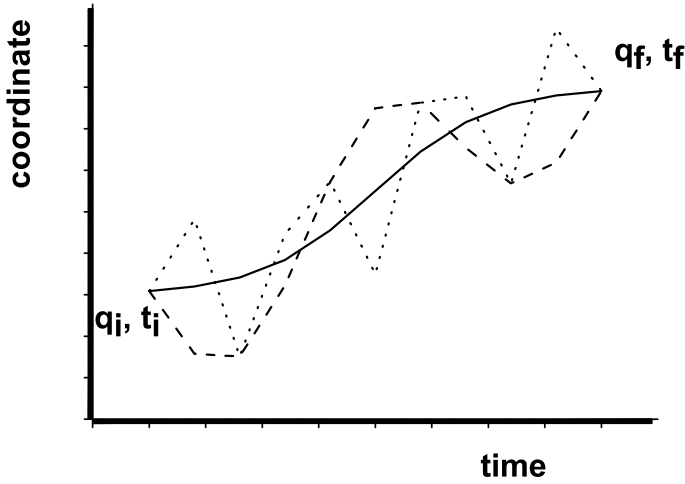


Fig. 2.3 Discrete versions of a continuous trajectory.

The Jacobian is given by

$$\mathcal{J} = \det \left(\frac{\partial W_j}{\partial q_k} \right) = \prod_{j=1}^N \left(1 - \epsilon \alpha \frac{df(q_j)}{dq_j} \right). \quad (2.13)$$

For $\epsilon \rightarrow 0$, it can be approximated as

$$\mathcal{J} = e^{-\epsilon \alpha \sum \frac{df(q_j)}{dq_j}}. \quad (2.14)$$

Now, remembering that $P(\{q_j\}) = \mathcal{J} P(\{W_j\})$, and taking into account that the conditional probability $P(q, t \mid q_0, t_0)$ is given as a sum over all the possible paths, we get

$$\begin{aligned} P(q, t \mid q_0, t_0) = & \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} \left(\frac{1}{4\pi\epsilon D} \right)^{N/2} dW_1 dW_2 \dots dW_N \delta(q_f - q_N) \\ & \times \exp \left(-\frac{1}{4D\epsilon} \sum_j (W_j - W_{j-1})^2 \right). \end{aligned} \quad (2.15)$$

Replacing (2.10) into (2.15) and going to the continuous limit, the different terms in the exponentials yield

$$\begin{aligned}
 \lim_{N \rightarrow \infty, \epsilon \rightarrow 0} \epsilon \alpha \sum_j \frac{df(q_j)}{dq_j} &\rightarrow \alpha \int_{t_0}^t ds \frac{df(q(s))}{dq} \\
 \lim_{N \rightarrow \infty, \epsilon \rightarrow 0} \frac{\epsilon}{2} \sum_j \left(\alpha f(q_{j+1}) + (1 - \alpha) f(q_j) \right)^2 &\rightarrow \frac{1}{2} \int_{t_0}^t ds f(q(s))^2 \\
 \lim_{N \rightarrow \infty, \epsilon \rightarrow 0} \frac{\epsilon}{2} \sum_j \left(\frac{(q_{j+1} - q_j)}{\epsilon} \right)^2 &\rightarrow \frac{1}{2} \int_{t_0}^t ds \dot{q}(s)^2 \\
 \lim_{N \rightarrow \infty, \epsilon \rightarrow 0} \sum_j (q_{j+1} - q_j) (\alpha f(q_{j+1}) + (1 - \alpha) f(q_j)) &\rightarrow \int_{t_0}^t dq f(q(s)).
 \end{aligned} \tag{2.16}$$

Hence, we can write

$$P(q, t \mid q_0, t_0) = \int \mathcal{D}[q(t)] e^{-\frac{1}{\hbar} \int_{t_0}^t ds \mathcal{L}[q(s), \dot{q}(s)]}, \tag{2.17}$$

where

$$\mathcal{L}[q(s), \dot{q}(s)] = \frac{1}{4} \left(\dot{q}(s) - f(q(s)) \right)^2 + \alpha \frac{df(q(s))}{dq}, \tag{2.18}$$

is the *stochastic Lagrangian*, also called Onsager–Machlup functional (Onsager and Machlup (1953a,b); Langouche *et al.* (1982)). The dependence of the Lagrangian on α is clearly seen in the last expression. In (2.17), $\mathcal{D}[q]$ corresponds to the differential of the path, that is, the continuous expression of the discrete product of differentials in (2.15). We can also identify the *stochastic action* through

$$\mathcal{S}[q(t)] = \int_{t_0}^t ds \mathcal{L}[q(s), \dot{q}(s)], \tag{2.19}$$

that allows to write Eq.(2.17) as

$$P(q, t \mid q_0, t_0) = \int \mathcal{D}[q(t)] e^{-\frac{1}{\hbar} \mathcal{S}[q(t)]}. \tag{2.20}$$

This last expression is the one we will exploit in the following.

