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# Models of Theoretical Physics

PROF. *Amos Maritan, Marco Baiesi*

UNIVERSITY OF PADOVA

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WRITTEN BY: *Francesco Manzali*

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# Introduction

*Francesco Manzali, 20/02/2019*

## 1.1 Course information

The goal of this course is to introduce a series of problems in modern physics (in particular of statistical mechanics), describing their origin and their solution, along with some useful mathematical tools. At the end of the lectures, one student should be able to formulate problems and solve them. Exercises will be published online, and the final exam will consist of a theoretical question and a problem to solve (similar to the ones seen during the course). It will be needed to bring an *exercise book* with all the written solutions of the course's exercises.

(Lesson 1 of  
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## 1.2 Introduction

In classical mechanics, if we know all forces  $\mathbf{F}$  that act on a certain particle, along with its initial condition (e.g. position  $\mathbf{x}(t=0)$  and velocity  $\mathbf{v}(t=0)$ ), we can compute its trajectory  $\mathbf{x}(t) \forall t$  by integrating the equations of motion. This is indeed true even for ensembles of particles - but it becomes very impractical for macroscopic objects. For example, a drop of water contains something in the order of  $10^{23}$  molecules, and so to completely describe its motion it is needed to integrate six times that many equations (3 for position, 3 for velocity for each single particle). Even if we had the computational capacity to do so, it would not be possible to know the necessary initial conditions with the required precision.

On the other hand, it is not very interesting to solve this kind of problem, because one could not possibly understand the intricacy of this motion, and so the task doesn't give much insight in the relevant physics. In fact, often we are most interested in the *macroscopic* properties of the object. That is the aim of *statistical mechanics*.

## 1.3 The diffusion problem

We start by considering a famous problem in statistical mechanics, the *diffusion problem*, which consists in describing what happens to a droplet of fluid in a bath of a different substance (e.g. ink in water).

There are two main results about diffusion:

- Fick's Law ( $\sim 1895$ )
- Einstein's paper on Brownian motion (1905).

### 1.3.1 Brownian motion

The explanation of Brownian motion proposed by Einstein in 1905 was the first demonstration of the discrete nature of matter, i.e. the fact that substances are made of smaller discrete particles: molecules.

Einstein observed that a fine powder, not containing any *living organisms*, moved erratically if suspended in still water.

If we assume that water is composed of particles, the single grains of powder behave like large objects hit by smaller particles. The number of hits on each side is almost the same, so the total force which acts on the large object is almost 0. However, if the grains are sufficiently small, the slight unbalance in the number of collisions can produce a significant acceleration, leading to a kind of *random motion*.

For example, let's consider a spherical grain submerged in the liquid. Let's call  $U$  the upper hemisphere, and  $L$  the lower one. Denote with  $\bar{N}_c$  the average number of collisions per second per surface unit. Then the number of hits on  $U$  is *almost* the same to that of  $L$ , up to a certain (binomial) error:

$$\bar{N}_c \cdot U = \bar{N}_c \cdot L \pm \sqrt{\bar{N}_c}$$

Thus, the relative error is given by:

$$\frac{\sqrt{\bar{N}_c}}{\bar{N}_c} = \frac{1}{\sqrt{\bar{N}_c}}$$

Note that if the grains are small,  $\bar{N}_c$  will be small too, and so the relative error will be high.

### 1.3.2 Time evolution and the continuity equation

Let's try to give a quantitative description of this kind of motion. We start by specifying the *initial conditions* as a *starting distribution*, i.e. a function  $\rho: \mathbb{R}^3 \times \mathbb{R} \rightarrow R$  such that  $\rho(\mathbf{r}, t)$  is the probability to find a particle in position  $\mathbf{r}$  at the instant  $t$ .

*Starting  
distribution*

1. For a discrete, point particle we have  $\rho(\mathbf{r}, 0) = \delta^3(\mathbf{r} - \mathbf{r}_0)$ , i.e. the particle is at the starting position with certainty.
2. For some quantity of matter (for example a droplet of ink), we have some uniform initial density, such as:

$$\rho(\mathbf{r}, 0) = \rho_0(\mathbf{r}) = \begin{cases} \bar{\rho}_0 & |\mathbf{r}| < R \\ 0 & \text{otherwise} \end{cases}$$

Note that  $\rho(\mathbf{r}, t)$  is a probability density, and not a usual density of matter. The difference is merely of normalization. If  $N$  is the total number of particles in ink, then  $N\rho(\mathbf{r}, t)$  is the density of ink particles at *the specific* position  $\mathbf{r}$  and time  $t$ , which will be denoted with  $\rho_n(\mathbf{r}, t)$ :

$$1 = \int_V d^3r \rho(\mathbf{r}, t)$$

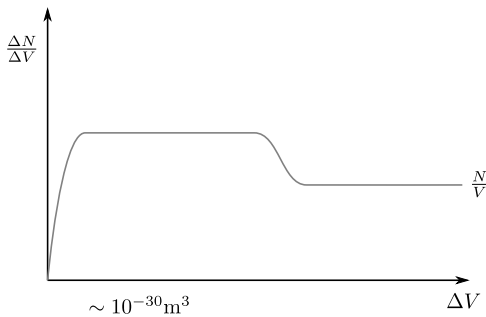
$$N = \int_V d^3r \underbrace{N\rho(\mathbf{r}, t)}_{\text{density at } \mathbf{r}}$$

The meaning of a point-wise density can be understood as a limit:

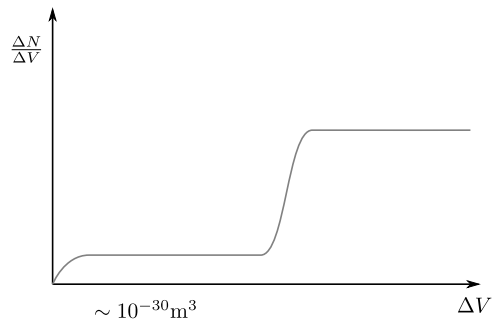
*Point-wise  
density*

$$N\rho(\mathbf{r}, t) = \text{density at } \mathbf{r}, \text{ time } t = \lim_{\Delta V \downarrow 0} \frac{\Delta N}{\Delta V}$$

Consider a patch of liquid of volume  $\Delta V$ , that contains a number  $\Delta N$  of ink particles. By letting it shrink “enough”,  $\Delta N/\Delta V$  reaches a constant value - that is the density in a macroscopically small patch of liquid. Of course,  $\Delta V$  cannot reach 0, because in that case  $\Delta N = 0$ . So, the limit is to be interpreted in a macroscopical sense ( $\Delta V$  is macroscopically vanishing,  $\Delta V \downarrow 0$ ) and not in a mathematical sense ( $\Delta V \rightarrow 0$ ).



**Figure (1.1)** – Density (ratio  $\Delta N/\Delta V$ ) as function of patch size  $\Delta V$  for a region centered around the ink distribution  $\rho_0$  ( $|\mathbf{r}| < R$  at  $t = 0$ ). If  $\Delta V$  is sufficiently large, the patch comprises also some space without ink, and so the density is lower.



**Figure (1.2)** – Density for a patch centered on a point  $|\mathbf{r}| > R$ . Here the density is higher for high  $\Delta V$ , as in these cases the patch comprises also the ink’s initial distribution ( $\rho_0$ ).

We now want to compute  $\rho(\mathbf{r}, t)$  for  $t > 0$ , given  $\rho(\mathbf{r}, 0)$ .

We start by considering the *continuity equation*. The idea is that particles do

*Continuity  
equation*

not move by “jumping” between far positions, but travel in a *continuous way*.

Consider a box of volume  $V$ , that contains a fixed number  $N$  of particles, with density:

$$N\rho(\mathbf{r}, t) \equiv \rho_n(\mathbf{r}, t)$$

Let  $A$  be a patch of  $V$ , with boundary  $\partial A$ . The number of particles inside  $A$  at time  $t$  is given by:

$$\int_A d^3r \rho_n(\mathbf{r}, t) = N_A(t) \quad (1.1)$$

And at a later time  $t + \Delta t$ :

$$\int_A d^3r \rho_n(\mathbf{r}, t + \Delta t) = N_A(t + \Delta t) \quad (1.2)$$

Let's introduce a new quantity, the *current*  $\mathbf{j}(\mathbf{r}, t)$  at position  $\mathbf{r}$  and time  $t$ . Consider a small area  $dS$  centered on  $\mathbf{r}$ , with  $\hat{n}(\mathbf{r}) \perp dS$ . The number of particles flowing through  $dS$  during an interval  $\Delta t$  is defined as:

$$\Delta t \mathbf{j}(\mathbf{r}, t) \cdot \hat{n}(\mathbf{r}) dS$$

and this can be used to compute  $\mathbf{j}$ .

For example, for a uniform flow of particles with density  $\rho_n$  and velocity  $\mathbf{v}$ , the *current* is  $\mathbf{j} = \rho_n \mathbf{v}$ .

Returning to the problem, we note that the *change* of  $N_A$  over time is explained by the **flux** of particles through the closed boundary  $\partial A$ , i.e. the surface integral of the current  $\mathbf{j}$ :

$$N_A(t + \Delta t) - N_A(t) = - \int_{\partial A} dS \hat{n} \cdot \mathbf{j}(\mathbf{r}, t) \Delta t \quad (1.3)$$

Here we define, by convention, the sign of  $\mathbf{j}(\mathbf{r}, t)$  to be positive if the current is *outward*, that is from  $A$  to  $V \setminus A$ . So, a positive current means that particles are *leaving*  $A$ , and this explains the  $-$  in (1.3).

Substituting (1.1) and (1.2) in (1.3) we arrive at:

$$\int_A d^3r \frac{1}{\Delta t} [\rho_n(\mathbf{r}, t + \Delta t) - \rho_n(\mathbf{r}, t)] = - \int_{\partial A} dS (\mathbf{r}) \mathbf{j}(\mathbf{r}, t) \cdot \hat{n}(\mathbf{r}) \Delta t$$

Taking the limit  $\Delta t \rightarrow 0$ :

$$\int_A d^3r \frac{\partial}{\partial t} \rho_n(\mathbf{r}, t) = - \int_{\partial A} dS \hat{n} \cdot \mathbf{j}(\mathbf{r}, t) \stackrel{(a)}{=} - \int_A d^3r \nabla \cdot \mathbf{j}(\mathbf{r}, t)$$

where in (a) we applied the Gauss divergence theorem.

Rearranging:

$$\int_A d^3r [\dot{\rho}_n(\mathbf{r}, t) + \nabla \cdot \mathbf{j}(\mathbf{r}, t)] = 0$$



This is the **continuity equation** in integral form. Note that it holds for any choice of volume  $A \subseteq \mathbb{R}^3$ . So, knowing that  $\mathbf{j}$  and  $\dot{\rho}$  are continuous functions, by the fundamental theorem of calculus we know that the same relation must hold everywhere *for the integrand*, meaning that:

$$\dot{\rho}_n(\mathbf{r}, t) + \nabla \cdot \mathbf{j}(\mathbf{r}, t) = 0 \quad \forall \mathbf{r}, \forall t \quad (1.4)$$

That is the **continuity equation** in differential form.

### 1.3.3 Fick's Law

If there are no other fields (EM, gravity, etc.), but we still observe a non-zero  $\mathbf{j}$ , where could it possibly be from?

The only other relevant physical vector in this situation, i.e. not depending on an arbitrary choice of reference frame, is the “spatial” rate of change of density, i.e. its gradient  $\nabla \rho_n$ . In fact, it is observed that particles tend to move *opposite* to that gradient - from regions where there are more particles to regions where there are less. This can be summarized by **Fick's Law**:

$$\mathbf{j}(\mathbf{r}, t) = -D \nabla \rho_n(\mathbf{r}, t) \quad (1.5)$$

Of course, there could be some other terms in this expression:

$$\mathbf{j}(\mathbf{r}, t) = -D \nabla \rho_n(\mathbf{r}, t) + C \nabla (\nabla \rho_n) + \dots$$

However, by dimensional analysis,  $\partial_x^k \rho_n \sim \rho_n / L^k$ , where  $L$  is the macroscopic dimension of the container. So, the higher order terms can be considered negligible.

### 1.3.4 The Diffusion Equation

Substituting (1.5) in (1.4) we arrive finally at the **diffusion equation**:

$$\dot{\rho}_n(\mathbf{r}, t) = \nabla \cdot (D \cdot \nabla \rho_n(\mathbf{r}, t)) \quad (1.6)$$

Knowing the initial density  $\rho_n(\mathbf{r}, 0)$  and some macroscopical details for the fluids (all contained in the *diffusion parameter*  $D$ ), we can now compute the density after a small interval  $\Delta t$ . For example, we can start by expanding  $\rho_n(\mathbf{r}, \Delta t)$  around  $\Delta t = 0$ :

$$\rho_n(\mathbf{r}, \Delta t) = \rho_n(\mathbf{r}, 0) + \Delta t \dot{\rho}_n(\mathbf{r}, 0) + O(\Delta t^2)$$

Ignoring the higher order terms, we can use (1.6) and compute  $\rho_n(\mathbf{r}, \Delta t)$ .

This may be more or less doable depending on the form of  $D$ , that can depend on both  $\mathbf{r}$  and  $t$ . The  $\mathbf{r}$ -dependence is characteristic of problems that are not translational invariant (e.g. a crystal). In fact, if  $D$  **does not** depend on  $\mathbf{r}$ , the diffusion equation becomes:

$$\dot{\rho}_n(\mathbf{r}, t) = D \nabla^2 \rho_n(\mathbf{r}, t) \quad (1.7)$$

Because the only spatial derivatives are of second order, then if  $\rho(\mathbf{r}, t)$  is a solution, also  $\rho(\mathbf{r} + \mathbf{R}, t)$  is a solution, for any choice of  $\mathbf{R}$ .

Note that (1.7) is quite similar to the Schrödinger equation for a free particle:

$$-i \partial_t \psi = + \frac{\hbar}{2m} \nabla^2 \psi$$

The yellow term is analogous to  $D$ , and the only difference is given by the green term. This can be resolved by a substitution  $\tau = it$  (passing to “imaginary time”).

**Example 1** (Particle diffusing in  $d = 1$ ):

Consider the simplest case of a single particle moving in one dimension, with  $D$  constant. Let  $\rho(x, 0) = \delta(x)$ .

The diffusion equation in  $d = 1$  is:

$$\dot{\rho}(x, t) = D \rho''(x, t) \quad (1.8)$$

The macroscopic quantities of interest are the expected position and velocity, defined as:

$$\langle x \rangle_t = \int_{-\infty}^{+\infty} \rho(x, t) x \, dx \quad \frac{d\langle x \rangle_t}{dt} = \int_{-\infty}^{+\infty} \dot{\rho}(x, t) x \, dx$$

From the normalization condition:

$$\int_{-\infty}^{+\infty} \rho(x, t) dx = 1$$

we note that  $\rho(\pm\infty, t) = 0$ , and also  $\rho'(x, t) \rightarrow 0$  for  $|x| \rightarrow \infty$  (otherwise, the density would diverge).

These limits allow us to compute the velocity by repeated integration by parts:

$$\begin{aligned} \frac{d\langle x \rangle_t}{dt} &= \frac{d}{dt} \int_{-\infty}^{+\infty} \rho(x, t) x \, dx = \int_{-\infty}^{+\infty} \dot{\rho}(x, t) x \, dx \stackrel{(1.8)}{=} D \int_{-\infty}^{+\infty} \rho''(x, t) x \, dx = \\ &= \underbrace{x \rho'(x, t) \Big|_{x=-\infty}^{x=+\infty}}_{=0} - \underbrace{\left( \frac{dx}{dx} \right) \rho(x, t) \Big|_{x=-\infty}^{x=+\infty}}_{=0} + D \int_{-\infty}^{+\infty} \rho(x, t) \underbrace{\left( \frac{d^2 x}{dx^2} \right)}_{=0} dx = 0 \end{aligned}$$

A similar calculation can be done for the expected value of the time derivative of a generic function  $f(x)$ :

$$\frac{d}{dt} \langle f(x) \rangle = D \int_{-\infty}^{\infty} \rho(x, t) \left( \frac{d^2 f(x)}{dx^2} \right) dx \quad (1.9)$$

As the velocity is 0, the position is constant, so that:

$$\langle x \rangle_t = \langle x \rangle_{t=0} = \int_{-\infty}^{+\infty} dx x \rho(x, 0) = 0$$

However, if we consider  $f(x) = x^2$ , thanks to (1.9) we arrive at:

$$\frac{d}{dt}\langle x^2 \rangle_t = \int_{-\infty}^{+\infty} \dot{\rho}(x, t) x^2 dx = D \int_{-\infty}^{+\infty} 2\rho(x, t) dx$$

As  $\rho(x, 0) = \delta(x)$ , we have:

$$\frac{d}{dt}\langle x^2 \rangle_0 = D \int_{-\infty}^{+\infty} 2\delta(x) dx = 2D$$

And integrating with respect to  $t$ :

$$\langle x^2 \rangle_t = 2Dt + \langle x^2 \rangle_0 = 2Dt$$

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## 1.4 Brownian motion and Markov Processes

Let's tackle the diffusion problem with a different approach.

Consider a particle moving in  $d = 1$ . We start by discretizing time and space intervals, so that we only focus on positions  $x_i$  at instants  $t_n$ :

$$x_i \equiv i \cdot l \quad t_n \equiv n \cdot \varepsilon \quad (1.10)$$

The diffusion process is intrinsically stochastic, meaning that the motion of grains is given by collisions at the microscopical level, which are essentially random.

So, suppose that the particle lies in a certain known position at  $t = 0$ . After an instant, the particle may have moved to the right (with probability  $P_+$ ) or to the left ( $P_-$ ), or have remained in the same position as before ( $P_0$ ). As these cases cover all the possibilities, it holds:

$$P_+ + P_- + P_0 = 1$$

Denote with  $w_i(t_n)$  the probability that the particle lies at position  $x_i$  at time  $t_n$ .

The probability for the next timestep is then given by the **Master Equation** :

$$w_i(t_{n+1}) = P_0 w_i(t_n) + P_+ w_{i-1}(t_n) + P_- w_{i+1}(t_n) \quad (1.11)$$

In fact, if the particle were at position  $i$  at time  $t_n$ , then it will remain in the same position with probability  $P_0$ . Otherwise, it could have been one position left and moved to the right ( $P_+$ ), or one position right and moved to the left ( $P_-$ ).