2.3 The Recovering of the Fokker–Planck Equation

As in the quantum mechanics case, it is interesting to reassure oneself that the indicated form of the propagator allows us to recover the original Fokker–Planck equation. To verify this point, and according to the previous results, we can write a discrete version of the propagator (or conditional probability) as

$$\begin{aligned}
 P(q, t + \epsilon \mid q_0, t_0) &= \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} \left(\frac{1}{4\pi\epsilon D} \right)^{\frac{N+2}{2}} dq_1 dq_2 \dots dq_{N+1} \\
 &\quad \times \exp \left(-\frac{\epsilon}{4D} \sum_j^{N+2} \left(\frac{q_j - q_{j-1}}{\epsilon} - f\left(\frac{q_j + q_{j-1}}{2}\right) \right)^2 \right) \\
 &= \int_{-\infty}^{\infty} \left(\frac{1}{4\pi\epsilon D} \right)^{\frac{1}{2}} \exp \left(-\frac{\epsilon}{4D} \left(\frac{q - q_{N+1}}{\epsilon} - f\left(\frac{q + q_{N+1}}{2}\right) \right)^2 \right) \\
 &\quad \times P(q_{N+1}, t \mid q_0, t_0), \tag{2.21}
 \end{aligned}$$

where in the last line we have extracted the final integration point, and identified the rest with $P(q_{N+1}, t \mid q_0, t_0)$. Note that the discretization form we have adopted here, as the noise is additive, results equivalent to the one we used previously. See also the brief comments about the discretization procedures after (2.10).

Now we define the following change of variables $\eta = q - q_{N+1}$ that could be written as $q_{N+1} = q - \eta$, and $d\eta = -dq_{N+1}$. We also have

$$\frac{q + q_{N+1}}{2} = \frac{q + q - \eta}{2} = q - \frac{\eta}{2}.$$

Hence, the previous equation can be written as

$$\begin{aligned}
 P(q, t + \epsilon \mid q_0, t_0) &= \int_{-\infty}^{\infty} d\eta \left(\frac{1}{4\pi\epsilon D} \right)^{1/2} \\
 &\quad \times \exp \left(-\frac{\epsilon}{4D} \left(\frac{\eta}{\epsilon} - f\left(q - \frac{\eta}{2}\right) \right)^2 \right) P(q - \eta, t \mid q_0, t_0) \\
 &\approx \int_{-\infty}^{\infty} d\eta \left(\frac{1}{4\pi\epsilon D} \right)^{1/2} \\
 &\quad \times \exp \left(-\frac{\epsilon}{4D} \left(\left(\frac{\eta}{\epsilon} \right)^2 - 2\frac{\eta}{\epsilon} f\left(q - \frac{\eta}{2}\right) + f\left(q - \frac{\eta}{2}\right)^2 \right) \right) \\
 &\quad \times P(q - \eta, t \mid q_0, t_0), \tag{2.22}
 \end{aligned}$$

that corresponds to a Gaussian integration in η . As ϵ is very small, only small values of η will contribute to the integral. Hence, we can expand $f(q - \frac{\eta}{2})$ and $P(q - \eta, t | q_0, t_0)$ around $\eta \approx 0$.

We have

$$P(q - \eta, t | q_0, t_0) \approx P(q, t | q_0, t_0) - \eta \frac{\partial}{\partial q} P(q, t | q_0, t_0) + \frac{\eta^2}{2} \frac{\partial^2}{\partial q^2} P(q, t | q_0, t_0) + O(\eta^3).$$

Inserting this and also the expansion of $f(q - \eta)$ we get

$$\begin{aligned} P(q, t + \epsilon | q_0, t_0) &\approx \int_{-\infty}^{\infty} \left(\frac{1}{4\pi\epsilon D} \right)^{1/2} d\eta \\ &\times \left(1 - \frac{1}{2D} \left[\eta f(q) - \frac{\eta^2}{2} f'(q) \right] - \frac{\epsilon}{4D} f(q)^2 \dots \right) \\ &\times \left(P(q, t | q_0, t_0) - \eta \frac{\partial}{\partial q} P(q, t | q_0, t_0) + \frac{\eta^2}{2} \frac{\partial^2}{\partial q^2} P(q, t | q_0, t_0) + \dots \right) \end{aligned}$$

whose integration yields

$$\begin{aligned} P(q, t + \epsilon | q_0, t_0) &\approx P(q, t | q_0, t_0) + \epsilon \left[\frac{\partial}{\partial q} (f(q) P(q, t | q_0, t_0)) \right. \\ &\quad \left. \dots \dots \dots + D \frac{\partial^2}{\partial q^2} P(q, t | q_0, t_0) + O(\epsilon^2) \right]. \quad (2.23) \end{aligned}$$

Now, taking the limit $\epsilon \rightarrow 0$, and identifying

$$\frac{1}{\epsilon} (P(q, t + \epsilon | q_0, t_0) - P(q, t | q_0, t_0)) \approx \frac{\partial}{\partial t} P(q, t | q_0, t_0),$$

we recover the original Fokker–Planck equation.

2.4 Path Integrals in Phase Space

Similarly to what is done in a quantum mechanical framework, we can also obtain, within the present context, a path integral representation for the propagator in phase space (Marinov (1980); Langouche *et al.* (1982)). In

order to show how to get it, we will exploit a notation that resembles the *bra* and *ket* representation in quantum mechanics (Landau and Lifshitz (1958)).

Let us recall the Fokker–Planck equation

$$\begin{aligned}\frac{\partial}{\partial t}P(q, t \mid q_0, t_0) &= -\frac{\partial}{\partial q}(f(x)P(q, t \mid q_0, t_0)) + D\frac{\partial^2}{\partial q^2}P(q, t \mid q_0, t_0) \\ &= -LP(q, t \mid q_0, t_0),\end{aligned}\tag{2.24}$$

and, as in Feynman and Hibbs (1965), we define the *temporal evolution* operator through

$$P(q, t \mid q_0, t_0) = \langle q, t \mid q_0, t_0 \rangle = \langle q \mid U(t, t_0) \mid q_0 \rangle.$$

The kinetic equation fulfilled by the operator U results

$$\frac{\partial}{\partial t}U(t, t') = -L(\hat{p}, \hat{q})U(t, t'),\tag{2.25}$$

whose solution is

$$U(t, t') = \exp(-L(\hat{p}, \hat{q})[t - t']),$$

where p will be defined latter, and with the initial condition

$$U(t, t) = 1,$$

and the condition $\langle q \mid q' \rangle = \delta(q - q')$.

As we have done before, we can now use this notation to express the propagator in terms of a set of integrations over intermediate times (or time slicing)

$$\langle q \mid U(t, t_0) \mid q_0 \rangle = \int \dots \int \prod_{j=1}^M dq_j \prod_{j=1}^{M+1} \langle q_j \mid U(t_j, t_{j-1}) \mid q_{j-1} \rangle,\tag{2.26}$$

where $t_j = t_{j-1} + \epsilon = t_0 + j\epsilon$, so $\epsilon = \frac{t-t_0}{M+1}$, and $t_{M+1} = t$.

We now resort to the so called Trotter's formula (see for instance Schulman (1981)). For operators A and B , and a parameter λ we have that

$$\exp(\lambda(A + B)) = \exp(\lambda A) \exp(\lambda B) \exp\left(\frac{\lambda^2}{2}[A, B] + O(\lambda^3)\right),$$

where $[A, B]$ indicates the commutator of operators A and B . For $\lambda \ll 1$ the above expression reduces to

$$\approx \exp(\lambda A) \exp(\lambda B) + O(\lambda^2).$$

Hence, for very small ϵ (or M large enough) we have

$$\langle q_j | U(t_j, t_{j-1}) | q_{j-1} \rangle \approx \exp(-\epsilon L(p_j, q_j)).$$

We define the operator p as

$$\frac{\partial}{\partial q} \rightarrow i\hat{p},$$

its eigenfunctions $\langle p_j |$ fulfilling

$$\langle p_j | q_j \rangle = \frac{1}{\sqrt{2\pi}} \exp(ip_j q_j),$$

and

$$\int dp_j | p_j \rangle \langle p_j | = 1.$$

We also have that

$$f(q) | q' \rangle = f(q') | q' \rangle,$$

as well as

$$\exp\left(\epsilon \frac{\partial}{\partial q} f(q)\right) | p \rangle \rightarrow \exp(\epsilon i p f(q)) | p \rangle,$$

$$\exp\left(\epsilon D \frac{\partial^2}{\partial q^2}\right) | p \rangle \rightarrow \exp(-\epsilon D p^2) | p \rangle.$$

According to these results, each contribution to the propagator could be written as

$$\begin{aligned} \langle q_j | U(t_j, t_{j-1}) | q_{j-1} \rangle &= \int dp_{j-1} \langle q_j | U(t_j, t_{j-1}) | p_{j-1} \rangle \langle p_{j-1} | q_{j-1} \rangle \\ &= \int dp_{j-1} \langle q_j | \exp\left(\epsilon \frac{\partial}{\partial q_j} f(q_j) - \epsilon D \frac{\partial^2}{\partial q_j^2}\right) \\ &\quad \times | p_{j-1} \rangle \langle p_{j-1} | q_{j-1} \rangle \\ &= \int dp_{j-1} \langle q_j | p_{j-1} \rangle \exp(\epsilon [ip_{j-1} f(q_j) - D p_{j-1}^2]) \\ &\quad \times \frac{1}{\sqrt{2\pi}} \exp(ip_{j-1} q_{j-1}) \\ &= \frac{1}{2\pi} \int dp_{j-1} \exp\left(i\epsilon p_{j-1} [f(q_j) - \frac{\Delta q_j}{\epsilon}] - \epsilon D p_{j-1}^2\right), \end{aligned}$$

with $\Delta q_j = q_j - q_{j-1}$.