Here we supposed that  $\varepsilon$  is sufficiently small, so that the particle will only take one step at a time.

Stochastic systems for which the state at a certain time depends only on the state one instant before are called **Markov's Processes** .

Note that, as the particle cannot “escape from the system”, its probability to be in *any* position is conserved at any given time:

$$\sum_{i=-\infty}^{\infty} w_i(t_{n+1}) = \sum_{i=-\infty}^{\infty} w_i(t_n) = \cdots = \sum_{i=-\infty}^{\infty} w_i(0)$$

Suppose that the particle “always moves”, that is  $P_0 = 0$ , and also that it “is balanced” ( $P_+ = P_- = 0.5$ ). The final position  $i$  at time  $t_n$  is given by the number of steps to the right  $n_+$  minus the number of steps to the left  $n_- \in \mathbb{N}$ :

$$\mathbb{Z} \ni i = n_+ - n_-$$

This process can be simulated by flipping a coin at each timestep: if it lands on heads the particle will move to the right, otherwise to the left. So, denoting the total number of steps as  $n = n_+ + n_-$ , then the probability for the particle to be in position  $x_i$  is given by a binomial distribution:

$$w_i(t_n) = \binom{n}{n_+} \frac{1}{2^{n_+}} \frac{1}{2^{n_-}} = \frac{1}{2^n} \binom{n}{n_+} = \binom{n}{n_-} \frac{1}{2^n} \quad (1.12)$$

This can be generalized to the case where  $P_+ \neq P_-$ :

$$w_i(t_n) = \binom{n}{n_-} P_+^{n_+} P_-^{n_-} \quad (1.13)$$

Note that (1.12) satisfies the Master Equation (1.11), that is:

$$w_i(t_{n+1}) = \frac{1}{2}(w_{i+1}(t_n) + w_{i-1}(t_n))$$

We start by noting that if  $i = n_+ - n_-$  and  $n = n_+ + n_-$ , then:

$$n_+ = \frac{n+i}{2} \quad n_- = \frac{n-i}{2}$$

And so:

$$\frac{1}{2}(w_{i+1}(t_n) + w_{i-1}(t_n)) = \frac{1}{2^{n+1}} \left[ \binom{n}{\frac{n+i+1}{2}} + \binom{n}{\frac{n+i-1}{2}} \right] \quad (1.14)$$

Recall now the recurrence relation for the binomial coefficient:

$$\binom{n}{k} = \binom{n-1}{k} + \binom{n-1}{k-1}$$

which leads to the desired result:

$$(1.14) = \frac{1}{2^{n+1}} \binom{n+1}{\frac{n+i+1}{2}} = w_i(t_{n+1})$$

## 1.5 Probability Generating Functions

Let's introduce a useful mathematical tool to deal with the binomial coefficient. Let  $X$  be a discrete random variables taking values in the non-negative integers ( $\mathbb{N}$ ). The **probability generating function** of  $X$  is defined as:

$$G(z) \equiv \mathbb{E}[z^X] = \sum_{x=0}^{+\infty} p(x)z^x$$

where  $p$  is the *probability mass function* of  $X$ , i.e.  $p(x)$  is the probability that  $X = x$  ( $p(x) = \mathbb{P}(X = x)$ ).

$G(z)$  is useful because we can retrieve  $p(k)$  for any  $k \in \mathbb{N}$  by simply differentiating  $k$  times with respect to  $z$  and setting  $z = 0$ :

$$G(z) = p(0) + p(1)z + p(2)z^2 + \dots \Rightarrow \frac{d^k}{dz^k} G(z) \Big|_{z=0} = p(k)$$

Note that  $G(1) = 1$  because of the normalization:

$$G(1) = \sum_{x=0}^{+\infty} p(x)1^x = \sum_{x=0}^{+\infty} p(x) = 1$$

Then, if we evaluate the first derivative for  $z = 1$  we get:

$$G'(1) = p(1) + 2p(2)z + 3p(3)z^2 + \dots \Big|_{z=1} = \sum_{x=1}^{+\infty} p(x)xz^{x-1} \Big|_{z=1} = \quad (1.15)$$

$$= \sum_{x=1}^{+\infty} xp(x) = (0 \cdot p(0)) + 1 \cdot p(1) + 2 \cdot p(2) + \dots = \mathbb{E}[X] \quad (1.16)$$

However, the second derivative of  $G$  evaluated at  $z = 1$  does not give the second moment:

$$\begin{aligned} G''(1) &= 2 \cdot 1p(2) + 3 \cdot 2p(3)z + 4 \cdot 3p(4)z^2 + \dots \Big|_{z=1} = \sum_{x=2}^{+\infty} x(x-1)z^{x-2}p(x) \Big|_{z=1} = \\ &= \mathbb{E}(X(X-1)) \end{aligned}$$

More generally:

$$G^{(k)}(1) = \mathbb{E}(X(X-1)\dots(X-k+1)) = \mathbb{E}\left(\frac{X!}{(X-k)!}\right)$$

which is called the  $k$ -th factorial moment of  $X$ .

But how can we get the “usual” moments from  $G$ ? One possibility is to “compensate” the difference between a factorial moment and a usual one by adding other terms. For example, note that:

$$G''(1) = \mathbb{E}(X(X-1)) = \mathbb{E}(X^2) - \mathbb{E}(X)$$

and so:

$$G''(1) + G'(1) = (\mathbb{E}(X^2) - \mathbb{E}(X)) + \mathbb{E}(X) = \mathbb{E}(X^2)$$

A more clever way is to consider the operator  $\theta(z)$  defined as:

$$\theta(z) \equiv z \frac{\partial}{\partial z}$$

on  $G$ . In fact:

$$\theta(z)G(z) = z \frac{\partial}{\partial z} \sum_{x=0}^{+\infty} p(x)z^x = z \sum_{x=1}^{+\infty} xp(x)z^{x-1} = \sum_{x=1}^{+\infty} xp(x)z^x$$

And setting  $z = 1$  leads back to the  $\mathbb{E}[X]$ . If we apply  $\theta(z)$  again, however, something interesting happens:

$$\theta(z)^2 G(z) = \left( z \frac{\partial}{\partial z} \right) \left( z \frac{\partial}{\partial z} \right) G(z) = z \frac{\partial}{\partial z} \sum_{x=1}^{+\infty} xp(x)z^x = \sum_{x=1}^{+\infty} x^2 p(x)z^x \quad (1.17)$$

Now setting  $z = 1$  leads to  $\mathbb{E}[X^2]$ . In general:

$$\theta(z)^k G(z) \Big|_{z=1} = \mathbb{E}[X^k]$$

Note how the exponent of  $z$  never changes, as it is lowered by 1 by the  $\partial_z$ , and then risen back by the  $z$  factor. So, every new application of the  $\theta(z)$  operator merely brings down another  $x$  factor, rising the  $x$  exponent inside the sum - which is exactly what we want to compute moments.

## 1.6 The Diffused Distribution

Let's focus on our specific (discrete) case, with the particle moving on a discretized line. At any given time  $t_n$  we can compute the mass probability function  $W_{t_n} : \mathbb{Z} \rightarrow \mathbb{R}_+$ , with  $W_{t_n}(x_i) \equiv w_i(t_n)$ . In other words, this is the function that maps every position  $x_i$  with the probability of containing a particle at time  $t_n$ .

We are interested in knowing the *shape* of  $W_{t_n}$ , that is its moments:

$$\langle x^q \rangle_{t_n} = \sum_{i=-\infty}^{+\infty} W_{t_n}(x_i) x_i^q \stackrel{(1.10)}{=} \sum_{i=-\infty}^{+\infty} w_i(t_n) (l \cdot i)^q \quad q \in \mathbb{N}$$

The first moment ( $q = 1$ ) gives the average position:

$$\begin{aligned} \langle x \rangle_{t_n} &= l \cdot \sum_{i=-\infty}^{+\infty} w_i(t_n) i = \\ &= l \sum_{i=-\infty}^{+\infty} w_i(t_n) (2n_+ - n) = \\ &\stackrel{(a)}{=} l (2 \langle n_+ \rangle_{t_n} - n) \end{aligned} \quad (1.18)$$

where in (a) we used the normalization condition ( $\forall n \in \mathbb{N}, \sum_i w_i(t_n) = 1$ ). Thus, we found that the average position  $\langle x \rangle$  of the particle at time  $t_n$  is related to the value of  $n_+$ .

So, let  $n_+$  be the random variable of interest. Recall that  $n_+$  is sampled from a binomial distribution (1.13), and that  $n_+ = (n+1)/2$  and so  $i = 2n_+ - n$ . Then, the *probability generating function* of  $n_+$  is given by:

$$\begin{aligned}\widetilde{W}(z, n) &\equiv \sum_{n_+=0}^n z^{n_+} w_i(t_n) \Big|_{i=2n_+-n} \stackrel{(1.13)}{=} \sum_{n_+=0}^n z^{n_+} \binom{n}{n_+} P_+^{n_+} P_-^{n-n_+} = \\ &\stackrel{(a)}{=} (P_+ z + P_-)^n\end{aligned}$$

where in (a) we used the binomial theorem.

We can now use the property (1.16) of the probability generating function to compute  $\langle n_+ \rangle$ :

$$\langle n_+ \rangle = \frac{\partial}{\partial z} \widetilde{W}(z, n) \Big|_{z=1} = n(P_+ z + P_-)^{n-1} P_+ \Big|_{z=1} = n \underbrace{(P_+ + P_-)}_{=1} P_+ = nP_+ \quad (1.19)$$

For computing the second moment, we apply the  $\theta(z)$  operator, as seen in (1.17):

$$\begin{aligned}\langle n_+^2 \rangle &= \left( z \frac{\partial}{\partial z} \right)^2 \widetilde{W}(z, n) \Big|_{z=1} = z \frac{\partial}{\partial z} z n (P_+ z + P_-)^{n-1} P_+ \Big|_{z=1} = \\ &= z (n(P_+ z + P_-)^{n-1} P_+ + z n P_+^2 (n-1) (P_+ z + P_-)^{n-2}) \Big|_{z=1} = \\ &= nP_+ (1 + (n-1)P_+) \quad (1.20)\end{aligned}$$

We can now compute  $\text{Var}(n_+)$  recalling that:

$$\text{Var}[X] = \mathbb{E}[X^2] - (E[X])^2$$

Thus:

$$\text{Var}[n_+] = \langle n_+^2 \rangle - \langle n_+ \rangle^2 = nP_+ (1 + P_+) \quad (1.21)$$

We now go back to  $\langle x \rangle_{t_n}$ , recalling the relation (1.18):

$$\langle x \rangle_{t_n} = l(2\langle n_+ \rangle_{t_n} - n) \stackrel{(1.19)}{=} nl(2P_+ - 1) \stackrel{(a)}{=} nl(P_+ - P_-)$$

where in (a) we used  $P_+ + P_- = 1$ .

For the variance, recall that:

$$\text{Var}[aX + b] = a^2 \text{Var}[X]$$

and so, starting again from (1.18):

$$\text{Var}[x]_{t_n} = 4l^2 \text{Var}[n_+] \stackrel{(1.21)}{=} 4nl^2 P_+ (1 - P_+) = 4nl^2 P_+ P_-$$

Note that the variance is always proportional to time ( $n$ ), even if  $P_+ \neq P_-$ . However, if we go back and compute the  $\langle x^2 \rangle_{t_n}$ , we will note that it is not linear in time:

$$\begin{aligned}\langle x^2 \rangle_{t_n} &= \text{Var}[x]_{t_n} + \langle x \rangle_{t_n}^2 = 4nl^2 P_+ (1 - P_+) + (nl(P_+ - P_-))^2 = \\ &= nl^2 (4P_+ P_- + n(P_+ - P_-)^2)\end{aligned}$$

Let's evaluate the previous quantities for the simple symmetrical case, where  $P_+ = P_- = 1/2$ :

$$\begin{aligned}\langle n_+ \rangle &= \frac{n}{2}; & \langle n_+^2 \rangle &= \frac{n}{4}(n+1); & \text{Var}[n_+] &= \frac{3}{4}n \\ \langle x \rangle_{t_n} &= 0; & \langle x^2 \rangle_{t_n} &= nl^2 & \text{Var}(x)_{t_n} &= nl^2\end{aligned}$$

As expected, the average number of steps to the right is half the total steps (as  $P_+ = 1/2$ ), and the average position is 0.

## 1.7 Continuum Limit

Recall that  $t_n = n\varepsilon$ , and so, for the symmetrical case ( $P_+ = P_-$ ):

$$\langle x \rangle_{t_n} = 0; \quad \langle x^2 \rangle_{t_n} = l^2 n = \frac{l^2}{\varepsilon} t_n \quad (1.22)$$

The analysis of the diffusion equation in  $d = 1$  showed that, for a particle starting at  $x(t=0) = 0$ :

$$\langle x^2 \rangle_t = 2Dt \quad (1.23)$$

The correct *continuum limit* should reproduce the result of (1.23) from (1.22). Notice that if we simply let  $\varepsilon \rightarrow 0$  and  $l \rightarrow 0$ ,  $\langle x^2 \rangle$  becomes undefined. Therefore, we need to fix the ratio  $l^2 \varepsilon^{-1}$  during the limit. If we define this ratio as:

$$\frac{l^2}{\varepsilon} \equiv 2D$$

then the limit of (1.22) leads to (1.23) as desired:

$$\langle x^2 \rangle_{t_n} = \frac{l^2}{\varepsilon} t_n \xrightarrow[l, \varepsilon \rightarrow 0]{l^2/\varepsilon = 2D} 2Dt = \langle x^2 \rangle_t$$

Note that  $[D] = \text{m}^2 \text{s}^{-1}$ , and so the previous expression is dimensionally correct.

This same result, however, can be also obtained in a more simple way.

The idea is to represent the final state of the random walk at time  $t_n$  as the sum of  $n$  steps:

$$x(t_n) = u_1 + u_2 + \cdots + u_n$$

Each step can be on the right or on the left according to some probability distribution. In other words,  $u_i$  is a random variable. If we suppose steps of *unit length* symmetrically distributed (i.e.  $P_+ = P_- = 1/2$ ) we get:

$$u_n = \begin{cases} +1 & p = 1/2 \\ -1 & p = 1/2 \end{cases}$$



Now it is easy to compute the average position:

$$\begin{aligned}\langle x(t_n) \rangle &= n \langle u \rangle = 0 \\ \langle u \rangle &= \frac{1}{2}(+1) + \frac{1}{2}(-1) = 0\end{aligned}$$

And the average of the square:

$$\begin{aligned}\langle x^2(t_n) \rangle &= \langle (u_1 + \dots + u_n)^2 \rangle = n \cdot \underbrace{\langle u^2 \rangle}_1 + \sum_{i \neq j} \underbrace{\langle u_i \cdot u_j \rangle}_{\langle u_i \rangle \langle u_j \rangle = 0} = n \\ \langle u^2 \rangle &= \frac{1}{2}(+1)^2 + \frac{1}{2}(-1)^2 = 1\end{aligned}$$

Note that  $\langle u_i \cdot u_j \rangle = \langle u_i \rangle \langle u_j \rangle$  because  $u_i$  and  $u_j$  are statistically independent. So we showed that  $\langle x^2 \rangle_{t_n}$  is linear in the number of time steps ( $n$ ). Here, the  $l^2$  factor from (1.22) is missing because the spatial step size is set to 1.

Another interesting observation comes from the relation:

$$i = 2n_+ - n$$

Note how  $i$  and  $n$  must have the same parity, as  $2n_+$  is always even. So the particle will be at an even position ( $x_i$  with  $i$  even) after an even number  $n$  of time steps, and at an odd  $x_i$  after an odd time  $t_n$ .

## 1.8 Evolution for large times

We can plot  $w_i(t_n)$  for a fixed  $t_n$  as a function of position ( $i$ ):

$$w_i(t_n) = \frac{n!}{\left(\frac{n+i}{2}\right)! \left(\frac{n-i}{2}\right)!} \frac{1}{2^n} \quad (1.24)$$

For  $n = 0$  (starting time), all the particles are at  $x_0$ . Then, after each timestep the probability distribution “expands”, meaning that more and more positions have a non-zero probability of being explored.

We now want to examine what happens after a *long period of time*, that is the asymptotic behaviour at  $n \rightarrow \infty$ .