Introducing this expression into (2.26) we obtain

$$\begin{aligned} \langle q \mid U(t, t_0) \mid q_0 \rangle &= \int \dots \int \prod_{j=1}^M dq_j \prod_{k=1}^{M+1} \frac{dp_k}{2\pi} \\ &\quad \times \prod_{j=1}^{M+1} \exp \left(i\epsilon p_{j-1} \left[f(q_j) - \frac{\Delta q_j}{\epsilon} \right] - \epsilon D p_{j-1}^2 \right) \\ &= \int \mathcal{D}[q(t)] \mathcal{D}[p(t)] \exp \left(-\frac{1}{D} S[q, p] \right), \end{aligned} \quad (2.28)$$

where the last line indicates the limit of $M \rightarrow \infty$. Here, the integration measures are such that

$$\mathcal{D}[q(t)] \approx \prod_{j=1}^M dq_j$$

and

$$\mathcal{D}[p(t)] \approx \prod_{k=1}^{M+1} \frac{dp_k}{2\pi}.$$

We have defined

$$S[q, p] = \int ds \left\{ ip(s) \dot{q}(s) - \mathcal{H}(q(s), p(s)) \right\}$$

with

$$\mathcal{H}(q(s), p(s)) = -ip(s)f(q(s)) - (ip(s))^2.$$

Equation (2.28) corresponds to the phase-space representation for the propagator, a form that we will exploit in some cases. Clearly, the Gaussian integrals over p_j can be readily done, yielding the different contributions in (2.16), and leading us to the usual configuration space path integral.

2.5 Generating Functional and Correlations

We now define the so called *Generating Functional* and its relation with the correlation functions. Starting from the form defined in (2.19), we define the following form of the action

$$\mathcal{S}_J[q(t)] = \int_{t_0}^t ds \left[\mathcal{L}[q(s), \dot{q}(s)] + DJ(s)q(s) \right]. \quad (2.29)$$



Introducing this form into the path integral we have the following functional

$$\mathcal{Z}[J(t)] = \int \mathcal{D}[q] \exp \left\{ -\frac{1}{D} \mathcal{S}_J[q(t)] \right\}, \quad (2.30)$$

this functional is called the *Generating Functional*. The reason for this name can be understood as follows. Let us take the functional derivatives of $\mathcal{Z}[J(t)]$ respect to $J(t)$. What we have is

$$\begin{aligned} \frac{\delta}{\delta J(t_1)} \mathcal{Z}[J(t)] &= - \int \mathcal{D}[q] q(t_1) \exp \left\{ -\frac{1}{D} \mathcal{S}_J[q(t)] \right\} \\ \frac{\delta^2}{\delta J(t_1) \delta J(t_2)} \mathcal{Z}[J(t)] &= \int \mathcal{D}[q] q(t_1) q(t_2) \exp \left\{ -\frac{1}{D} \mathcal{S}_J[q(t)] \right\} \\ &\dots = \dots \\ \frac{\delta^n}{\delta J(t_1) \dots \delta J(t_n)} \mathcal{Z}[J(t)] &= (-1)^n \int \mathcal{D}[q] q(t_1) \dots q(t_n) \exp \left\{ -\frac{1}{D} \mathcal{S}_J[q(t)] \right\}. \end{aligned}$$

When these expressions are evaluated at $J = 0$ we obtain

$$\begin{aligned} \left. \frac{\delta}{\delta J(t_1)} \mathcal{Z}[J(t)] \right|_{J=0} &= - \int \mathcal{D}[q] q(t_1) \exp \left\{ -\frac{1}{D} \mathcal{S}[q(t)] \right\} \\ &\dots \dots \\ &= -\langle q(t_1) \rangle \\ \left. \frac{\delta^2}{\delta J(t_1) \delta J(t_2)} \mathcal{Z}[J(t)] \right|_{J=0} &= \int \mathcal{D}[q] q(t_1) q(t_2) \exp \left\{ -\frac{1}{D} \mathcal{S}[q(t)] \right\} \\ &\dots \dots \\ &= -\langle q(t_1) q(t_2) \rangle, \\ &\dots = \dots \\ \left. \frac{\delta^n}{\delta J(t_1) \dots \delta J(t_n)} \mathcal{Z}[J(t)] \right|_{J=0} &= (-1)^n \int \mathcal{D}[q] q(t_1) \dots q(t_n) \exp \left\{ -\frac{1}{D} \mathcal{S}[q(t)] \right\} \\ &\dots \dots \\ &= -\langle q(t_1) \dots q(t_n) \rangle, \end{aligned} \quad (2.31)$$

where $\langle \dots \rangle$ indicates the average of the inserted quantity. It is clear that such averages correspond to the one, two, n -time correlation functions. In

general we could define

$$\langle q(t_1) \dots q(t_n) \rangle = (-1)^n \frac{\delta^n}{\delta J(t_1) \dots \delta J(t_n)} \mathcal{Z}[J(t)] \Big|_{J=0}, \quad (2.32)$$

that makes clear the reason for the name of $\mathcal{Z}[J(t)]$.

This functional also allows us to obtain the average of a function $\mathcal{G}[q(t)]$, if it accepts the following expansion

$$\mathcal{G}[q(t)] = \sum_{n=0}^{\infty} G_n q(t)^n. \quad (2.33)$$

Hence, we can define its average as

$$\begin{aligned} \langle \mathcal{G}[q(t)] \rangle &= \int \mathcal{D}[q] \mathcal{G}[q(t)] \exp \left\{ -\frac{1}{D} \mathcal{S}[q(t)] \right\} \\ &= \sum_{n=0}^{\infty} G_n \int \mathcal{D}[q] q(t)^n \exp \left\{ -\frac{1}{D} \mathcal{S}[q(t)] \right\}, \end{aligned} \quad (2.34)$$

and could be finally written as

$$\langle \mathcal{G}[q(t)] \rangle = \mathcal{G} \left[\frac{\delta}{\delta J(t)} \right] \mathcal{Z}[J(t)] \Big|_{J=0}. \quad (2.35)$$

Chapter 3

Generalized Path Expansion Scheme I

3.1 Expansion Around the Reference Path

The scheme we describe here is due to Davison (1954), and has been generalized by Levit and Smilansky (1985). Originally, this scheme was applied to the quantum case and we will adapt it here to the present stochastic framework.

Let $q_r(t)$ be a reference trajectory, which is an arbitrary function of t , satisfying the conditions

$$\begin{aligned}q_r(t_0) &= q(t_0) = q_0 \\ q_r(t_f) &= q(t_f) = q_f.\end{aligned}\tag{3.1}$$

Let $\{u^\nu(t)\}$ be an infinite orthogonal basis which spans the space of functions defined in the interval $[t_0, t_f]$ and vanishing at both its ends (i.e.: $u^\nu(t_0) = u^\nu(t_f) = 0$). This set can be conveniently chosen as the normalized eigenfunctions of an arbitrary Sturm–Liouville differential operator defined in this space. However we will see that just the problem under study provides the form of the most adequate operator. A completely arbitrary path can be split and written as

$$q(t) = q_r(t) + \sum_{\nu=1}^{\infty} a_\nu u^\nu(t).\tag{3.2}$$

Even though the reference trajectory $q_r(t)$ could be arbitrarily chosen, for convenience we select the one that makes extreme the action (2.19). The



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first variation of the action gives

$$\begin{aligned}\delta\mathcal{S}[q(t)] &= \int_{t_0}^t ds \left\{ \frac{\partial\mathcal{L}}{\partial q} \delta q + \frac{\partial\mathcal{L}}{\partial \dot{q}} \delta \dot{q} \right\} \\ &= \int_{t_0}^t ds \left\{ \frac{\partial\mathcal{L}}{\partial q} - \frac{d}{dt} \frac{\partial\mathcal{L}}{\partial \dot{q}} \right\} \delta q,\end{aligned}\quad (3.3)$$

where the variations fulfill $\delta q(t_0) = \delta q(q_f) = 0$. Then, the reference (sometimes called classical, or in the present context “most probable” (Langouche *et al.* (1982))) trajectory, chosen as the one that makes extreme the action, implies $\delta\mathcal{S}[q(t)] = 0$. Hence, it is the solution of the corresponding Euler–Lagrange equation

$$\frac{d}{dt} \frac{\partial\mathcal{L}}{\partial \dot{q}} - \frac{\partial\mathcal{L}}{\partial q} = 0. \quad (3.4)$$

We can expand the action about this classical path obtaining to the lowest order

$$\mathcal{S}[q(t)] = \mathcal{S}[q_r(t)] + \frac{1}{2} \delta^2 \mathcal{S}[q_r(t)]. \quad (3.5)$$

The second variation of $\mathcal{S}[q(t)]$, indicated by $\delta^2 \mathcal{S}[q_r(t)]$ leads to

$$\begin{aligned}\delta^2 \mathcal{S}[q_r(t)] &= \int_{t_0}^t ds \left\{ \delta q \frac{\partial^2 \mathcal{L}}{\partial q^2} \delta q + \delta q \frac{\partial^2 \mathcal{L}}{\partial q \partial \dot{q}} \delta \dot{q} \right. \\ &\quad \left. + \delta \dot{q} \frac{\partial^2 \mathcal{L}}{\partial \dot{q} \partial q} \delta q + \delta \dot{q} \frac{\partial^2 \mathcal{L}}{\partial \dot{q}^2} \delta \dot{q} \right\}_{q_r(t)},\end{aligned}\quad (3.6)$$

where all the second order derivatives must be evaluated along the classical path. We call

$$\mathcal{R}[q_r, \dot{q}_r] = \left(\frac{\partial^2 \mathcal{L}}{\partial q^2} \right)_{q_r} \quad (3.7)$$

$$\mathcal{Q}[q_r, \dot{q}_r] = \left(\frac{\partial^2 \mathcal{L}}{\partial q \partial \dot{q}} \right)_{q_r} \quad (3.8)$$

$$\tilde{\mathcal{Q}}[q_r, \dot{q}_r] = \left(\frac{\partial^2 \mathcal{L}}{\partial \dot{q} \partial q} \right)_{q_r} \quad (3.9)$$

$$\mathcal{P}[q_r, \dot{q}_r] = \left(\frac{\partial^2 \mathcal{L}}{\partial \dot{q}^2} \right)_{q_r}. \quad (3.10)$$