We start by computing the logarithm of (1.24):

$$\ln w_i(t_n) = -n \ln 2 + \ln n! - \ln \left( \frac{n+i}{2} \right)! - \ln \left( \frac{n-i}{2} \right)!$$

In this way, we can use the Stirling approximation:

$$\begin{aligned}\ln k! &= \ln k + \ln(k-1) + \dots + \ln 2 + \ln 1 = \\ &\approx k \ln k - k + \frac{1}{2} \ln(2\pi k)\end{aligned}$$

Thus arriving at a complicated expression:

$$\begin{aligned} \ln w_i(t_n) \underset{n \gg 1}{\approx} & -n \ln 2 + n \ln n - \cancel{x} + \frac{1}{2} \ln(2\pi n) \\ & - \frac{n+i}{2} \ln \left( \frac{n+i}{2} \right) + \cancel{\frac{n+i}{2}} - \frac{1}{2} \ln \left( 2\pi \frac{n+i}{2} \right) \\ & - \frac{n-i}{2} \ln \left( \frac{n-i}{2} \right) + \cancel{\frac{n-i}{2}} - \frac{1}{2} \ln \left( 2\pi \frac{n-i}{2} \right) \end{aligned}$$

Let's gradually simplify it. We start by collecting all the  $n$ :

$$\begin{aligned} & n \left( -\ln 2 + \ln n - \frac{1}{2} \ln \left( \frac{n+i}{2} \right) - \frac{1}{2} \ln \left( \frac{n-i}{2} \right) \right) = \\ & = n \ln \left( \frac{n}{2\sqrt{\frac{n+i}{2}}\sqrt{\frac{n-i}{2}}} \right) = n \ln \left( \frac{n}{\sqrt{n^2 - i^2}} \right) = n \ln \left( \frac{1}{\sqrt{1 - i^2/n^2}} \right) = \\ & \underset{(a)}{=} n \ln \left( 1 + \frac{1}{2} \frac{i^2}{n^2} + O \left( \frac{i^3}{n^3} \right) \right) \underset{(b)}{=} \frac{n}{2} \frac{i^2}{n^2} + O \left( \frac{i^3}{n^3} \right) \approx \frac{i^2}{2n} \end{aligned} \quad (1.25)$$

where in (a) and in (b) we used respectively the following Taylor expansions (as  $n \rightarrow \infty$  and so  $1/n \rightarrow 0$ ):

$$(1 \pm x)^n = 1 \pm nx + O(x^2) \quad \ln(1+x) = x + O(x^2) \quad (1.26)$$

Then we collect the  $i/2$ :

$$\begin{aligned} & -\frac{i}{2} \left[ \ln \left( \frac{n+i}{2} \right) - \ln \left( \frac{n-i}{2} \right) \right] = -\frac{i}{2} \ln \left( \frac{n+i}{n-i} \right) = \\ & = -\frac{i}{2} \ln \left( \frac{1+i/n}{1-i/n} \right) \underset{(a)}{=} -\frac{i}{2} \ln \left( \left( 1 + \frac{i}{n} \right) \left( 1 + \frac{i}{n} + O \left( \frac{i^2}{n^2} \right) \right) \right) = \\ & = -\frac{i}{2} \ln \left( 1 + \frac{2i}{n} + O \left( \frac{i^2}{n^2} \right) \right) \underset{(b)}{=} -\frac{i}{2} \left( \frac{2i}{n} + O \left( \frac{i^2}{n^2} \right) \right) \approx -\frac{i^2}{n} \end{aligned} \quad (1.27)$$

And finally we consider the remaining terms:

$$\begin{aligned} & \frac{1}{2} \left[ \ln(2\pi n) - \frac{1}{2} \ln \left( 2\pi \frac{n+i}{2} \right) - \ln \left( 2\pi \frac{n-i}{2} \right) \right] = \\ & = \frac{1}{2} \ln \left( \frac{2\pi n}{2\pi \frac{n+i}{2} 2\pi \frac{n-i}{2}} \right) = \frac{1}{2} \ln \left( \frac{2n}{\pi(n^2 - i^2)} \right) = \frac{1}{2} \ln \left( \frac{2}{\pi n} \frac{1}{1 - \frac{i^2}{n^2}} \right) = \\ & = \frac{1}{2} \ln \left( \frac{2}{\pi n} + O \left( \frac{i^2}{n^2} \right) \right) \approx \frac{1}{2} \ln \left( \frac{2}{\pi n} \right) \end{aligned} \quad (1.28)$$

Putting it all back together:

$$\ln w_i(t_n) \underset{n \gg 1}{\approx} (1.25) + (1.27) + (1.28) = \frac{1}{2} \ln \left( \frac{2}{\pi n} \right) - \frac{i^2}{2n}$$

And by exponentiating we get:

$$w_i(t_n) \underset{n \gg 1}{\approx} \sqrt{\frac{2}{\pi n}} \exp \left( -\frac{i^2}{2n} \right) \quad (1.29)$$

We now want to obtain a *continuous* pdf from the mass probability  $w_i(t_n)$ . Note that if we regard  $w_i(t_n)$  as a function of position at a fixed time  $W_{t_n}(x_i)$ , and extend the domain to all  $\mathbb{R}$  we get a really “bumpy” function, as it is non-zero only on  $x_i = li$  with  $i \in \mathbb{Z}$ . However, if we *integrate* over every *small patch* of  $W_{t_n}(x_i)$ , we can “smooth” all the “bumpyness”, and get a nice pdf. Let’s formalize that more carefully. Starting from  $W_{t_n}(x_i)$ , we can compute the probability to find a particle in an interval  $I \subseteq \mathbb{R}$  by simply summing the mass probabilities  $w_j(t_n)$  for all the  $x_j \in I$ .

The idea is now to define a *continuous* pdf  $W(x, t)$  as follows:

$$W(x, t_n)\Delta x = \mathbb{P}\left(x \in \left[x - \frac{\Delta x}{2}; x + \frac{\Delta x}{2}\right], t_n\right) \quad \Delta x \ll 1, \Delta x \gg l$$

That is,  $W(x, t_n)\Delta x$  is the probability that a particle lies “near” a certain position  $x \in \mathbb{R}$  at an instant  $t_n$  (i.e. within an interval  $I$  centered on  $x$  with width  $\Delta x$  sufficiently small, but large with respect to the discretization). We will then “cure” the discreteness of time by considering the asymptotic behaviour for  $t \rightarrow \infty$ .

By expanding the previous expression we get:

$$\mathbb{P}\left(x \in \left[x - \frac{\Delta x}{2}, x + \frac{\Delta x}{2}\right]\right) \underset{(a)}{\approx} \mathbb{P}\left(i \in \left[i_0 - \frac{\Delta x}{2l}; i_0 + \frac{\Delta x}{2l}\right]\right) = \sum_{j=i_0-\Delta x/(2l)}^{i_0+\Delta x/(2l)} w_j(t_n) \quad (1.30)$$

where in (a)  $i_0$  is such that  $x_{i_0}$  is closest to  $x$ , that is  $i_0 = \lfloor x/l \rfloor$  (recall that  $x_i = il \Rightarrow i = x_i/l$ ).

Note that this specific choice of  $I$  contains  $\Delta x/l$  points (supposing  $\Delta x \gg l$ ). However, depending on the parity of  $n$  (fixed by the choice of the instant  $t_n$ ), only half of the positions  $x_j$  can be explored, as  $n$  and  $j$  must have the same parity. For the other half, we approximate and compute  $w_j(t_n)$  at the center point  $j = i_0$ . Thus:

$$(1.30) \approx \frac{\Delta x}{l} \left( \frac{1}{2} \cdot 0 + \frac{1}{2} w_{i_0}(t_n) \right) = \frac{\Delta x}{2l} w_{i_0}(t_n) \quad (1.31)$$

We have now an expression for  $W(x, t_n)$ , which is continuous with respect to  $x$ :

$$W(x, t_n) \Delta x = \frac{\Delta x}{2l} w_{i_0}(t_n) \quad (1.32)$$

If we now take the limit  $n \rightarrow 0$  we can substitute (1.29) in (1.32), leading to:

$$W(x, t) = \frac{1}{2l} \sqrt{\frac{2}{\pi n}} \exp\left(-\frac{i^2}{2n}\right)$$

Substituting  $x = il$  and  $t = n\varepsilon$  we get:

$$W(x, t) = \sqrt{\frac{2\varepsilon}{4l^2\pi t}} \exp\left(-\frac{x^2}{2\frac{l^2}{\varepsilon}t}\right)$$

As  $l^2 \epsilon^{-1} = 2D$ :

$$W(x, t) = \frac{1}{\sqrt{4\pi Dt}} \exp\left(-\frac{x^2}{4Dt}\right)$$

We can now compute the first two moments of  $x$ :

$$\begin{aligned}\langle x \rangle_t &= \int_{\mathbb{R}} W(x, t) x \, dx = 0 \\ \langle x^2 \rangle_t &= \int_{\mathbb{R}} W(x, t) x^2 \, dx = 2Dt\end{aligned}$$

This last integral can be done in many ways. For example, recall the gaussian integral:

$$I = \sqrt{\frac{\pi}{\mu}} = \int_{-\infty}^{\infty} e^{-\mu y^2} \, dy$$

Differentiating (according to Leibniz integral rule) with respect to  $\mu$ :

$$\frac{\partial I}{\partial \mu} = - \int_{\mathbb{R}} e^{-\mu y^2} y^2 \, dy = -\frac{1}{2} \sqrt{\frac{\pi}{\mu^3}} \quad (1.33)$$

and so:

$$\begin{aligned}\langle x^2 \rangle_t &= \frac{1}{\sqrt{4\pi Dt}} \int_{-\infty}^{+\infty} x^2 \exp\left(-\frac{x^2}{4Dt}\right) \, dx = \\ &= \frac{1}{\sqrt{4\pi Dt}} \int_{-\infty}^{+\infty} e^{-\mu x^2} x^2 \, dx \Big|_{\mu=(4Dt)^{-1}} \stackrel{(1.33)}{=} \frac{1}{\sqrt{4\pi Dt}} \frac{1}{2} \sqrt{\pi(4Dt)^3} = 2Dt\end{aligned}$$

**Summary of the last lessons.** Analysing the dynamics of the Diffusion Problem led to the Master Equation, which in the symmetrical case reduces to:

$$w_i(t_{n+1}) = \frac{1}{2}(w_{i-1}(t_n) + w_{i+1}(t_n)) \quad (1.34)$$

where  $w_i(t_n)$  is the (mass) probability function for a particle, i.e.  $w_i(t_n)$  is the probability that a particle will be at position  $x_i = i \cdot l$  at time  $t_n = n \cdot \epsilon$ .

Further evaluation, in terms of the Binomial distribution, leads to the exact solution:

$$w_i(t_n) = \frac{1}{2^n} \binom{n}{n_+} \quad (1.35)$$

where  $n_+$  is a random variable representing the number of steps in which the particle moves to the *right*.

Then we considered the continuum limit, with  $l, \epsilon \downarrow 0$  (keeping  $l^2 \epsilon^{-1} = 2D$  constant), arriving to:

$$w_i(t_n) = \frac{1}{\sqrt{4\pi Dt}} \exp\left(-\frac{x^2}{4Dt}\right) \quad (1.36)$$

which is the pdf for a particle that starts at  $x = 0$  at  $t = 0$ .

(Lesson 4 of  
14/10/19)  
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## 1.9 Continuum limit of the Master Equation

The same result can be obtained by taking directly the continuum limit of the ME (1.34), which will lead to a differential equation that can *then* be solved. We start by recalling that, for a fine discretization,  $w_i(t_n)$  is approximately equal to the probability of being around a generic  $(x, t)$  (i.e.  $W(x, t)\Delta x$ ), up to a normalization constant:

$$W(x_0, t_n)\Delta x = \mathbb{P}(x \in [x_0 - \Delta x/2, x_0 + \Delta x/2]) \approx \frac{\Delta x}{2l} w_{i_0}(t_n) \quad i_0 = \lfloor \Delta x/l \rfloor$$

And so, with a slight abuse of notation:

$$w_i(t_n) \approx 2lW(x, t) \quad i = \lfloor x/l \rfloor, n = \lfloor t/\epsilon \rfloor$$

Substituting in (1.34) leads to:

$$2lW(x, t + \epsilon) = 2l \frac{1}{2} (W(x - l, t) + W(x + l, t)) \quad (1.37)$$

which means that an analogous Master Equation holds even for  $W(x, t)$ , which is a continuous pdf, and thus can be differentiated. In particular, we can compute  $W(x, t + \epsilon)$  in terms of  $W(x, t)$  (and derivatives) by expanding around  $\epsilon = 0$ :

$$W(x, t + \epsilon) = W(x, t) + \epsilon \frac{\partial}{\partial \tau} W(\chi, \tau) \Big|_{(x, t)} + \frac{\epsilon^2}{2} \frac{\partial^2}{\partial \tau^2} W(\chi, \tau) \Big|_{(x, t)} + O(\epsilon^3) \quad (1.38)$$

And also  $W(x \pm l, t)$  by expanding around  $l = 0$ :

$$W(x \pm l, t) = W(x, t) \pm l \frac{\partial}{\partial \chi} W(\chi, \tau) \Big|_{(x, t)} + \frac{l^2}{2} \frac{\partial^2}{\partial \chi^2} W(\chi, \tau) \Big|_{x, t} + O(l^3) \quad (1.39)$$

We then introduce the following notation for the space and time derivatives:

$$\dot{W}(x, t) = \frac{\partial}{\partial \tau} W(\chi, \tau) \Big|_{(x, t)} \quad W'(x, t) = \frac{\partial}{\partial \chi} W(\chi, \tau) \Big|_{(x, t)}$$

so that a space derivative is denoted with  $a'$  ( $a''$  for the second derivative), and a time derivative with  $\dot{a}$  ( $\ddot{a}$  for the second derivative).

We can now substitute back in (1.37). We start with the right side:

$$W(x + l, t) + W(x - l, t) = 2W(x, t) + l^2 W''(x, t) + O(l^4)$$

where the  $O(l^4)$  is given by the cancellation of the odd powers (including  $l^3$ ). Equating to the left side of (1.37) leads to:

$$\cancel{W(x, t)} + \epsilon \dot{W}(x, t) + \frac{\epsilon^2}{2} \ddot{W}(x, t) = \cancel{W(x, t)} + \frac{l^2}{2} W''(x, t) + O(l^4)$$

Dividing by  $\epsilon$ :

$$\begin{aligned} \dot{W}(x, t) + \frac{\epsilon}{2} \ddot{W}(x, t) &= \underbrace{\frac{l^2}{2\epsilon}}_D W''(x, t) + O\left(\frac{l^4}{\epsilon}\right) \\ &= DW''(x, t) + O(4\epsilon D^2) \end{aligned}$$

*Not so sure about this part*

If we now take the continuum limit, then  $\epsilon, l \rightarrow 0$  with the ratio  $D = l^2/(2\epsilon)$  fixed, both  $\ddot{W}(x, t)$  and the error term vanish, leading to the **diffusion equation**:

$$\dot{W}(x, t) = DW''(x, t) \quad (1.40)$$

### 1.9.1 Solution of the Continuous Master Equation

We want now to solve (1.40), and show that the solution will be the same we previously derived in (1.36).

So, we start from:

$$\partial_t W(x, t) = D\partial_x^2 W(x, t)$$

This is a second order partial differential equation. To be able to solve it, we must first define its **boundary conditions**. In this case, we suppose that the particle is unconstrained, and so the spatial domain coincides with  $\mathbb{R}$ .

As  $W(x, t)$  is a pdf, the following conditions must hold:

$$W(x, t) \geq 0 \quad \forall(x, t) \quad \int_{\mathbb{R}} W(x, t) = 1$$

From the normalization, it follows that  $W(x, t)$  - and its spatial derivative  $W'(x, t)$  - must vanish as  $|x| \rightarrow \infty$ , so that the integral does not diverge:

$$\lim_{|x| \rightarrow \infty} W(x, t) = 0 \quad \lim_{|x| \rightarrow \infty} W'(x, t) = 0 \quad (1.41)$$

However, it is not obvious that  $W(x, t) \geq 0$  will always hold, assuming we choose an initial condition  $W(x, t_0) \geq 0$ . This will be obvious *a posteriori* - and in fact can be justified by the peculiar properties of this differential equation.

To solve (1.40), as the spatial domain is all  $\mathbb{R}$ , one standard technique is that of the Fourier integral transform, which allows us to “remove” derivatives by replacing  $\partial_x \psi \rightarrow ik\psi$ ,  $\partial_{xx} \rightarrow -k^2\psi$ . Thus, if we can “remove” the second-order space derivative, we will be left with a much more simpler first order differential equation in the time variable.

**Translational invariance.** This approach is suggested by the translational invariance of solutions of (1.40). In fact, if  $W(x, t)$  is a solution, then also  $\tilde{W}(x, t) = W(x - a, t)$  is a solution.

The generator of the translations is the *momentum*, and its eigenfunctions are the *plane waves*, i.e. the Fourier basis. So, by expressing a function in this base, we will harness the equation’s symmetry - simplifying the problem.

In other words, the Fourier basis diagonalizes the Laplacian operator which appears in (1.40):

$$\partial_x^2 \varphi_k(x) = \lambda_k \varphi_k(x) \quad \lambda_k \equiv -k^2 \quad \varphi_k(x) = A_k e^{\pm ikx}, k \in \mathbb{R}$$

In a general case, the Fourier integral trick can be tried for every variable, starting from the one with the higher order derivative, and then the case which

leads to the most simplification can be pursued.

We start by rewriting  $W(x, t)$  as a (infinite) linear combination of vectors of the Fourier basis:

$$W(x, t) = \int_{\mathbb{R}} \frac{dk}{2\pi} e^{ikx} c_k(t) \quad (1.42)$$

where the  $2\pi$  factor is just a normalization convention.

Let  $\varphi_k(x) = e^{ikx}$ . Then, as the Fourier basis is orthonormal, the following holds (recalling the Fourier transform of the  $\delta$  function):

$$\begin{aligned} \langle \varphi_k, \varphi_{k'} \rangle &= \int_{\mathbb{R}} dx \varphi_k^*(x) \varphi_{k'}(x) = \int_{\mathbb{R}} dx e^{i(k'-k)x} = 2\pi \delta(k - k') \\ \langle \tilde{\varphi}_x, \tilde{\varphi}_{x'} \rangle &= \int_{\mathbb{R}} dk \varphi_k^*(x) \varphi_k(x') = 2\pi \delta(x - x') \end{aligned} \quad (1.43)$$

We then apply a Fourier transform to both members of (1.42), by multiplying by  $e^{-ik'x}$  and integrating over  $x$ :

$$\int_{\mathbb{R}} W(x, t) e^{-ik'x} dx = \int_{\mathbb{R}} \frac{dk}{2\pi} \int_{\mathbb{R}} dx e^{i(k-k')x} c_k(t)$$

If we now apply the ON relation (1.43) we can solve the integral in the right side:

$$\int_{\mathbb{R}} W(x, t) e^{-ik'x} dx = \int_{\mathbb{R}} dk \delta(k - k') c_k(t) = c_{k'}(t)$$

And substituting  $k' \rightarrow k$  we arrive at an expression for  $c_k(t)$ :

$$c_k(t) = \int_{\mathbb{R}} dx e^{-ikx} W(x, t) \quad (1.44)$$

Starting from (1.40) we can write a corresponding differential equation for the coefficients  $c_k(t)$  in the Fourier basis, and then solve it.

**Braket notation.** Let the solution be  $|W(t)\rangle$ , so that  $\langle x|W(t)\rangle = W(x, t)$ . Then in (1.42) we just did a change of basis (by using Dirac completeness):

$$|W(t)\rangle = \mathbb{I} |W(t)\rangle = \int_k |k\rangle \underbrace{\langle k|W(t)\rangle}_{c_k(t)}$$

where  $|k\rangle$  are elements of the Fourier basis ( $\langle x|k\rangle = e^{ikx}$ ) and so:

$$c_k(t) = \langle k|W(t)\rangle = \int_x \langle k|x\rangle \langle x|W(t)\rangle = \int_{\mathbb{R}} dx e^{-ikx} W(x, t)$$

So the initial differential equation (1.40) is expressed in the position basis, while the following equation involving  $c_k(t)$  is expressed in the Fourier basis.