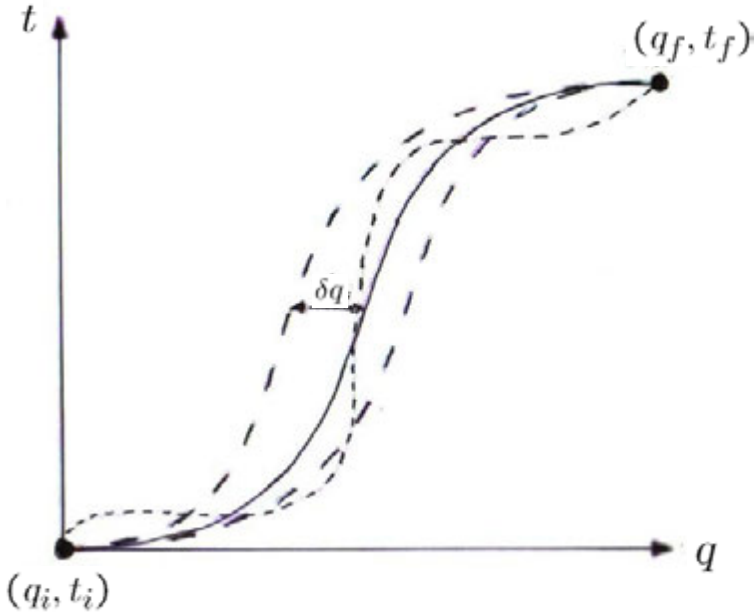


Fig. 3.1 Departure from the reference trajectory.

Now, we rewrite (3.6) as

$$\delta^2 \mathcal{S}[q_r(t)] = \int_{t_0}^t ds \left\{ \delta q \mathcal{R} \delta q + \delta q \mathcal{Q} \delta \dot{q} + \delta \dot{q} \tilde{\mathcal{Q}} \delta q + \delta \dot{q} \mathcal{P} \delta \dot{q} \right\}, \quad (3.11)$$

and after integrating by parts (once only), we obtain

$$\begin{aligned} \delta^2 \mathcal{S}[q_r(t)] &= \int_{t_0}^t ds \, \delta q \left\{ \mathcal{R} + \mathcal{Q} \frac{d}{dt} - \frac{d}{dt} \tilde{\mathcal{Q}} - \frac{d}{dt} \mathcal{P} \frac{d}{dt} \right\} \delta q \\ &= \int_{t_0}^t ds \, \delta q \Lambda \delta q. \end{aligned} \quad (3.12)$$

The explicit form of the operator Λ , also called Jacobi equation (Goldstein (1980)), is

$$\Lambda = - \left\{ \frac{d}{dt} \left(\frac{\partial^2 \mathcal{L}}{\partial \dot{q}^2} \right)_{q_r} \frac{d}{dt} + \frac{d}{dt} \left(\frac{\partial^2 \mathcal{L}}{\partial \dot{q} \partial q} \right)_{q_r} - \left(\frac{\partial^2 \mathcal{L}}{\partial q \partial \dot{q}} \right)_{q_r} \frac{d}{dt} - \left(\frac{\partial^2 \mathcal{L}}{\partial q^2} \right)_{q_r} \right\}, \quad (3.13)$$

and we reiterate that the coefficients obtained by derivatives of the Lagrangian should be evaluated at $q_r(t)$.

3.2 Fluctuations Around the Reference Path

We now choose the basis $u^\nu(t)$ as the solutions of the Sturm–Liouville problem associated with the operator Λ

$$\Lambda u^\nu(t) + \lambda^\nu u^\nu(t) = 0, \quad (3.14)$$

$$\int_{t_0}^t ds u^\nu(t) u^\eta(t) = \delta_{\nu\eta}, \quad (3.15)$$

with eigenvalues λ^ν and with the boundary conditions $u^\nu(t_0) = u^\nu(t) = 0$. Then we have

$$\delta^2 \mathcal{S}[q_r(t)] = \sum_{\nu, \eta} \int_{t_0}^t ds a_\nu a_\eta u^\nu(t) \Lambda u^\eta(t), \quad (3.16)$$

leading to

$$\delta^2 \mathcal{S}[q_r(t)] = \sum_{\nu} a_\nu^2 \lambda^\nu. \quad (3.17)$$

This result makes obvious the reason for choosing the basis $\{u^\nu(t)\}$ as was done in (3.14).

Returning to (2.20) and taking into account the expansion (3.5) and the last results, we obtain

$$\begin{aligned} P(q, t \mid q_0, t_0) &\cong \int \mathcal{D}[q(t)] e^{-\mathcal{S}[q_r(t)] - \frac{1}{2} \delta^2 \mathcal{S}[q_r(t)]} \\ &\simeq e^{-\mathcal{S}[q_r(t)]/D} \int_{\delta q(t_0)=\delta q(t_f)=0} \mathcal{D}[\delta q(t)] e^{-\frac{1}{2} \delta^2 \mathcal{S}[q_r(t)]} \\ &\simeq e^{-\mathcal{S}[q_r(t)]/D} \mathcal{K}(t_f \mid t_0). \end{aligned} \quad (3.18)$$

The procedure leading to (3.18) is equivalent to the usual stationary-phase approximation in the path-integral picture of standard quantum mechanics (Schulman (1981); Langouche *et al.* (1982); Levit and Smilansky (1985); Kleinert (1990b); Khandekar and Lawande (1986); Khandekar *et al.* (2000)). The first term represents the naive (classical) approximation for the propagator, while the last integral includes the fluctuations around the classical (or also deterministic) trajectory. What remains is to evaluate the

integral giving $\mathcal{K}(t_f | t_0)$, but transforming from $\{\delta q(t)\}$ to the set $\{a_\nu\}$. Since this is a linear transformation, and thus independent of the a_ν , what remains are several independent Gaussian integrals

$$\begin{aligned}\mathcal{K}(t_f | t_0) &= \int_{\lambda} \prod_{\nu} da_{\nu} \mathcal{J} e^{\sum_{\nu} \lambda^{\nu} a_{\nu}^2} \\ &= \mathcal{J} \prod_{\nu} \left(\frac{2\pi D}{\lambda^{\nu}} \right)^{1/2}.\end{aligned}\quad (3.19)$$

The Jacobian $\mathcal{J}$ must be invariant, in such a way that

$$\mathcal{K}(t_f | t_0) \prod_{\nu} (\lambda^{\nu})^{1/2} = \mathcal{K}(t_f | t_0)^{free} \prod_{\nu} (\lambda_{free}^{\nu})^{1/2}, \quad (3.20)$$

where *free* means the case without drift (that is $f(q) = 0$). In such a case the Sturm–Liouville operator takes the simple form

$$\Lambda^{free} = -\frac{d}{dt} \mathcal{P} \frac{d}{dt} = -\frac{d^2}{dt^2}. \quad (3.21)$$

From (3.19) and (3.20) it is clear how we can proceed in order to obtain approximate results for the propagator. If we only consider the set that includes the first N functions $u^{\nu}(t)$, we have an N th-order approximation to the propagator through

$$P(q, t | q_0, t_0)_N = e^{-S[q_r(t)]} \left(\prod_{\nu}^N \frac{\lambda_{free}^{\nu}}{\lambda^{\nu}} \right)^{1/2} \mathcal{K}(t_f | t_0)^{free}, \quad (3.22)$$

which is equivalent to the usual polygonal approximation to the path-integral (Feynman and Hibbs (1965); Schulman (1981); Langouche *et al.* (1982); Wio (1990); Khandekar and Lawande (1986); Khandekar *et al.* (2000)). This could be a good starting point for numerical procedures. However, what we want is to find more general results.

Before continuing with this calculation we now show a different result (initially using a quite simple example) related to the exploitation of space-time transformations, that will allow us to go a little further in this approach.

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Chapter 4

Space-Time Transformation I

4.1 Introduction

One aspect recently studied by several authors concerns the application of space-time transformation, within the realm of path integral schemes, in order to “map” a “difficult” (in principle unsolvable) problem into a “more simple” (solvable) one. One of the most outstanding examples is the possibility of solving the Coulomb problem, within a path integral framework, via the so called *Duru–Kleinert* transformations (Duru and Kleinert (1979, 1982); Ho and Inomata (1982); Duru (1983); Inomata (1983, 1984); Pak and Sokman (1984a,b); Kleinert (1989a,b, 1990a,b); Pelster and Kleinert (1997)). However, the use of these transformations within the realm of the path integral approach to stochastic processes is scarce or almost nonexistent (Deininghaus and Graham (1979)).

In this chapter we present a simple application of such a kind of transformation for the case of diffusion in a time-dependent harmonic potential. It is well known that a closed expression exists for the transition probability of such a system (Hänggi and Thomas (1975); van Kampen (2004)). Also, a very thorough study of the most general Gaussian path integral form can be found in Grosjean (1988). However, our aim is to show, through such a simple example, the possibility of exploiting these transformation techniques, within a path integral framework, in more complicated cases. We will follow the procedure presented in Felsager (1985) for the quantum case, translating it to the stochastic (i.e. *imaginary time*) case. In what follows we present the procedure to be used, and the way to get the *classical* (or *most probable*) trajectories necessary to write the general solution (that is reduced to quadratures). In so doing, we will follow the paper of Batista *et al.* (1996). We also discuss the application of the previous re-

sults to the problem of a *fluctuation theorem* within an out of equilibrium Onsager–Machlup approach (Deza *et al.* (2009)).