So, we start by differentiating (1.44) with respect to  $t$ :

$$\begin{aligned}
\dot{c}_k(t) &= \int_{\mathbb{R}} dx e^{-ikx} \dot{W}(x, t) \stackrel{(a)}{=} D \int_{-\infty}^{\infty} e^{-ikx} W''(x, t) dx = \\
&\stackrel{(b)}{=} \cancel{D W'(x, t) e^{-ikx}} \Big|_{-\infty}^{\infty} - D \int_{-\infty}^{\infty} \partial_x (e^{-ikx}) W'(x, t) dx = \\
&\stackrel{(c)}{=} -D \underbrace{(\partial_x e^{-ikx})}_{-ike^{-ikx}} W(x, t) \Big|_{-\infty}^{\infty} + D \int_{\mathbb{R}} \underbrace{\partial_x^2 (e^{-ikx})}_{-k^2 e^{-ikx}} W(x, t) dx = \\
&= -Dk^2 \underbrace{\int_{-\infty}^{+\infty} dx e^{-ikx} W(x, t)}_{c_k(t)} = -Dk^2 c_k(t)
\end{aligned}$$

where in (a) we substituted (1.40), and in (b) and (c) we performed two integrations by parts. Note that the  $W(x, t)$  and  $W'(x, t)$  terms vanish because of the boundary conditions (1.41).

Summarizing:

$$\dot{c}_k(t) = \int_{\mathbb{R}} dx e^{-ikx} \dot{W}(x, t) = -Dk^2 c_k(t)$$

This is a first-order ordinary differential equation, which can be solved by separation of variables:

$$\frac{d}{dt} c_k(t) = -Dk^2 c_k(t) \Rightarrow \int \frac{dc_k(t)}{c_k(t)} = \int -Dk^2 dt \Rightarrow \ln c_k(t) = -Dk^2 t + C$$

And rearranging:

$$c_k(t) = A e^{-Dk^2 t} \quad (1.45)$$

To find the integration constant  $A$  we impose the initial conditions, i.e. that  $c_k(t)$  be equal to a known  $c_k(t_0)$  at time  $t_0$ :

$$c_k(t_0) \stackrel{!}{=} A e^{-Dk^2 t_0} \Rightarrow A = c_k(t_0) e^{Dk^2 t_0} \quad (1.46)$$

And substituting (1.46) back in (1.45) we arrive at the general integral:

$$c_k(t) = c_k(t_0) e^{-Dk^2(t-t_0)} \quad (1.47)$$

We can now go back to  $W(x, t)$  by plugging (1.47) into (1.42):

$$\begin{aligned}
W(x, t) &= \int_{\mathbb{R}} \frac{dk}{2\pi} e^{ikx} c_k(t) = \int_{\mathbb{R}} \frac{dk}{2\pi} e^{ikx - Dk^2(t-t_0)} c_k(t_0) = \\
&\stackrel{(1.44)}{=} \int_{\mathbb{R}} \frac{dk}{2\pi} e^{ikx - Dk^2(t-t_0)} \int_{\mathbb{R}} dy e^{-iky} W(y, t_0) = \\
&= \int_{\mathbb{R}} dy W(y, t_0) \int_{\mathbb{R}} \frac{dk}{2\pi} \exp \left( -Dk^2(t-t_0) + ik(x-y) \right) \quad (1.48)
\end{aligned}$$

Recall (CFR 17/10 lecture) that:

$$\int_{-\infty}^{+\infty} \frac{dk}{2\pi} e^{-iak^2 - ibk} = \frac{1}{\sqrt{4\pi ai}} \exp \left( \frac{ib^2}{4a} \right)$$



and so with  $ia = D(t - t_0)$  and  $b = -(x - y)$  we arrive at:

$$\int_{\mathbb{R}} \frac{dk}{2\pi} \exp(-Dk^2(t - t_0) + ik(x - y)) = \frac{1}{\sqrt{4\pi D(t - t_0)}} \exp\left(-\frac{(x - y)^2}{4D(t - t_0)}\right)$$

Substituting back in (1.48):

$$W(x, t) = \frac{1}{\sqrt{4\pi D(t - t_0)}} \int_{\mathbb{R}} dy W(y, t_0) \exp\left(-\frac{(x - y)^2}{4D(t - t_0)}\right) \quad (1.49)$$

### 1.9.2 Propagators

Suppose we know with certainty that the particle is in  $y = x_0$  at time  $t = t_0$ , that is:

$$W(y, t_0) = \delta(y - x_0)$$

Then, substituting in (1.49) leads to:

$$W(x, t|x_0, t_0) \equiv \frac{1}{\sqrt{4\pi D(t - t_0)}} \exp\left(-\frac{(x - x_0)^2}{4D(t - t_0)}\right) \quad (1.50)$$

where with  $W(x, t|x_0, t_0)$  we denote the probability that the particle will be *around* position  $x$  at time  $t$ , **given** it was certainly in  $x_0$  at time  $t_0$ .  $W(x, t|x_0, t_0)$  is also called **propagator**, as it “propagates” the particle from  $(x_0, t_0)$  to  $(x, t)$  as a sort of *continuous transition probability*. This is much more evident if we rewrite (1.49) as follows (with  $y \rightarrow x_0$  for simplicity):

$$W(x, t) = \int dx_0 W(x, t|x_0, t_0) W(x_0, t_0) \quad (1.51)$$

### 1.9.3 Properties

Let’s explore some properties of (1.51).

1. **ESCK property.** Let’s propagate a particle from a starting point  $(x_0, t_0)$  to two different end points  $(x_1, t_1)$  and  $(x_2, t_2)$ :

$$W(x_1, t_1) = \int dx_0 W(x_1, t_1|x_0, t_0) W(x_0, t_0) \quad (1.52)$$

$$W(x_2, t_2) = \int dx_0 W(x_2, t_2|x_0, t_0) W(x_0, t_0) \quad (1.53)$$

We can also propagate to  $(x_2, t_2)$  starting from  $(x_1, t_1)$ :

$$W(x_2, t_2) = \int dx_1 W(x_2, t_2|x_1, t_1) W(x_1, t_1) \quad (1.54)$$

Now, if we substitute (1.52) in (1.54) we get:

$$W(x_2, t_2) = \iint dx_1 dx_0 W(x_2, t_2|x_1, t_1) W(x_1, t_1|x_0, t_0) W(x_0, t_0)$$

By comparing this expression with (1.53), we find that:

$$W(x_2, t_2 | x_0, t_0) = \int dx_1 W(x_2, t_2 | x_1, t_1) W(x_1, t_1 | x_0, t_0)$$

That is, the propagator between two *points*  $A$  and  $B$  can be obtained by multiplying the propagators between  $A \rightarrow C$  and  $C \rightarrow B$  and summing over *all possible choices* of  $C$ . This property is the Einstein-Smoluchowski-Kolmogorov-Chapman relation (**ESCK**).

2. **Moments.** Consider two instants  $t_1 \neq t_2$ , and suppose we want to compute  $\langle x(t_2)x(t_1) \rangle$ , supposing that the particle started in  $x = 0$  at  $t = 0$ . Applying the definition of an expected value:

$$\langle x(t_2)x(t_1) \rangle = \iint dx_1 dx_2 \mathbb{P}(x_2, t_2; x_1, t_1 | 0, 0) x_2 x_1$$

where  $\mathbb{P}(x_2, t_2; x_1, t_1 | 0, 0)$  is the *joint pdf* of a particle being around  $x_1$  at  $t_1$  and around  $x_2$  at  $t_2$ , given the *initial position* in  $x = 0$  at  $t = 0$ .

Recall from probability theory that:

$$\begin{aligned} \mathbb{P}(x_2, t_2; x_1, t_1; 0, 0) &= \mathbb{P}(x_2, t_2; x_1, t_1 | 0, 0) \mathbb{P}(0, 0) \\ \Rightarrow \mathbb{P}(x_2, t_2; x_1, t_1 | 0, 0) &= \frac{\mathbb{P}(x_2, t_2; x_1, t_1; 0, 0)}{\mathbb{P}(0, 0)} = \frac{W(x_2, t_2 | x_1, t_1) W(x_1, t_1 | 0, 0) \cancel{W(0, 0)}}{\cancel{W(0, 0)}} \\ &= W(x_2, t_2 | x_1, t_1) W(x_1, t_1 | 0, 0) \end{aligned}$$

Recalling the result in (1.50) we can now compute:

$$\langle x(t_2)x(t_1) \rangle = \iint_{\mathbb{R}^2} dx_1 dx_2 x_1 x_2 \frac{\exp\left(-\frac{(x_2-x_1)^2}{4D(t_2-t_1)}\right)}{\sqrt{4\pi D(t_2-t_1)}} \frac{\exp\left(-\frac{x_1^2}{4Dt_1}\right)}{\sqrt{4\pi Dt_1}}$$

By changing variables ( $x_1 = y_1$ ,  $x_2 - x_1 = y_2$ ) we arrive at:

$$\begin{aligned} &= \frac{1}{\sqrt{4\pi D(t_2-t_1)}} \frac{1}{\sqrt{4\pi Dt_1}} \iint_{\mathbb{R}^2} dy_1 dy_2 y_1(y_1 + y_2) \exp\left(-\frac{y_2^2}{4D(t_2-t_1)} - \frac{y_1^2}{4Dt_1}\right) = \\ &\stackrel{(a)}{=} \frac{1}{\sqrt{4\pi D(t_2-t_1)}} \frac{1}{\sqrt{4\pi Dt_1}} \int dy_1 y_1^2 \exp\left(-\frac{y_1^2}{4Dt_1}\right) \cdot \int dy_2 \exp\left(-\frac{y_2^2}{4D(t_2-t_1)}\right) = \\ &\stackrel{(b)}{=} \frac{1}{\sqrt{4\pi D(t_2-t_1)}} \frac{1}{\sqrt{4\pi Dt_1}} (2Dt_1 \sqrt{4\pi Dt_1}) (\sqrt{4\pi D(t_2-t_1)}) = 2Dt_1 \end{aligned}$$

In (a) we note that by expanding  $y_1(y_1 + y_2)$ , the term with  $y_1 y_2$  is an odd function integrated over a symmetric domain, that results in 0. So, only the term with  $y_1^2$  remains, allowing the integral's factorization. Then, in (b), we compute the Gaussian integrals, *supposing*  $t_1 < t_2$  (so that  $t_2 - t_1 > 0$ ) and recalling:

$$\begin{aligned} \int_{-\infty}^{+\infty} \exp\left(-\frac{1}{2}ax^2\right) dx &= \sqrt{\frac{2\pi}{a}} \\ \int_{-\infty}^{+\infty} x^2 \exp\left(-\frac{1}{2}ax^2\right) dx &= -2 \frac{d}{da} \int_{-\infty}^{+\infty} \exp\left(-\frac{1}{2}ax^2\right) dx = \sqrt{\frac{2\pi}{a}} \frac{1}{a} \end{aligned}$$

The case when  $t_1 > t_2$  leads to a similar result, with  $t_1 \leftrightarrow t_2$ . Thus, in general:

$$\langle x(t_1)x(t_2) \rangle = 2D \min(t_1, t_2)$$

Generalizing:

$$\begin{aligned}\mathbb{P}(x_i, t_i; i = 0, \dots, n) &= \mathbb{P}(x_n, t_n; x_{n-1}, t_{n-1}; \dots; x_1, t_1; x_0, t_0) = \\ &= \prod_{i=1}^n W(x_i, t_i | x_{i-1}, t_{i-1}) W(x_0, t_0)\end{aligned}$$

This is the joint probability for a *discrete trajectory*, meaning that we care only about what happens at certain discrete times.

For the average value of a generic function  $f$  of the trajectory points:

$$\langle f(x(t_n), x(t_{n-1}), \dots, x(t_0)) \rangle$$

we need to use the joint probability:

$$= \int \prod_{i=0}^n W(x_i, t_i; i = 0, \dots, n) \cdot f(x_n, x_{n-1}, \dots, x_0)$$

In the next lecture we will try to see how to generalize this kind of calculation to a function that also depends on the *in between points*, that is on a *infinite set of values of the trajectory*. For example:

$$\left\langle \exp \left( - \int_0^t a(\tau) x(\tau) d\tau \right) \right\rangle$$

depends on the *whole* trajectory.

(Lesson 4 of  
21/10/19)  
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## 1.10 Wiener's integral

Consider an *unconstrained* Brownian particle, moving on the real line, starting in  $x_0$  at  $t_0$ . By solving the diffusion equation we found that the probability of finding the particle in  $[x, x + dx]$  at time  $t > t_0$  is given by the **propagator**:

$$\begin{aligned}\mathbb{P}\{x(t) \in [x, x + dx] | x(t_0) = x_0\} &= W(x, t | x_0, t_0) dx = \\ &= \frac{1}{\sqrt{4\pi D(t - t_0)}} \exp \left( - \frac{(x - x_0)^2}{4D(t - t_0)} \right) dx\end{aligned}\tag{1.55}$$

By integrating (1.55) we can then find the probability of finding the particle inside an interval  $[A, B]$  at time  $t$ :

$$\mathbb{P}\{x(t) \in [A, B] | x(t_0) = x_0\} = \int_A^B dx W(x, t | x_0, t_0) \quad t > t_0$$

We are now interested in computing the expected value  $\langle f \rangle$  of **functionals**  $f$  of the trajectory, i.e. of quantities depending on several (or all) points of the trajectory  $x(\tau)$  of a Brownian particle.

- The simplest example is the **correlation function**, which is defined as the product of the particle's position at two different times  $t_1 < t_2$ :

$$f(\{x(t_1), x(t_2)\}) = x(t_1)x(t_2) \quad t_1 < t_2$$

- A more general (and difficult) case is given by a function of the *entire* trajectory, such as:

$$f(\{x(\tau) : 0 < \tau \leq t\}) = g \left( \int_0^t x(\tau) a(\tau) d\tau \right) \quad a, g: \mathbb{R} \rightarrow \mathbb{R}$$

### 1.10.1 Functions of a discrete number of points

Let's start from the simplest case, and consider the **correlation function**:

$$f(\{x(t_1), x(t_2)\}) = x(t_1)x(t_2) \quad t_1 < t_2$$

To compute  $\langle f \rangle$  we will need the *joint probability distribution*  $g(x_1, x_2)$  that gives the probability of  $x(t_1)$  being “close to”  $x_1$  **and**  $x(t_2)$  “close to”  $x_2$  *for the same trajectory*. Let us denote the three events of interest:

$A$ : Particle starts in  $x_0$  at  $t_0$

$B$ : Particle is close to  $x_1$  at  $t_1$  ( $x(t_1) \in [x_1, x_1 + dx_1]$ )

$C$ : Particle is close to  $x_2$  at  $t_2$  ( $x(t_2) \in [x_2, x_2 + dx_2]$ )

We are interested in the joint probability  $\mathbb{P}(C, B|A)$  (the order is defined by  $t_2 > t_1 > t_0$ ). From probability theory:

$$\mathbb{P}(C, B|A) = \mathbb{P}(C|B, A)\mathbb{P}(B|A)$$

We already now how to compute probabilities like  $\mathbb{P}(B|A)$ , but not like  $\mathbb{P}(C|B, A)$ . Fortunately, that is not needed.

Recall, in fact, that Brownian motion is a *Markovian process*, meaning that the *future* depends only on the *present state*, i.e. the particle *has no memory*. So, **subsequent displacements are independent**: the probability of the particle going from  $x_1$  to  $x_2$  is the same whether it has started at  $x_0$  or at any other point  $\tilde{x}_0$ . In other words, if we take the *present state* as the particle being in  $x_1$  at  $t_1$ , the future (position at  $t_2 > t_1$ ) depends only on that, and not on the past (position at  $t_0$ ). So:

$$\mathbb{P}(C|B, A) = \mathbb{P}(C|B)$$

leading to:

$$\mathbb{P}(C, B|A) = \mathbb{P}(C|B)\mathbb{P}(B|A)$$

Inserting the *propagators* (1.55):

$$d\mathbb{P}_{t_1, t_2}(x_1, x_2) \equiv W(x_2, t_2|x_1, t_1)W(x_1, t_1|x_0, t_0) dx_1 dx_2$$

This is the joint probability we need to compute  $\langle f \rangle$ . Of course, nothing stops us from considering  $N$  “jumps” instead of only 2:

$$\begin{aligned} d\mathbb{P}_{t_1, \dots, t_n}(x_1, \dots, x_n|x_0, t_0) &\equiv W(x_n, t_n|x_{n-1}, t_{n-1}) \dots W(x_1, t_1|x_0, t_0) dx_1 dx_2 \dots dx_n = \\ &= \exp\left(-\sum_{i=1}^n \frac{(x_i - x_{i-1})^2}{4\pi D \Delta t_i}\right) \prod_{i=1}^n \frac{dx_i}{\sqrt{4\pi D \Delta t_i}} \quad (1.56) \end{aligned}$$

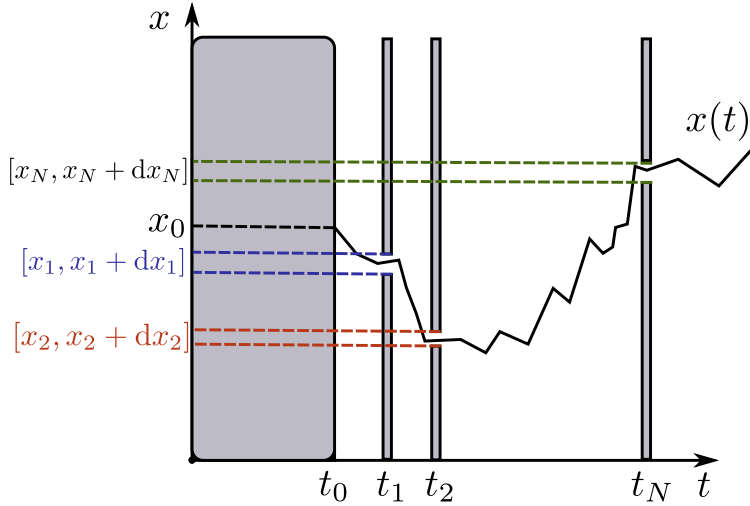
Then, the average of a generic function  $f(x(t_1), \dots, x(t_n))$  of the positions of the particle at times  $t_1 < t_2 < \dots < t_n$  is defined as:

$$\langle f(x(t_1), \dots, x(t_n)) \rangle_w = \int_{\mathbb{R}^n} f(x_1, \dots, x_n) d\mathbb{P}_{t_1, \dots, t_n}(x_1, \dots, x_n|x_0, t_0)$$

### 1.10.2 Functionals of the whole trajectory

The quantity in (1.56) can be interpreted as the *infinitesimal volume element* spanned by all the *trajectories* passing through a set of *tiny gates*, as represented in figure 1.3.

The underlying idea is that *probabilities* satisfy the axioms of *measures*, that is *functions that assign a measure*, i.e. a generalization of “size”, to *all sets included in a specific collection*.



**Figure (1.3)** – All trajectories that pass through the set of *gates*  $[x_i, x_i + dx_i]$  at times  $t_i$  (such as the  $x(t)$  here represented) contribute to the *volume*  $d\mathbb{P}_{t_1, \dots, t_n}(x_1, \dots, x_N)$

We now try to formalize this idea in order to extend the results of the previous section to the case of functions depending on a *infinite* number of trajectory points.

1. **Space definition.** Let  $T \subset \mathbb{R}$  (**index set**), denote with  $\mathbb{R}^T$  the set of all functions (**stochastic processes**)  $k: T \rightarrow \mathbb{R}$ . The idea is that an element of  $\mathbb{R}^T$  is a collection of *random variables* indexed by  $T$ .

In our case  $T$  is a collection of time instants (e.g.  $T = [0, +\infty)$ ) and a generic element of  $\mathbb{R}^T$  is made of *all the traversed points of a trajectory at times  $T$* :

$$\{x(t): t \in T\} \in \mathbb{R}^T$$

2. **Probability measure on finite points.** The expression in (1.56), as observed, allows us to *measure* the volumes spanned by trajectories traversing a set of gates. Let's formalize this idea. Consider a *finite* set of times  $T = \{t_i\}_{i=1, \dots, n}$  with  $n \in \mathbb{N}$ ,  $t_i \in \mathbb{R}$  and  $t_1 < t_2 < \dots < t_n$ , each associated to a *gate*  $H_i = [a_i, b_i]$ , with  $a_i, b_i \in \mathbb{R}$  and  $a_i < b_i$ . All the trajectories  $\mathbb{R}^T$  traversing each  $H_i$  at a time  $t_i \in T$  span a **cylindrical set**  $A$  of the form:

$$A = \{x(t): x(t_1) \in H_1, \dots, x(t_n) \in H_n\} \subset \mathbb{R}^T$$

Using (1.56) and integrating over the *gates* we can define the measure of  $A$ -like sets as:

$$P_w(A) \equiv \int_{\mathbb{R}^n} d\mathbb{P}_{t_1, \dots, t_n}(x_1, \dots, x_n | x_0, t_0) \mathbb{I}_{H_1}(x_1) \dots \mathbb{I}_{H_n}(x_n)$$

where  $\mathbb{I}_{H_i}(x_i)$  are **characteristic functions** of the gates:

$$\mathbb{I}_{H_i}(x) = \begin{cases} 1 & x \in H_i \\ 0 & \text{otherwise} \end{cases}$$

In our case  $H_i$  are just intervals, and so:

$$P_w(A) \equiv \mathbb{P}_{t_1, \dots, t_n}(A) \stackrel{(1.56)}{=} \int_{H_1} dx_1 \int_{H_2} dx_2 \dots \int_{H_n} dx_n \prod_{i=1}^n \frac{1}{\sqrt{4\pi D \Delta t_i}} \exp\left(-\frac{(x_i - x_{i-1})^2}{4D \Delta t_i}\right) \quad (1.57)$$

with  $\Delta t_i = t_i - t_{i-1}$ .

3. **Generalization on infinite points.** Note that (1.57) holds for any  $n$ . So, using  $A$ -like sets, we can construct a  $\sigma$ -algebra<sup>1</sup>  $\mathcal{F}$  of  $\mathbb{R}^T$ . Then, by applying **Kolmogorov extension theorem** we can extend the measure  $P_w$  we just found to the entire  $\mathcal{F}$ .
4. **Probability space.** We now have a set of *all possible outcomes*  $\mathbb{R}^T$  (in our case, all the possible trajectories that can be produced by a Brownian motion). We also have the collection of all *events*  $\mathcal{F}$ , that is subsets of  $\mathbb{R}^T$  for which is meaningful to assign a *probability measure*  $P_w: \mathcal{F} \rightarrow [0, 1]$ . The triad  $(\mathbb{R}^T, \mathcal{F}, P_w)$  forms a **probability space**, that gives a rigorous meaning to the concept of “computing the probability of a trajectory”.

The **measure** so obtained is called **Wiener measure**, and denoted as the following:

$$P_w(A) \equiv \int_A d_w x(\tau)$$

Then we can compute expected values. For example, if  $f(\{x(\tau): \tau \in T\})$  is a function depending on the points traversed at times in a set  $T$ , then:

$$\langle f \rangle_w \equiv \int_{\mathbb{R}^T} f(x(\tau)) d_w x(\tau) \quad T = [0, \infty)$$

Note that the Wiener measure *exists* and it's well defined (Kolmogorov's theorem), but we know it explicitly only in specific *finite cases*. So, to compute the expected value of functionals  $F(\{x(t)\})$  over *continuous trajectories* we first *discretize* the trajectory, and then take a *continuum limit*.

1. Suppose we have a functional  $F(\{x(\tau): 0 < \tau < t\})$ , and we want to compute  $\langle F \rangle$ .

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<sup>1</sup> A  $\sigma$ -algebra on a set  $X$  is a collection  $\Sigma$  of subsets of  $X$  that includes  $X$  itself, is closed under complement, and is closed under countable unions

2. We *discretize* the problem by *arbitrarily* subdividing the time interval  $[0, t]$  in  $n$  parts  $0 = t_0 < t_1 < t_2 < \dots < t_n = t$ . Then we consider an *approximated* functional  $F_N(\{x(t_0), \dots, x(t_n)\})$  (for example approximating the path  $x(\tau)$  with a piecewise linear function, depending only on  $x(t_0), \dots, x(t_n)$ ), so that:

$$F = \text{“} \lim_{N \rightarrow \infty} \text{”} F_N$$

where  $N \rightarrow \infty$  means that  $\max \Delta t_i \rightarrow 0$ , with  $\Delta t_i = t_i - t_{i-1}$ . This limit needs to be properly defined (by using the Wiener measure to define a norm in a space of *integrable* functionals, etc.), but we will not do that here.

3. Then the **Weiner path integral** is defined as:

$$\begin{aligned} \langle F \rangle_w &= \int d_w x(\tau) F(\{x(\tau) : 0 < \tau < t\}) \equiv \text{“} \lim_{N \rightarrow \infty} \text{”} \langle F_N \rangle_w = \\ &= \text{“} \lim_{N \rightarrow \infty} \text{”} \int d\mathbb{P}_{t_1, \dots, t_n} (x_1, \dots, x_n | x_0, t_0) F_N(x(t_0), \dots, x(t_n)) \end{aligned}$$

Geometrically, we are evaluating  $F$  for every possible Brownian path  $x(\tau)$ , and then averaging all these results, each weighted by the *probability* of the corresponding path.

**Example 2** (Correlation function and ESCK property):

As expected, the more general definition of the Wiener measure - involving the continuum limit  $N \rightarrow \infty$  - reduces to (1.56) when evaluated for a function depending only on a finite set of particle's positions.

For example, consider the expected value of the *correlation function* (assume the particle starting in 0 at time 0 for simplicity):

$$\begin{aligned} \langle x(t'_1) x(t'_2) \rangle &= \int d_w x x_1(t'_1) x_2(t'_2) = \\ &= \text{“} \lim_{N \rightarrow \infty} \text{”} \int d\mathbb{P}_{t_1, \dots, t_N} (x_1, \dots, x_N | 0, 0) x(t_k) x(t_n) = \end{aligned}$$

where we chose the discretization so that  $t_k = t'_1$  and  $t_n = t'_2$ . Then, by expanding the measure and applying the ESCK property we get (the limit is omitted):

$$\begin{aligned} &= \int dx_1 \dots dx_N W(x_N, t_N | x_{N-1}, t_{N-1}) \dots W(x_1, t_1 | 0, 0) x_k x_n = \\ &\stackrel{(a)}{=} \int dx_k dx_n W(x_n, t_n | x_k, t_k) W(x_k, t_k | 0, 0) x_k x_n \end{aligned}$$

which is the same result we could have obtained directly from (1.56):

$$\langle x(t'_1) x(t'_2) \rangle = \int dx'_1 dx'_2 W(x'_2, t'_2 | x'_1, t'_1) W(x'_1, t'_1 | 0, 0) x'_1 x'_2$$

## 1.11 Change of random variables

Consider a random variable  $X \sim q(x)$ , with  $q(x)$  being a generic distribution (e.g.  $q(x) = \mu e^{-\mu x}$ ). Now consider a function  $y(x)$ , e.g.  $y(x) = x^2$ .  $Y$  is then a new random variable, with a certain distribution  $p(y)$ . We now want to compute  $p(y)$  starting from  $q(x)$  and  $y(x)$ .

Suppose that  $y(x)$  is invertible. Then, if we extract a value from  $X$ , it will be inside  $[x, x + dx]$  with a probability  $q(x) dx$ . Knowing  $X$ , we can use the relation  $y(x)$  to uniquely determine  $Y$ , that will be in  $[y, y + dy]$  with the same probability. So, the following holds:

$$q(x) dx = p(y) dy \quad (1.58)$$

We can compute  $dy$  by nudging  $y(x)$ , and expanding in Taylor series:

$$y(x + dx) \equiv y + dy + O(dy^2) = y(x) + \underbrace{dx y'(x)}_{dy} + O(dx^2)$$

and so  $dy = dx y'(x)$ . Substituting in (1.58) we get:

$$q(x) dx = p(y) dy = p(y(x)) y'(x) dx \Rightarrow p(y) = q(x(y)) \frac{dx}{dy} \quad (1.59)$$

For a more general  $y(x)$ ,  $x \sim q(x)$  and  $y = y(x)$ , the expected value of a function  $f$  in terms of  $q(x)$ :

$$\begin{aligned} \langle f(y) \rangle &= \int_{\mathbb{R}} dx f(y(x)) q(x) = \\ &= \int_{\mathbb{R}} dx f(y(x)) q(x) \underbrace{\int_{\mathbb{R}} dz \delta(z - y(x))}_{=1} = \\ &\stackrel{(a)}{=} \int_{\mathbb{R}} dz f(z) \underbrace{\int_{\mathbb{R}} dx q(x) \delta(z - y(x))}_{\langle \delta(z - y(x)) \rangle_{q(x)}} \end{aligned} \quad (1.60)$$

where in (a) we used the fact that  $\delta(z - y(x)) = 1$  only when  $z = y(x)$ , and it's 0 otherwise, and so:

$$f(y(x)) = \int_{\mathbb{R}} dz f(z) \delta(z - y(x))$$

Of course we can rewrite  $\langle f \rangle$  directly in terms of  $p(y)$ :

$$\langle f(y) \rangle = \int_{\mathbb{R}} dy f(y) p(y) \quad (1.61)$$

Comparing (1.60) with (1.61) and renaming  $y \rightarrow z$  leads to:

$$p(z) = \int_{\mathbb{R}} dx q(x) \delta(z - y(x)) = \langle \delta(z - y(x)) \rangle_{q(x)} \quad (1.62)$$

which, in general, is not the same as the previously obtained result:

$$p(z) \neq q(x(z)) \frac{dx(z)}{dz}$$



To retrieve this special case we must assume  $y(x)$  to be invertible, with inverse  $x(y)$ . This means that  $\text{sgn } y'(x) = A$ , with  $A \in \mathbb{R} \setminus \{0\}$  constant. We want now to compute  $\delta(z - y(x))$  in this case. Recall that  $\delta \circ g$ , if  $g$  is a continuously differentiable function with  $g(x_0) = 0$  and  $g'(x) \neq 0 \forall x$  is:

$$\delta(g(x)) = \frac{\delta(x - x_0)}{|g'(x_0)|}$$

So, if we let  $g(x) = z - y(x)$ , the only zero is at  $x = x(z)$ , as then  $y(x(z)) = z$ . So:

$$\delta(z - y(x)) = \frac{\delta(x - x(z))}{|y'(x(z))|}$$

Substituting back in (1.62):

$$\begin{aligned} p(z) &= \left\langle \frac{\delta(x - x(z))}{|y'(x(z))|} \right\rangle_{q(x)} = \int_{\mathbb{R}} dx q(x) \frac{\delta(x - x(z))}{|y'(x(z))|} = q(x(z)) |y'(x(z))|^{-1} = \\ &= q(x(z)) \frac{dx(y)}{dy} \Big|_{y=x(z)} \end{aligned} \quad (1.63)$$

which is the same rule found in (1.59).

## 1.12 The 1st integral

Thanks to the Wiener measure we have a way to assign probabilities to *paths*  $x(\tau)$ . We can recover from this the *transition probabilities* we started from, by considering the functional that *evaluates* a path at an instant  $t$ :  $x(\tau) \mapsto x(t) \equiv x_t$ . Then, by applying (1.62) we can compute the distribution followed by  $x_t$ :

$$p(x_t) = W(x_t, t|0, 0) = \langle \delta(x_t - x(\tau)) \rangle_w = \int d_W x(\tau) \delta(x_t - x(\tau)) \quad (1.64)$$

(The starting condition  $x(t_0) = x_0$  is *contained* in the definition of the measure  $d_W x(\tau)$ ).

So we can now write:

$$\begin{aligned} W(x, t|0, 0) &= \int d_W x \delta(x(t) - x) = \\ &= \lim_{N \rightarrow \infty} \int \prod_{i=1}^{N+1} \frac{dx_i}{\sqrt{4\pi D \Delta t_i}} \exp \left( - \sum_{i=1}^N \frac{(x_i - x_{i-1})^2}{4D \Delta t_i} \right) \delta(x_{N+1} - x) \end{aligned}$$

where  $t_n = t$ ,  $x(t_n) = x_{N+1}$ .

Recall that:

$$W(x_t, t|0, 0) = \frac{1}{\sqrt{4\pi Dt}} \exp \left( - \frac{x_t^2}{4Dt} \right)$$

If we set  $x_t = 0$  (for simplicity), we get:

$$W(0, t|0, 0) = \frac{1}{\sqrt{4\pi Dt}} \quad (1.65)$$

As an exercise to get some familiarity with Wiener integrals, we want now to *re-derive* this result, by evaluating the Wiener path integral in (1.64), with  $x_t = 0$ :

$$W(0, t|0, 0) = \langle \delta(0 - x(\tau)) \rangle_w = \int d_W x(\tau) \delta(x(\tau)) \equiv I_1 \quad (1.66)$$

First, it is convenient to establish some additional notation. Let  $T = [0, \infty)$ . We denote with  $\mathcal{C}\{0, 0; t'\}$  the subset of trajectories in  $\mathbb{R}^T$  starting from  $x = 0$  at  $t = 0$ , and lasting a time span  $t'$ . Then,  $\mathcal{C}\{0, 0; x', t'\}$  is the subset of  $\mathcal{C}\{0, 0; t'\}$  when even the end-point is fixed to be  $x(t') = x'$ . The following *normalization* property holds:

$$\langle 1 \rangle_w = \int_{\mathcal{C}\{0, 0; t\}} 1 \cdot d_W x(\tau) = 1$$

We can then rewrite (1.66) as:

$$I_1 = \int_{\mathcal{C}\{0, 0; 0, t\}} d_W x(\tau)$$

Geometrically,  $W(0, t|0, 0) = I_1$  is the probability that a Brownian particle starting at the origin *returns* in it after a finite amount of time  $t$ .

The standard way to compute a Wiener integral is to *discretize* it, and then take a *continuum* limit. So, consider for simplicity a **uniform** time discretization  $\{t_i\}_{i=1, \dots, N+1}$ , with instants  $\epsilon$ -apart from each other, so that:

$$t_i - t_{i-1} \equiv \epsilon = \frac{t}{N+1} \quad \forall i = 1, \dots, N+1$$

Note that the end-points are  $x_0 = x_{N+1} = 0$ .

Then:

$$I_1 \equiv \lim_{\substack{\epsilon \rightarrow 0 \\ N \rightarrow \infty}} I_1^{(N)} \quad (1.67)$$

$$I_1^{(N)} \equiv \frac{1}{(\sqrt{4\pi D\epsilon})^{N+1}} \int_{-\infty}^{+\infty} dx_1 \int_{-\infty}^{+\infty} dx_2 \cdots \int_{-\infty}^{+\infty} dx_N \exp \left( -\frac{1}{4D\epsilon} \sum_{i=0}^N (x_{i+1} - x_i)^2 \right) \quad (1.68)$$

Let's focus on the summation in the exponential:

$$\begin{aligned} \sum_{i=0}^N (x_{i+1} - x_i)^2 &= x_1^2 + \cancel{x_0^2} - 2x_0x_1 + x_2^2 + x_1^2 - 2x_1x_2 + \cdots + \cancel{x_{N+1}^2} + x_N^2 - 2x_Nx_{N+1} = \\ &= 2(x_1^2 + \cdots + x_N^2) - 2(x_1x_2 + x_2x_3 + \cdots + x_{N-1}x_N) = \\ &= 2 \left( \sum_{i=1}^N x_i^2 \right) - 2 \left( \sum_{i=1}^{N-1} x_i x_{i+1} \right) \end{aligned}$$

This is a *quadratic form*, i.e. a polynomial with all terms of order 2. So, it can be written in *matrix form*:

$$= \sum_{k,l=1}^N x_k A_{kl} x_l = \mathbf{x}^T A_N \mathbf{x}$$

for an appropriate choice of entries  $A_{kl}$  of the  $N \times N$  matrix  $A_N$ :

$$A_{kk} = 2; A_{kl} = -(\delta_{kl} + 1 + \delta_{k+1,l}) \Rightarrow A_N = \begin{pmatrix} 2 & -1 & 0 & \cdots & 0 \\ -1 & 2 & -1 & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & -1 & 2 & -1 \\ 0 & \cdots & 0 & -1 & 2 \end{pmatrix}$$

Substituting back in (1.68):

$$I_1^{(N)} = \frac{1}{(\sqrt{4\pi D\epsilon})^{N+1}} \int_{-\infty}^{+\infty} dx_1 \cdots \int_{-\infty}^{+\infty} dx_N \exp\left(-\frac{\mathbf{x}^T A_N \mathbf{x}}{4D\epsilon}\right)$$

Recall the multivariate Gaussian integral:

$$\int_{-\infty}^{+\infty} dx_1 \cdots dx_N \exp\left(-\sum_{ij} B_{ij} x_i x_j\right) = \frac{(\sqrt{\pi})^N}{\sqrt{\det B}}$$

leading to:

$$I_1^{(N)} = \frac{1}{(\sqrt{4\pi D\epsilon})^{N+1}} \sqrt{\frac{\pi^N}{\det\left(A_N \left[\frac{1}{4D\epsilon}\right]^N\right)}} \stackrel{(a)}{=} \frac{1}{(\sqrt{4\pi D\epsilon})^{N+1}} \frac{\sqrt{4\pi D\epsilon}^N}{\sqrt{\det A_N}} = \frac{1}{\sqrt{4\pi D\epsilon}} \frac{1}{\sqrt{\det A_N}} \quad (1.69)$$

where in (a) we used the property of the determinant  $\det(cA) = c^n \det(A) \forall c \in \mathbb{R}$ .