4.2 Simple Example

Our starting point is to consider the following Langevin equation

$$\dot{x}(t) = h(x, t) + \xi(t), \quad (4.1)$$

where $\xi(t)$, as usual, is an additive *white noise* (van Kampen (2004)). It is well known that in one dimension a multiplicative noise problem can be reduced to an additive one (van Kampen (2004); Gardiner (2009)). Equation (4.1) corresponds to describing the overdamped motion of a particle in a time-dependent potential. In the present case we assume that $h(x, t) = -a(t)x$. As indicated, in Chapter 3, the path integral representation of the transition probability associated with this Langevin equation is given by:

$$P(x_b, t_b \mid x_a, t_a) = \int_{x(t_a)=x_a}^{x(t_b)=x_b} \mathcal{D}[x(t)] e^{-\int_{t_a}^{t_b} L(x(\tau), \dot{x}(\tau), \tau) d\tau}. \quad (4.2)$$

Here the stochastic *Lagrangian* or *Onsager–Machlup* functional is given, in a midpoint ($\alpha = 1/2$) discretization (Langouche *et al.* (1982)), by

$$L(x, \dot{x}, t) = \frac{1}{2D} (\dot{x} - h(x, t))^2 + \frac{1}{2} \frac{dh(x, t)}{dx}. \quad (4.3)$$

Replacing the actual form of $h(x, t)$, the previous expression can be expanded to yield:

$$L(x, \dot{x}, t) = \frac{1}{2D} (\dot{x}^2 + a^2 x^2 + 2 a x \dot{x}) + \frac{1}{2} a = L_o + \frac{d\Phi(t)}{dt}, \quad (4.4)$$

$$\Phi(t) = -\frac{1}{2} \int_{t_a}^t a(t') dt' + \frac{a(t)}{2D} x^2, \quad (4.5)$$

$$L_o = \frac{1}{2D} (\dot{x}^2 + (a^2(t) - \dot{a}(t)) x^2). \quad (4.6)$$

At this point, as the Lagrangian of our problem is at most quadratic in x and $\dot{x}$, we can obtain the exact result through the use of the usual

procedure of expanding around a reference (*classical* or *most probable*) trajectory ($x(t) = x_{clas}(t) + q(t)$) and, apart from the problem of getting such a trajectory, our problem reduces to evaluating the following expression:

$$P(x_b, t_b | x_a, t_a) = e^{-[\Phi(t_b) - \Phi(t_a)]} e^{-S_o^{cl}(t_b, t_a)} \int_{q(t_a)=0}^{q(t_b)=0} \mathcal{D}[q(t)] e^{-\delta^2 S_o(t_b, t_a)}. \quad (4.7)$$

The effective action to be solved in order to perform the path integral indicated in (4.7) is then

$$\delta^2 S_o(t_b, t_a) = \frac{1}{2D} \int_{t_a}^{t_b} (\dot{q}^2 + (a^2 - \dot{a})q^2) dt. \quad (4.8)$$

After partial integration, we get

$$\delta^2 S_o(t_b, t_a) = -\frac{1}{2D} \int_{t_a}^{t_b} (q\ddot{q} - (a^2 - \dot{a})q^2) dt. \quad (4.9)$$

Hence, the path integral in (4.7) adopts the form

$$P(x_b, t_b | x_a, t_a) = e^{-[\Phi(t_b) - \Phi(t_a)]} e^{-S_o^{cl}(t_a, t_b)} \int_{q(t_a)=0}^{q(t_b)=0} \mathcal{D}[q(t)] \exp \left[\frac{1}{2D} \int_{t_a}^{t_b} dt q \left(\frac{d^2}{dt^2} - (a^2 - \dot{a}) \right) q \right]. \quad (4.10)$$

In order to evaluate this path integral we need to diagonalize the operator

$$\frac{d^2}{dt^2} - [a^2 - \dot{a}]. \quad (4.11)$$

However, there is an alternative way involving a change of variables that transforms the action in (4.8) into the one corresponding to the free diffusion problem. In following this approach we will make use of results in Chapter 5 of Felsager (1985). Let us call $f(t)$ the solution of the equation

$$\left\{ \frac{d^2}{dt^2} - w(t) \right\} f(t) = 0, \quad (4.12)$$

where $w(t) = a^2 - \dot{a}$, and with the condition $f(t_a) \neq 0$. It is easy to verify that

$$f(t) = A e^{\left\{ -\int_{t_a}^t a(s) ds \right\}}, \quad (4.13)$$

is a solution of (4.12) fulfilling the required condition. We will use now the function $f(t)$ to perform the change of variables $q(t) \Rightarrow y(t)$ according to

$$q(t) = f(t) \int_{t_a}^t \frac{\dot{y}(s)}{f(s)} ds, \quad (4.14)$$