Now, all that's left is to compute the determinant of  $A_N$ . Fortunately, as  $A_N$  is a *tri-diagonal* matrix, there is a recurrence relation in terms of the leading principal minors of  $A_N$ , which turns out to be multiples of the determinants of  $A_{N-1}$  and  $A_{N-2}$ .

Explicitly, consider  $A_N$ :

$$\det A_N \equiv \begin{vmatrix} 2 & -1 & 0 & \cdots & 0 \\ -1 & 2 & -1 & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & -1 & 2 & -1 \\ 0 & \cdots & 0 & -1 & 2 \end{vmatrix}_{N \times N}$$

and start computing the determinant following the last column. The only non-

zero contributions are:

$$\det A_N = \underbrace{(-1)^{(N-1)+N}}_{+1} (-1) \begin{vmatrix} 2 & -1 & 0 & \cdots & 0 \\ -1 & 2 & -1 & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & -1 & 2 & -1 \\ 0 & \cdots & 0 & 0 & -1 \end{vmatrix}_{(N-1) \times (N-1)} + (-1)^{2N} (2) \det A_{N-1} =$$

$$= (-1)^{2(N-1)} (-1) \det A_{N-2} + 2 \det A_{N-1} = 2 \det A_{N-1} - \det A_{N-2} \quad (1.70)$$

where the terms in blue are just the alternating signs from the determinant expansion, and the other colours identify the matrix entries that are being used.

Then, it is just a matter of computing the first two terms of the succession ( $|A_N| = \det A_N$  for brevity):

$$|A_1| = 2 \quad |A_2| = \begin{vmatrix} 2 & -1 \\ -1 & 2 \end{vmatrix} = 4 - 1 = 3$$

And now we can use (1.70) to iteratively compute all  $|A_N|$ , e.g.  $|A_3| = 2 \cdot 3 - 2 = 4$ . To find  $|A_N|$  for a *generic*  $N$ , we need to make an hypothesis, and then verify that it is compatible with (1.70). In this case, note that  $|A_N| = N + 1$  (\*) for all the examples we explicitly computed. Then, by induction:

$$|A_{N+1}| \stackrel{(1.70)}{=} 2 \cdot |A_N| - |A_{N-1}| \stackrel{(*)}{=} 2 \cdot (N + 1) - (N - 1 + 1) = 2N + 2 - N = (N + 1) + 1$$

which is indeed compatible with (\*). So, substituting back in (1.69) we get:

$$I_1^{(N)} = \frac{1}{\sqrt{4\pi D\epsilon}} \frac{1}{\sqrt{N+1}} \stackrel{(a)}{=} \frac{1}{\sqrt{4\pi Dt}}$$

where in (a) we used  $\epsilon = t/(N + 1) \Rightarrow N + 1 = t/\epsilon$  from the discretization. Note that this result is *constant* with respect to  $\epsilon$  or  $N$  (recall that  $t$  is fixed beforehand) and so taking the *continuum* limit leads immediately to  $I_1$  (1.67):

$$I_1 \equiv \lim_{\substack{\epsilon \rightarrow 0 \\ N \rightarrow \infty}} \frac{1}{\sqrt{4\pi Dt}} = \frac{1}{\sqrt{4\pi Dt}}$$

which is coherent with the result we previously computed (1.65).

## 1.13 A first functional

Consider a Brownian trajectory  $x(\tau)$  (from now on, we will assume that all trajectories start in  $x = 0$  at  $t = 0$ ), and a functional that *weights* every traversed point  $x(\tau)$  with a function  $a: \mathbb{R} \rightarrow \mathbb{R}$ , and then applies another function  $F: \mathbb{R} \rightarrow \mathbb{R}$  to the total integral:

$$F[x(\tau)] = F\left(\int_0^t a(\tau)x(\tau) d\tau\right)$$

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For simplicity, we set  $D = 1/4$ , so that:

$$d\mathbb{P}_{t_1, \dots, t_n}(x_1, \dots, x_n | 0, 0) = \exp \left( - \sum_{i=1}^n \frac{(x_i - x_{i-1})^2}{\pi \Delta t_i} \right) \prod_{i=1}^n \frac{dx_i}{\sqrt{\pi \Delta t_i}}$$

This is equivalent to a time rescaling  $t \rightarrow \tau = 4Dt$ .

We want now to compute  $\langle F \rangle$ :

$$I_3 \equiv \langle F[x(\tau)] \rangle_w = \int_{\mathcal{C}\{0,0;t\}} d_W x(\tau) F[x(\tau)]$$

**Note:** the next computations will follow the book. Prof. Maritan's method for evaluating  $I_3$  is quicker, but more advanced, and will be presented at the end.

Then we start by discretizing, by choosing a time grid  $0 = t_0 < t_1 < \dots < t_N = t$ :

$$I_3 = \lim_{N \rightarrow \infty} I_3^{(N)}$$

$$I_3^{(N)} = \int_{-\infty}^{+\infty} \frac{dx_1}{\sqrt{\pi \Delta t_1}} \dots \int_{-\infty}^{+\infty} \frac{dx_N}{\sqrt{\pi \Delta t_N}} F \left( \sum_{i=1}^N a_i x_i \Delta t_i \right) \exp \left( - \sum_{i=1}^N \frac{(x_i - x_{i-1})^2}{\Delta t_i} \right) \quad \begin{array}{l} a_i \equiv a(t_i) \\ x_i \equiv x(t_i) \end{array}$$

This integral can be evaluated by transforming it to a *gaussian integral* that we already know. So we start by changing variables:

$$x_i - x_{i-1} = y_i \quad i = 1, \dots, N \quad (1.71)$$

Note that:

$$\sum_{j=1}^i y_j = \cancel{x_1} - \underbrace{x_0}_{=0} + x_2 - \cancel{x_1} + \dots + x_i - \cancel{x_{i-1}} = x_i \quad 1 \leq i \leq N$$

So, when we compute the transformation of the volume element:

$$\det \left| \frac{\partial \{x_i\}}{\partial \{y_j\}} \right| = \det \begin{vmatrix} 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ \vdots & \vdots & \ddots & 0 \\ 1 & 1 & \dots & 1 \end{vmatrix}_{N \times N} = 1$$

as the determinant of a lower triangular matrix is equal to the product of the diagonal entries.

All that's left is to transform the argument of  $F$ . Let's start by writing the

first terms of the sum and apply the change of variables:

$$\begin{aligned}
\sum_{i=1}^N a_i x_i \Delta t_i &= a_1 x_1 \Delta t_1 + a_2 x_2 \Delta t_2 + \dots = \\
&= a_1 (y_1) \Delta t_1 + a_2 (y_1 + y_2) \Delta t_2 + \dots = \\
&= y_1 \left( \sum_{j=1}^N a_j \Delta t_j \right) + y_2 \left( \sum_{j=2}^N a_j \Delta t_j \right) + \dots + y_N a_N \Delta t_N = \\
&= \sum_{i=1}^N y_i \underbrace{\left( \sum_{j=i}^N a_j \Delta t_j \right)}_{A_i} \equiv \sum_{i=1}^N A_i y_i \tag{1.72}
\end{aligned}$$

Substituting everything back:

$$I_3^{(N)} = \int_{-\infty}^{+\infty} \frac{dy_1}{\sqrt{\pi \Delta t_1}} \dots \int_{-\infty}^{+\infty} \frac{dy_N}{\sqrt{\pi \Delta t_N}} F \left( \sum_{i=1}^N A_i y_i \right) \exp \left( - \sum_{i=1}^N \frac{y_i^2}{\Delta t_i} \right) \quad A_i = \sum_{j=i}^N a_j \Delta t_j$$

We can simplify this integral a bit more by rescaling the  $y_i$ :

$$z_i = A_i y_i \quad dy_i = \frac{dz_i}{A_i}$$

As each  $y_i$  is transformed independently, the jacobian is diagonal.

$$I_3^{(N)} = \int_{-\infty}^{+\infty} \frac{dz_1}{\sqrt{\pi A_1^2 \Delta t_1}} \dots \int_{-\infty}^{+\infty} \frac{dz_N}{\sqrt{\pi A_N^2 \Delta t_N}} F(z_1 + \dots + z_N) \exp \left( - \sum_{i=1}^N \frac{z_i^2}{A_i^2 \Delta t_i} \right)$$

This is the expected value of a function of the *sum* of  $N$  normally distributed random variables  $\{z_i\}$ . The idea is now to *isolate* one of them from the argument of  $F$ , integrate over it, and reiterate. This is done by changing variables yet again:

$$\begin{cases} \eta = z_1 + z_2 \\ \xi = z_2 \end{cases} \Rightarrow \begin{cases} z_1 = \eta - \xi \\ z_2 = \xi \end{cases} \Rightarrow \det \left| \frac{\partial \{z_1, z_2\}}{\partial \{\eta, \xi\}} \right| = \begin{vmatrix} 1 & -1 \\ 0 & 1 \end{vmatrix} = 1$$

leading to:

$$\begin{aligned}
I_3^{(N)} &= \int_{-\infty}^{+\infty} \frac{d\eta}{\sqrt{\pi A_1^2 \Delta t_1}} \int_{-\infty}^{+\infty} \frac{d\xi}{\sqrt{\pi A_2^2 \Delta t_2}} \int_{-\infty}^{+\infty} \frac{dz_3}{\sqrt{\pi A_3^2 \Delta t_3}} \dots \int_{-\infty}^{+\infty} \frac{dz_N}{\sqrt{\pi A_N^2 \Delta t_N}} \\
&\quad \cdot F(\eta + z_3 + \dots + z_N) \exp \left( - \frac{(\eta - \xi)^2}{A_1^2 \Delta t_1} - \frac{\xi^2}{A_2^2 \Delta t_2} - \sum_{i=3}^N \frac{z_i^2}{A_i^2 \Delta t_i} \right)
\end{aligned}$$

Note how  $\xi$  does not enter in the  $F$  argument, and so we can integrate over it:

$$\begin{aligned}
I_\xi &= \int_{-\infty}^{+\infty} d\xi \frac{1}{\sqrt{\pi A_1^2 \Delta t_1} \sqrt{\pi A_2^2 \Delta t_2}} \exp \left( - \frac{(\eta - \xi)^2}{A_1^2 \Delta t_1} - \frac{\xi^2}{A_2^2 \Delta t_2} \right) = \\
&= \int_{-\infty}^{+\infty} d\xi (\dots) \exp \left( - \frac{\xi^2 (A_2^2 \Delta t_1 + A_2^2 \Delta t_2) - (2\eta A_2^2 \Delta t_2) - (-\eta^2 A_2^2 \Delta t_2)}{A_1^2 A_2^2 \Delta t_1 \Delta t_2} \right)
\end{aligned}$$

Recall the gaussian integral formula:

$$\int_{-\infty}^{+\infty} \exp\left(-\textcolor{yellow}{a}x^2 + \textcolor{blue}{b}x + \textcolor{green}{c}\right) dx = \sqrt{\frac{\pi}{a}} \exp\left(\frac{b^2}{4a} + c\right) \quad (1.73)$$

which evaluates to:

$$I_\xi = \frac{1}{\sqrt{\pi(A_1^2\Delta t_1 + A_2^2\Delta t_2)}} \exp\left(-\frac{\eta^2}{A_1^2\Delta t_1 + A_2^2\Delta t_2}\right)$$

and substituting back in  $I_3^{(N)}$ :

$$\begin{aligned} I_3^{(N)} &= \int_{-\infty}^{+\infty} \frac{d\eta}{\sqrt{\pi A_1^2\Delta t_1 + \pi A_2^2\Delta t_2}} \int_{-\infty}^{+\infty} \frac{dz_3}{\sqrt{\pi A_3^2\Delta t_3}} \cdots \int_{-\infty}^{+\infty} \frac{dz_N}{\sqrt{\pi A_N^2\Delta t_N}} \\ &\quad \cdot F(\eta + z_3 + \cdots + z_N) \exp\left(-\frac{\eta^2}{A_1^2\Delta t_1 + A_2^2\Delta t_2} - \sum_{i=3}^N \frac{z_i^2}{A_i^2\Delta t_i}\right) \end{aligned}$$

We can now reiterate this procedure until only one integration is left:

$$I_3^{(N)} = \int_{-\infty}^{+\infty} \frac{dz}{\sqrt{\pi \sum_{i=1}^N A_i^2\Delta t_i}} F(z) \exp\left(-\frac{z^2}{\sum_{i=1}^N A_i^2\Delta t_i}\right)$$

We are now finally ready to take the continuum limit  $\Delta t_i \rightarrow 0$ ,  $N \rightarrow \infty$ . Note that:

$$\lim_{\Delta t_i \rightarrow 0} A_i = \int_{\tau}^t a(s) ds = A(\tau) \quad (1.74)$$

as the discrete sum goes from  $t_i = \tau$  to  $t_N = t$ . Then:

$$R \equiv \lim_{\Delta t \rightarrow 0} \sum_{i=1}^N A_i^2\Delta t_i = \int_0^t d\tau \left( \int_{\tau}^t ds a(s) \right)^2$$

and so:

$$I_3 = \lim_{N \rightarrow \infty} I_3^{(N)} = \int_{-\infty}^{+\infty} dz \frac{F(z)}{\sqrt{\pi R}} \exp\left(-\frac{z^2}{R}\right)$$

And to recover  $D$  we can just substitute  $R \rightarrow 4DR$ .

### 1.13.1 Alternative method

We consider now a different (quicker) technique to compute  $I_3$ . So we start again from:

$$I_3 \equiv \langle F[x(\tau)] \rangle_w = \int_{C\{0,0;t\}} d_W x(\tau) F\left(\int_0^t a(\tau)x(\tau) d\tau\right)$$

It is convenient to apply the change of variables we did in (1.72). We can do *before* discretizing, by defining  $A(\tau)$  as in (1.74):

$$A(\tau) \equiv \int_{\tau}^t a(s) ds \quad (1.75)$$

Note that  $\dot{A}(\tau) = -a(\tau)$ , and so the argument of  $F$  becomes:

$$\int_0^t a(\tau)x(\tau) d\tau = - \int_0^t \partial_\tau A(\tau)x(\tau) d\tau$$

Integrating by parts:

$$= -[x(\tau)A(\tau)]_{\tau=0}^{\tau=t} + \int_0^t A(\tau)\dot{x}(\tau) d\tau$$

And now we discretize the path over the instants  $0 = t_0 < t_1 < \dots < t_N$ , so that:

$$\begin{aligned} \int_0^t A(\tau)\dot{x}(\tau) d\tau &= \lim_{\Delta t_i \rightarrow 0} \sum_{i=1}^N A(t_i) \frac{x(t_i) - x(t_{i-1})}{\Delta t_i} \Delta t_i = \\ &= \lim_{N \rightarrow \infty} \sum_{i=1}^N A_i(x_i - x_{i-1}) = \lim_{N \rightarrow \infty} \sum_{i=1}^N A_i \Delta x_i \quad \begin{array}{l} x_i \equiv x(t_i) \\ A_i \equiv A(t_i) \end{array} \end{aligned}$$

Substituting back (here  $D = 1/4$  for simplicity):

$$\begin{aligned} I_3 &= \lim_{N \rightarrow \infty} I_3^{(N)} \\ I_3^{(N)} &= \int_{\mathbb{R}^N} \left( \prod_{i=1}^N \frac{dx_i}{\sqrt{\pi \Delta t_i}} \right) \exp \left( - \sum_{i=1}^N \frac{(\Delta x_i)^2}{\Delta t_i} \right) F \left( \sum_{i=1}^N A_i \Delta x_i \right) \end{aligned}$$

The idea is now to *apply* a change of random variable, rewriting the average  $\langle F[x(\tau)] \rangle_w$  (according to the distribution of *paths*) as the average  $\langle F(z) \rangle_{p(z)}$ , where  $p(z)$  is the distribution followed by the argument of  $F$ :

$$\sum_{i=1}^N A_i \Delta x_i$$

So, we begin by inserting the appropriate  $\delta$ :

$$I_3^{(N)} = \int_{\mathbb{R}^N} \left( \prod_{i=1}^N \frac{dx_i}{\sqrt{\pi \Delta t_i}} \right) \exp \left( - \sum_{i=1}^N \frac{(\Delta x_i)^2}{\Delta t_i} \right) F \left( \sum_{i=1}^N A_i \Delta x_i \right) \underbrace{\int_{\mathbb{R}} dz \delta \left( z - \sum_{i=1}^N A_i \Delta x_i \right)}_{=1}$$

Exchanging the integrals leads to:

$$\begin{aligned} \langle F \left( \sum_{i=1}^N A_i \Delta x_i \right) \rangle_w &= \langle F(z) \rangle_{p(z)} = \\ &= \int_{\mathbb{R}} dz F(z) \underbrace{\int_{\mathbb{R}^N} \left( \prod_{i=1}^N \frac{dx_i}{\sqrt{\pi \Delta t_i}} \right) F \left( \sum_{i=1}^N A_i \Delta x_i \right) \delta \left( z - \sum_{i=1}^N A_i \Delta x_i \right) \exp \left( - \sum_{i=1}^N \frac{(\Delta x_i)^2}{\Delta t_i} \right)}_{p(z)} \end{aligned}$$

We can evaluate  $I_3^{(N)}$  by transforming it to a *gaussian integral*. First, we remove the  $\delta$  with a Fourier transform:

$$2\pi\delta(x) = \int_{\mathbb{R}} e^{i\alpha x} d\alpha$$



which, in this case, leads to:

$$\delta \left( z - \sum_{i=1}^N A_i \Delta x_i \right) = \int_{\mathbb{R}} \frac{d\alpha}{2\pi} \exp \left( i\alpha \left( z - \sum_{i=1}^N A_i \Delta x_i \right) \right)$$

Substituting back:

$$I_3^{(N)} = \int_{\mathbb{R}} \frac{d\alpha}{2\pi} \int_{\mathbb{R}} dz F(z) e^{i\alpha z} \int_{\mathbb{R}^N} \left( \prod_{i=1}^N \frac{dx_i}{\sqrt{\pi \Delta t_i}} \right) \exp \left( - \sum_{i=1}^N \frac{\Delta x_i^2}{\Delta t_i} - i\alpha \sum_{i=1}^N A_i \Delta x_i \right)$$

We see that the last term is similar to a multivariate gaussian with a imaginary term, that we know how to integrate. We just need to remove the *differences* in the exponential with a change of variables (as in (1.71)):

$$\begin{aligned} y_1 &= \Delta x_1 = x_1 - \overbrace{x_0}^{=0} = x_1 \\ y_2 &= \Delta x_2 = x_2 - x_1 \\ &\vdots \\ y_N &= \Delta x_N = x_N - x_{N-1} \end{aligned}$$

The volume element will be transformed by the determinant of the Jacobian:

$$J = \det \frac{\partial(x_1 \dots x_N)}{\partial(y_1 \dots y_N)} = \left[ \det \frac{\partial(y_1 \dots y_N)}{\partial(x_1 \dots x_N)} \right]^{-1} = \begin{vmatrix} 1 & 0 & 0 & \dots & 0 \\ -1 & 1 & 0 & \dots & 0 \\ 0 & -1 & 1 & 0 & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & 1 \end{vmatrix}^{-1} = 1$$

where we used the fact that  $\det A^{-1} = (\det A)^{-1}$ , and that the determinant of a lower triangular matrix is just the product of the diagonal entries.

The integral then becomes:

$$\begin{aligned} I_3^{(N)} &= \int_{\mathbb{R}} \frac{d\alpha}{2\pi} \int_{\mathbb{R}} dz F(z) e^{i\alpha z} \int_{\mathbb{R}^N} \left( \prod_{i=1}^N \frac{dy_i}{\sqrt{\pi \Delta t_i}} \right) \exp \left( - \sum_{i=1}^N \frac{y_i^2}{\Delta t_i} - i\alpha \sum_{i=1}^N A_i y_i \right) = \\ &= \int_{\mathbb{R}} \frac{d\alpha}{2\pi} \int_{\mathbb{R}} dz F(z) e^{i\alpha z} \left[ \prod_{i=1}^N \int_{\mathbb{R}} \frac{dy_i}{\sqrt{\pi \Delta t_i}} \exp \left( - \frac{y_i^2}{\Delta t_i} - i\alpha A_i y_i \right) \right] \end{aligned}$$

The terms in the product are all independent gaussian integrals. Recall that:

$$\int_{\mathbb{R}} dk e^{-iak^2 - ibk} = \sqrt{\frac{\pi}{ia}} \exp \left( \frac{ib^2}{4a} \right) \quad (1.76)$$

So, with  $ia = 1/\Delta t_i$  and  $b = \alpha A_i$  we get:

$$\int_{\mathbb{R}} \frac{dy_i}{\sqrt{\pi \Delta t_i}} \exp \left( - \frac{y_i^2}{\Delta t_i} - i\alpha A_i y_i \right) = \exp \left( - \frac{\alpha^2 A_i^2 \Delta t_i}{4} \right)$$

and substituting back in the integral leads to:

$$\begin{aligned} I_3^{(N)} &= \int_{\mathbb{R}} \frac{d\alpha}{2\pi} \int_{\mathbb{R}} dz F(z) e^{i\alpha z} \left[ \prod_{i=1}^N \exp \left( -\frac{\alpha^2 A_i^2 \Delta t_i}{4} \right) \right] = \\ &= \int_{\mathbb{R}} \frac{d\alpha}{2\pi} \int_{\mathbb{R}} dz F(z) e^{i\alpha z} \exp \left( -\frac{\alpha^2}{4} \sum_{i=1}^N A_i^2 \Delta t_i \right) \end{aligned}$$

Applying the continuum limit ( $N \rightarrow \infty$ ,  $\Delta t_i \rightarrow 0$ ), the exponential argument becomes the limit of a Riemann sum, i.e. a integral:

$$\sum_{i=1}^N A(t_i)^2 \Delta t_i \xrightarrow{N \rightarrow \infty} \int_0^t A^2(\tau) d\tau \stackrel{(1.75)}{=} \int_0^t d\tau \left( \int_{\tau}^t ds a(s) \right)^2 \equiv R(t)$$

Substituting back:

$$I_3 \equiv \langle F \left( \int_0^t a(\tau) x(\tau) d\tau \right) \rangle = \lim_{N \rightarrow \infty} I_3^{(N)} = \int_{\mathbb{R}} dz \int_{\mathbb{R}} \frac{d\alpha}{2\pi} \exp \left( -\frac{\alpha^2}{4} R(t) + i\alpha z \right)$$

All that's left is to evaluate the last gaussian integral thanks to (1.76) with  $ia = R(t)/4$  and  $b = -z$ , leading to:

$$I_3 = \int_{\mathbb{R}} dz F(z) \frac{1}{2\pi} \sqrt{\frac{4\pi}{R(t)}} \exp \left( -\frac{z^2}{R(t)} \right) = \frac{1}{\sqrt{\pi R(t)}} \int_{\mathbb{R}} dz F(z) \exp \left( -\frac{z^2}{R(t)} \right)$$

So, we showed that:

$$\langle F \left( \int_0^t a(\tau) x(\tau) d\tau \right) \rangle_w = \sqrt{\frac{1}{\pi R(t)}} \int_{\mathbb{R}} dz F(z) \exp \left( -\frac{z^2}{R(t)} \right); \quad R(t) \equiv \int_0^t d\tau \left( \int_{\tau}^t a(s) ds \right)^2 \quad (1.77)$$

**Example 3** (Generating function):

Let  $F(z) = e^{hz}$ . Inserting in (1.77) results in:

$$\langle \exp \left( h \int_0^t a(\tau) x(\tau) d\tau \right) \rangle_w = \frac{1}{\sqrt{\pi R}} \int_{\mathbb{R}} dz \exp \left( -\frac{z^2}{R} + hz \right) \stackrel{(a)}{=} \exp \left( \frac{h^2 R}{4} \right) \equiv G(h) \quad (1.78)$$

where in (a) we used formula (1.73) with  $a = 1/R$  and  $b = h$ .

Note that  $G(h)$  is the **generating function** (CFR def. in 10/10 notes) of the integral:

$$I = \int_0^t a(\tau) x(\tau) d\tau$$

We can then retrieve the  $n$ -th moment of  $I$  by computing the  $n$ -th derivative of  $G(h)$ :

$$\left. \frac{d^n}{dh^n} G(h) \right|_{h=0} = \langle I^n \rangle_w$$

We can see this by differentiating the left side of (1.78):

$$G'(h) = \left\langle \int_0^t a(\tau) x(\tau) d\tau \exp \left( h \int_0^t a(\tau) x(\tau) d\tau \right) \right\rangle_w$$

and then setting  $h = 0$ :

$$G'(0) = \left\langle \int_0^t a(\tau) x(\tau) d\tau \right\rangle_w = \langle I \rangle_w$$

Then, differentiating the right side of (1.78) we have immediately the result:

$$\langle I \rangle_w = G'(h) \Big|_{h=0} = \frac{h}{2} R \exp \left( \frac{h^2 R}{4} \right) \Big|_{h=0} = 0$$

If we differentiate again we get the second moment:

$$G''(h) = \frac{R}{2} \exp \left( \frac{h^2 R}{4} \right) + \frac{h^2}{4} R^2 \exp \left( \frac{h^2 R}{4} \right) \Rightarrow G''(0) = \langle I^2 \rangle_w = \frac{R}{2}$$

Consider now a generic odd moment:

$$\left\langle \left( \int_0^t a(\tau) x(\tau) d\tau \right)^{2k+1} \right\rangle_w = 0 \quad \forall k \in \mathbb{N}$$

In fact, if we expand  $G(h)$ , we get:

$$G(h) = \sum_{n=0}^{\infty} \left( \frac{R}{4} \right)^n \frac{1}{n!} h^{2n}$$

Since all the powers are even, if we differentiate an odd number of times and set  $h = 0$  we are “selecting” an odd power - which just is not there - and so the result will be 0.

On the other hand, an even moment leads to:

$$\left\langle \left( \int_0^t a(\tau) x(\tau) d\tau \right)^{2k} \right\rangle_w = \left( \frac{R}{2} \right)^k \frac{(2k)!}{2^k k!}$$

(computations omitted).

## 1.14 Exponential functional

We consider now the following functional:

$$F[x(\tau)] = \exp \left( - \int_0^t d\tau P(\tau) x^2(\tau) \right)$$

As before, we wish to compute  $\langle F \rangle_w$ . We start by discretizing the path over a **uniform**<sup>2</sup> grid  $0 = t_0 < t_1 < \dots < t_N = t$  so that  $\Delta t_i = t_i - t_{i-1} \equiv \epsilon = t/N$ .

$$\begin{aligned} I_4 &\equiv \int_{\mathcal{C}\{0,0;t\}} d_W x(\tau) \exp \left( - \int_0^t d\tau P(\tau) x^2(\tau) \right) = \lim_{N \rightarrow \infty} I_4^{(N)} \\ I_4^{(N)} &= \int_{-\infty}^{+\infty} \frac{dx_1}{\sqrt{\pi\epsilon}} \cdots \int_{-\infty}^{+\infty} \frac{dx_N}{\sqrt{\pi\epsilon}} \exp \left( - \sum_{i=1}^N P_i x_i^2 \epsilon - \sum_{i=1}^N \frac{(x_i - x_{i-1})^2}{\epsilon} \right) \quad \begin{array}{l} x_i \equiv x(t_i) \\ P_i \equiv P(t_i) \end{array} \end{aligned} \quad (1.79)$$

The exponential argument is a **quadratic form**:

$$\begin{aligned} & - \epsilon (P_1 x_1^2 + \dots + P_N x_N^2) - \frac{1}{\epsilon} [x_0^2 + x_1^2 - 2x_0 x_1 + x_1^2 + x_2^2 - 2x_1 x_2 + \dots + x_{N-1}^2 + x_N^2 - 2x_{N-1} x_N] = \\ & = - \epsilon \sum_{i=1}^N P_i x_i^2 - \frac{1}{\epsilon} \left[ 2 \sum_{i=1}^{N-1} x_i^2 + x_N^2 - 2 \sum_{i=1}^N x_{i-1} x_i \right] = \\ & = - \left[ x_1^2 \left( \epsilon P_1 + \frac{2}{\epsilon} \right) + \dots + x_{N-1}^2 \left( \epsilon P_{N-1} + \frac{2}{\epsilon} \right) + x_N^2 \left( \epsilon P_N + \frac{1}{\epsilon} \right) + \frac{2}{\epsilon} \sum_{i=1}^N x_i x_{i-1} \right] = \\ & = - \sum_{i,j=1}^N A_{ij} x_i x_j \end{aligned}$$

where  $A_{ij}$  are matrix elements of a matrix  $A_N$ :

$$\begin{aligned} A_{ij} &= \delta_{ij} a_i - \frac{1}{\epsilon} (\delta_{i,j-1} + \delta_{i-1,j}) \quad a_i = P_i \epsilon + \frac{1}{\epsilon} (2 - \delta_{iN}) \\ A_N &= \begin{pmatrix} a_1 & -1/\epsilon & 0 & \dots & 0 \\ -\epsilon^{-1} & a_2 & -\epsilon^{-1} & 0 & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ 0 & 0 & -\epsilon^{-1} & a_{N-1} & -\epsilon^{-1} \\ 0 & 0 & 0 & -\epsilon^{-1} & a_N \end{pmatrix} \end{aligned}$$

We can now rewrite  $I_4^{(N)}$  as:

$$I_4^{(N)} = \int_{\mathbb{R}^N} \left( \prod_{i=1}^N \frac{dx_i}{\sqrt{\pi\epsilon}} \right) e^{-\mathbf{x}^T A_N \mathbf{x}} \quad \mathbf{x}^T = (x_1, \dots, x_N)$$

This is the integral of a multivariate gaussian, and evaluates to:

$$I_4^{(N)} = \frac{1}{\epsilon^{N/2} (\det A_N)^{1/2}} = \frac{1}{(\det(\epsilon A_N))^{1/2}}$$

---

<sup>2</sup>^The same result can be proved without this assumption, but which a much more heavy notation.

as for a  $N \times N$  matrix we have  $\det(\epsilon A_N) = \epsilon^N \det A_N$ . This has the advantage of removing all denominators in  $A_N$ .

To compute this determinant we use a method suggested by Gelfand and Yaglom (1960). We start by denoting with  $D_k^{(N)}$  the determinant of the matrix obtained by removing the first  $k-1$  rows and columns from  $\epsilon A_N$ :

$$D_k^{(N)} \equiv \begin{vmatrix} \epsilon a_k & -1 & 0 & \dots & 0 \\ -1 & \epsilon a_{k+1} & -1 & 0 & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & -1 & a_{N-1} & -1 \\ 0 & \dots & 0 & -1 & \epsilon a_N \end{vmatrix}$$

So that  $D_1^{(N)} = \det \epsilon A_N$  is the determinant we want to compute.

Expanding  $D_k^{(N)}$  from the first row we get:

$$\begin{aligned} D_k^{(N)} &= \epsilon a_k D_{k+1} - (-1) \begin{vmatrix} -1 & -1 & 0 & \dots & 0 \\ 0 & \epsilon a_{k+2} & -1 & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & -1 & a_{N-1} & -1 \\ 0 & 0 & 0 & -1 & \epsilon a_N \end{vmatrix} = \\ &\stackrel{(a)}{=} \epsilon a_k D_{k+1} + (-1) D_{k+2} = \epsilon \left( \epsilon P_k + \frac{2}{\epsilon} \right) D_{k+1} - D_{k+2} = \\ &= (\epsilon^2 P_k + 2) D_{k+1} - D_{k+2} \end{aligned}$$

where in (a) we expanded the last determinant following the first column.

Rearranging:

$$\frac{D_k^{(N)} - 2D_{k+1}^{(N)} + D_{k+2}^{(N)}}{\epsilon^2} = P_k D_{k+1}^{(N)} \quad (1.80)$$

We introduce now the variable  $\tau = (k-1)t/N$ , representing the *fraction* of removed rows/columns in each determinant, rescaled to the final time  $t$ . Performing a continuum limit  $N \rightarrow \infty$  we can then map  $D_k^{(N)} \xrightarrow[N \rightarrow \infty]{} D(s)$ . Then, the relation (1.80) becomes a *differential equation*:

$$\frac{d^2 D(\tau)}{d\tau^2} = P(\tau) D(\tau) \quad (1.81)$$

In fact, note that the first term of (1.80) is a second derivative in the *finite difference* approximation. This can be shown by Taylor expanding a generic function  $f(x)$  to get the points immediately before and after:

$$\begin{aligned} f(x + \Delta x) &= f(x) + f'(x)\Delta x + \frac{1}{2}f''(x)(\Delta x)^2 + O((\Delta x)^3) \\ f(x - \Delta x) &= f(x) - f'(x)\Delta x + \frac{1}{2}f''(x)(\Delta x)^2 + O((\Delta x)^3) \end{aligned}$$

Summing side by side, and denoting  $f(x) \equiv f_i$ ,  $f(x - \Delta x) \equiv f_{i-1}$  and  $f(x + \Delta x) \equiv f_{i+1}$ :

$$f_{i+1} + f_{i-1} = 2f_i + f_i''(\Delta x)^2 + O((\Delta x)^3)$$

Rearranging, shifting  $i \rightarrow i + 1$  and ignoring the higher order terms leads to:

$$\frac{f_{i+2} - 2f_{i+1} + f_i}{(\Delta x)^2} = f_{i+1}''$$

Analogously, this can be seen by computing the second derivative as *the derivative of the first derivative* in terms of incremental ratios:

$$\begin{aligned} f''(x) &= \lim_{\Delta x \rightarrow 0} \frac{1}{\Delta x} \left( \frac{f(x + \Delta x) - f(x)}{\Delta x} - \frac{f(x) - f(x - \Delta x)}{\Delta x} \right) = \\ &= \lim_{\Delta x \rightarrow 0} \frac{f(x + \Delta x) - 2f(x) + f(x - \Delta x)}{(\Delta x)^2} \end{aligned}$$

Returning to the problem, we note that the determinant of the full matrix, in the continuum limit, is given by:

$$\det(\epsilon A_N) = D_1^{(N)} \xrightarrow{N \rightarrow \infty} D(0)$$

(as  $s = (k - 1)t/N \Big|_{k=1} \equiv 0$ ). So, we just need to solve (1.81) and evaluate it at  $\tau = 0$ .

To do this, we first need *two* boundary conditions, as (1.81) is a second order differential equation.

Noting that  $D_N^{(N)}$  is just the last diagonal entry, we have:

$$D_N^{(N)} = \epsilon a_N = \epsilon^2 p_N + 1 \xrightarrow[N \rightarrow \infty]{\epsilon \rightarrow 0} 1$$

As  $s = (k - 1)t/N \Big|_{k=N} = t$  for  $N \rightarrow \infty$ , this means that:

$$D(t) = 1$$

For the second boundary condition, we search a relation for the first derivative at  $\tau = t$ :

$$\frac{dD(\tau)}{d\tau} \Big|_{\tau=t} = \lim_{N \rightarrow \infty} \frac{D_N^{(N)} - D_{N-1}^{(N)}}{\epsilon}$$

$D_{N-1}^{(N)}$  can be computed directly:

$$D_{N-1}^{(N)} = \begin{vmatrix} P_{N-1}\epsilon^2 + 2 & -1 \\ -1 & P_N\epsilon^2 + 1 \end{vmatrix} = P_{N-1}P_N\epsilon^4 + \epsilon^2(P_{N-1} + 2P_N) + 1$$

leading to:

$$\frac{dD(\tau)}{d\tau} \Big|_{\tau=t} = \lim_{\epsilon \rightarrow 0} \frac{\epsilon^2 P_N + 1 - P_{N-1}P_N\epsilon^4 - \epsilon^2(P_{N-1} + 2P_N) - 1}{\epsilon} = 0$$

Summarizing, we found that:

$$I_4 \equiv \langle \exp \left( - \int_0^t d\tau P(\tau) x^2(\tau) \right) \rangle_w = \frac{1}{\sqrt{D(0)}}$$

where  $D(\tau)$  is the solution of the differential equation:

$$\frac{d^2 D(\tau)}{d\tau^2} = P(\tau) D(\tau)$$

with the following boundary conditions:

$$\begin{cases} D(t) = 1 \\ \dot{D}(t) = \left. \frac{dD(\tau)}{d\tau} \right|_{\tau=t} = 0 \end{cases}$$

**Example 4** ( $P(\tau) = k^2$ , free end-point):

Let's compute  $I_4$  with the choice of  $P(\tau) = k^2$ . The differential equation becomes:

$$\frac{d^2 D(\tau)}{d\tau^2} = k^2 D(\tau)$$

which is that of a *harmonic repulsor*. The solution is a linear combination of exponentials:

$$D(\tau) = Ae^{k\tau} + Be^{-k\tau} \quad (1.82)$$

Differentiating:

$$\dot{D}(\tau) = k(Ae^{k\tau} - Be^{-k\tau})$$

We can now impose the boundary conditions:

$$\begin{cases} D(t) \stackrel{!}{=} 1 = Ae^{kt} + Be^{-kt} & (a) \\ \dot{D}(t) \stackrel{!}{=} 0 = k(Ae^{kt} - Be^{-kt}) & (b) \end{cases}$$

leading to:

$$\begin{aligned} (a) + (b): 2Ae^{kt} &= 1 \Rightarrow A = \frac{1}{2}e^{-kt} \\ (a) - (b): 2Be^{-kt} &= 1 \Rightarrow B = \frac{1}{2}e^{kt} \end{aligned}$$

So the solution is:

$$D(\tau) = \frac{1}{2} [e^{k(t-\tau)} + e^{-k(t-\tau)}] = \cosh(k(t-\tau)) \quad (1.83)$$

from which:

$$I_4 = \lim_{N \rightarrow \infty}^{(N)} = \frac{1}{\sqrt{D(0)}} = \frac{1}{\sqrt{\cosh(kt)}}$$

### 1.14.1 Fixed endpoint

We consider now a small variation of  $I_4$ , where we integrated on paths with a fixed *end-point*  $x(t) \equiv x_t$ :

$$\hat{I}_4 = \langle \exp \left( - \int_0^t P(\tau) x^2(\tau) d\tau \right) \delta(\mathbf{x} - x(t)) \rangle_w = \int_{\mathcal{C}\{0,0;x_t,t\}} \exp \left( - \int_0^t P(\tau) x^2(\tau) d\tau \right)$$

First, we rewrite the  $\delta$  in terms of a Fourier transform:

$$I'_4 = \int_{-\infty}^{+\infty} \frac{d\alpha}{2\pi} e^{i\alpha x} \langle \exp \left( - \int_0^t P(\tau) x^2(\tau) d\tau \right) e^{-i\alpha x(t)} \rangle_w$$

Then we discretize the path as before, with  $0 = t_0 < t_1 < \dots < t_N = t$  uniformly distributed ( $\Delta t_i = t_i - t_{i-1} \equiv \epsilon = t/N$ ):

$$\hat{I}_4 = \lim_{N \rightarrow \infty} \hat{I}_4^{(N)} \\ \hat{I}_4^{(N)} = \int_{\mathbb{R}} \frac{d\alpha}{2\pi} e^{i\alpha x} \int_{\mathbb{R}^N} \left( \prod_{i=1}^N \frac{dx_i}{\sqrt{\pi\epsilon}} \right) \exp \left( - \sum_{i=1}^N P_i x_i^2 \epsilon - \sum_{i=1}^N \frac{(x_i - x_{i-1})^2}{\epsilon} - i\alpha x_N \right)$$

where the red terms are the only differences from (1.79). We can rewrite the quadratic form with the matrix  $A_N$  as before:

$$\hat{I}_4^{(N)} = \int_{\mathbb{R}} \frac{d\alpha}{2\pi} e^{i\alpha x} \int_{\mathbb{R}^N} \left( \prod_{i=1}^N \frac{dx_i}{\sqrt{\pi\epsilon}} \right) \exp(-\mathbf{x}^T A_N \mathbf{x} - i\alpha x_N)$$

Also, we can express  $i\alpha x_N$  as a scalar product:

$$i\alpha x_N = \mathbf{h}^T \mathbf{x} \quad h_l = \delta_{lN}(-i\alpha)$$

So that we can now use the gaussian integral:

$$\int_{\mathbb{R}^N} d^N \mathbf{x} \exp \left( -\frac{1}{2} \mathbf{x}^T A \mathbf{x} + \mathbf{b} \cdot \mathbf{x} \right) = \exp \left( \frac{1}{2} \mathbf{b} \cdot A^{-1} \mathbf{b} \right) (2\pi)^{N/2} (\det A)^{-1/2}$$

with  $A = 2A_N$  and  $\mathbf{b} = \mathbf{h}$ :

$$\begin{aligned} I' &\equiv \frac{1}{\sqrt{(\pi\epsilon)^N}} \int_{\mathbb{R}^N} d^N \mathbf{x} \exp(-\mathbf{x}^T A \mathbf{x} + \mathbf{h}^T \mathbf{x}) = \frac{1}{\sqrt{(\pi\epsilon)^N}} \exp \left( \frac{1}{4} \mathbf{h}^T A^{-1} \mathbf{h} \right) (2\pi)^{N/2} (2^N \det A_N)^{-1/2} = \\ &= \frac{1}{\sqrt{(\pi\epsilon)^N}} \sqrt{\frac{\pi^N}{\det A_N}} \exp \left( \frac{1}{4} (-i\alpha)^2 (A_N^{-1})_{NN} \right) = \underbrace{\sqrt{\frac{1}{\epsilon^N \det A_N}}}_{I_0} \exp \left( -\frac{1}{4} \alpha^2 (A_N^{-1})_{NN} \right) \end{aligned}$$

where  $(A_N^{-1})_{NN}$  is the last diagonal element of the inverse matrix of  $A_N$ . Substituting back:

$$\hat{I}_4^{(N)} = I_0 \int_{\mathbb{R}} \frac{d\alpha}{2\pi} \exp \left( i\alpha x - \frac{1}{4} \alpha^2 (A_N^{-1})_{NN} \right)$$



which is again a gaussian integral, and following formula (1.76) with  $a = (A_N^{-1})_{NN}/4$  and  $b = -x$  leads to:

$$\hat{I}_4^{(N)} = \frac{I_0}{2\pi} \sqrt{\frac{4\pi}{(A_N^{-1})_{NN}}} \exp\left(-\frac{x^2}{(A_N^{-1})_{NN}}\right) = \frac{I_0}{\sqrt{\pi(A_N^{-1})_{NN}}} \exp\left(-\frac{x^2}{(A_N^{-1})_{NN}}\right) \quad (1.84)$$

All that's left is to compute  $(A_N^{-1})_{NN}$  and take the continuum limit. Recall from linear algebra that:

$$A^{-1} = \frac{1}{\det A} C_{ji}$$

where  $C_{ij}$  are the *cofactors* of  $A$ , i.e. the determinants of the matrices obtained from  $A$  by removing the  $i$ -th row and  $j$ -th column. In our case:

$$(A_N^{-1})_{NN} = \frac{C_{NN}}{\det A_N}$$

Before, we obtained  $\det A_N$  by means of  $D_k^{(N)}$ , i.e. the determinants of the matrices obtained by removing the first  $k-1$  rows and columns, so that  $D_1^{(N)} = \epsilon^N \det A_N$ . This leads to:

$$(A_N^{-1})_{NN} = \frac{\epsilon^N}{D_1^{(N)}} C_{NN}$$

For  $C_{NN}$  we have to compute the determinant of the  $(N-1) \times (N-1)$  matrix  $A_*^{(N-1)}$ , obtained by removing the last row and column from  $A_N$ . Note that  $A_*^{(N-1)} \neq A^{(N-1)}$ , as they differ for the *last diagonal element* which is:

$$(A_*^{(N-1)})_{N-1,N-1} = P_{N-1}\epsilon + \frac{2}{\epsilon} \neq (A_{N-1,N-1}^{(N-1)}) = P_{N-1}\epsilon + \frac{1}{\epsilon} \quad (1.85)$$

We proceed in a similar manner, defining  $\hat{D}_k^{(N-1)}$  to be the determinant of the matrix obtained by removing the first  $k-1$  rows and columns from  $\epsilon A_*^{(N-1)}$  (again, we multiply by  $\epsilon$  to remove denominators):

$$\hat{D}_k^{(N-1)} = \begin{vmatrix} \epsilon a_k & -1 & 0 & \dots & 0 \\ -1 & \epsilon a_{k-1} & -1 & 0 & \vdots \\ 0 & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & -1 & \epsilon a_{N-2} & -1 \\ 0 & \dots & \dots & -1 & \epsilon a_{N-1} \end{vmatrix}$$

So  $\hat{D}_1^{(N-1)} = \epsilon^{N-1} \det A_*^{(N-1)} = \epsilon^{N-1} C_{NN}$  leading to:

$$(A_N^{-1})_{NN} = \frac{\epsilon^N}{D_1^{(N)}} \frac{1}{\epsilon^{N-1}} \hat{D}_1^{(N-1)} = \epsilon \frac{\hat{D}_1^{(N-1)}}{D_1^{(N)}}$$

For simplicity, it is convenient to define  $\tilde{D}_1^{(N-1)} \equiv \epsilon \hat{D}_1^{(N-1)}$ , so that:

$$(A_N^{-1})_{NN} = \frac{\tilde{D}_1^{(N-1)}}{D_1^{(N)}} \quad (1.86)$$

Repeating the steps for the continuum limit, we get the same differential equation for  $\tilde{D}(\tau)$ :

$$\partial_\tau^2 \tilde{D}(\tau) = P(\tau) \tilde{D}(\tau)$$

However, due to (1.85), the boundary conditions are now different:

$$\begin{aligned} \tilde{D}_{N-1}^{(N-1)} &= \epsilon(\epsilon^2 P_{N-1} + 2) = P_{N-1} \epsilon^3 + 2\epsilon \xrightarrow{\epsilon \rightarrow 0} 0 = \tilde{D}(t) \\ \tilde{D}_{N-2}^{(N-1)} &= \epsilon \begin{vmatrix} P_{N-2} \epsilon^2 + 2 & -1 \\ -1 & P_{N-1} \epsilon^2 + 2 \end{vmatrix} = \epsilon(P_{N-1} P_{N-2} \epsilon^4 + 2(p_{N-1} + P_{N-2}) \epsilon^2 + 3) \\ \frac{\tilde{D}_{N-1}^{(N-1)} - \tilde{D}_{N-2}^{(N-1)}}{\epsilon} &= -1 + O(\epsilon^2) \xrightarrow{\epsilon \rightarrow 0} -1 = \left. \frac{d\tilde{D}(\tau)}{d\tau} \right|_{\tau=t} \end{aligned}$$

Then, substituting (1.86) in (1.84) we get:

$$\begin{aligned} \hat{I}_4^{(N)} &= \frac{I_0}{\sqrt{\pi(A_N^{-1})_{NN}}} \exp\left(-x^2 \frac{D_1^{(N)}}{\tilde{D}_1^{(N-1)}}\right) \quad I_0 = \frac{1}{\sqrt{\epsilon^N \det A_N}} = \frac{1}{\sqrt{D_1^{(N)}}} \\ I_4 &= \lim_{N \rightarrow \infty} \hat{I}_4^{(N)} = \frac{1}{\sqrt{\pi \tilde{D}(0)}} \exp\left(-x^2 \frac{D(0)}{\tilde{D}(0)}\right) \end{aligned} \quad (1.87)$$

Where  $D(\tau)$  and  $\tilde{D}(\tau)$  are solutions of the following differential equations with the following boundary conditions:

$$\begin{aligned} \tilde{D}''(\tau) &= P(\tau) \tilde{D}(\tau) & \begin{cases} \tilde{D}(t) = 0 \\ \left. \frac{d\tilde{D}(\tau)}{d\tau} \right|_{\tau=t} = -1 \end{cases} \\ D''(\tau) &= P(\tau) D(\tau) & \begin{cases} D(t) = 1 \\ \left. \frac{dD(\tau)}{d\tau} \right|_{\tau=t} = 0 \end{cases} \end{aligned}$$

**Example 5** ( $P(\tau) = k^2$  with fixed end-point):

Let  $P(\tau) = k^2$ , with  $k \in \mathbb{R}$  constant. We already solved the equation for  $D(\tau)$  with the right boundary conditions in (1.83):

$$D(\tau) = \cosh(k(t - \tau))$$

For  $\tilde{D}(\tau)$  we start from the general integral (1.82) and impose the appropriate boundary conditions:

$$\begin{cases} \tilde{D}(t) = \tilde{A}e^{kt} + \tilde{B}e^{-kt} = 0 & (a) \\ \left. \frac{d\tilde{D}(\tau)}{d\tau} \right|_{\tau=t} = k(\tilde{A}e^{kt} - \tilde{B}e^{-kt}) = -1 & (b) \end{cases}$$

so that:

$$\begin{aligned} k(a) + (b): 2\tilde{A}ke^{kt} = -1 &\Rightarrow \tilde{A} = -\frac{1}{2k}e^{-kt} \\ k(a) - (b): 2Bke^{-kt} = 1 &\Rightarrow \tilde{B} = \frac{1}{2k}e^{kt} \end{aligned}$$

leading to the solution:

$$\tilde{D}(\tau) = \frac{1}{2k}(e^{k(t-\tau)} - e^{-k(t-\tau)}) = \frac{1}{k} \sinh(k(t-\tau))$$

Finally, using the result we found in (1.87):

$$\begin{aligned} \langle \exp \left( -k^2 \int_0^t x^2(\tau) d\tau \delta(x - x(t)) \right) \rangle_w &= \int_{\mathcal{C}_{\{0,0;x_t,t\}}} \exp \left( -k^2 \int_0^t x^2(\tau) d\tau \right) d_W x(\tau) = \\ &= \sqrt{\frac{k}{\sinh(kt)}} \exp(-kx_t^2 \coth(kt)) \end{aligned}$$

## 1.15 Continuity of Brownian Path

(Lesson 6 of  
04/11/19)  
Compiled:  
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Consider a particle starting in  $x = 0$  at  $t = 0$ , and traversing  $N$  points  $\{x_i\}_{i=1,\dots,N}$  such that all increments  $\Delta x_i = x_i - x_{i-1}$  are *independent* and described by a *gaussian pdf*. The density function for such a trajectory  $\{x_i\}$  is the usual product of transition probabilities:

$$d\mathbb{P}_{t_1,\dots,t_N}(x_1,\dots,x_N) = \left( \prod_{i=1}^N \frac{dx_i}{\sqrt{4\pi\Delta t_i D}} \right) \exp \left( -\sum_{i=1}^N \frac{(\Delta x_i)^2}{4D\Delta t_i} \right) \quad \begin{matrix} \Delta t_i = t_i - t_{i-1} \\ \Delta x_i = x_i - x_{i-1} \end{matrix} \quad (1.88)$$

We now show that, taking the continuum limit  $\max_i \Delta t_i \rightarrow 0$  leads to paths  $\{x(\tau)\}$  that are *almost surely continuous*. In other words, for any interval  $T \subseteq \mathbb{R}$ , the subset  $N \subset \mathbb{R}^T$  of functions that are discontinuous has 0 Wiener measure.

Mathematically, we want to show that, as  $\Delta t_i \rightarrow 0$ , the probability that  $\Delta x_i$  is close to 0 approaches certainty:

$$\lim_{\Delta t_i \rightarrow 0} \mathbb{P}(|\Delta x_i| < \epsilon) = 1 \quad \forall \epsilon > 0$$

This is just the probability that, during time  $\Delta t_i$ , the particle makes a jump of size lower than  $\epsilon$ :

$$\begin{aligned} \mathbb{P}(|\Delta x_i| < \epsilon) &= \mathbb{P}(x_{i-1} - \epsilon < x_i < x_{i-1} + \epsilon | x(t_{i-1}) = x_i) = \\ &= \int_{x_{i-1}-\epsilon}^{x_{i-1}+\epsilon} \frac{dx_i}{\sqrt{4\pi D \Delta t_i}} \exp \left( -\frac{(x_i - x_{i-1})^2}{4D\Delta t_i} \right) = \\ &\stackrel{(a)}{=} \int_{-\epsilon}^{+\epsilon} \frac{d\Delta x_i}{\sqrt{4\pi D \Delta t_i}} \exp \left( -\frac{(\Delta x_i)^2}{4D\Delta t_i} \right) \end{aligned}$$

where in (a) we translated the variable of integration  $\Delta x_i = x_i - x_{i-1}$ .  
With another change of variables:

$$\frac{(\Delta x_i)^2}{\Delta t_i} = z^2 \Rightarrow z = \frac{\Delta x_i}{\sqrt{\Delta t_i}} \Rightarrow d\Delta x_i = dz \sqrt{\Delta t_i}$$

we get:

$$\mathbb{P}(|\Delta x_i| < \epsilon) = \int_{|z| < \epsilon/\sqrt{\Delta t_i}} \frac{dz \sqrt{\Delta t_i}}{\sqrt{4\pi D \Delta t_i}} \exp\left(-\frac{z^2}{4D}\right)$$

And taking the continuum limit leads to:

$$\lim_{\Delta t_i \rightarrow 0} \mathbb{P}(|\Delta x_i| < \epsilon) = \int_{-\infty}^{+\infty} \frac{dz}{\sqrt{4\pi D}} \exp\left(-\frac{z^2}{4D}\right) = 1$$

## 1.16 Differentiability of Brownian Path

With a very similar calculation (here omitted) we can also show that:

$$\lim_{\Delta t_i \downarrow 0} \left( \left| \frac{\Delta x_i}{\Delta t_i} \right| > k \right) = 1 \quad \forall k > 0$$

meaning that Brownian paths are *almost surely everywhere non-differentiable*.

Nonetheless, it is sometimes useful to consider “formal derivatives” of a Brownian path, that acquire a definite meaning only when considering a *finite discretization*. For example, we can start from (1.88) and rewrite it as:

$$d\mathbb{P}_{t_1, \dots, t_N}(x_1, \dots, x_N) = \left( \prod_{i=1}^N \frac{dx_i}{\sqrt{4\pi \Delta t_i}} \right) \exp\left(-\frac{1}{4D} \sum_{i=1}^N \Delta t_i \left( \frac{\Delta x_i}{\Delta t_i} \right)^2\right)$$

Then, in the continuum limit  $\Delta t_i \rightarrow 0$ , the sum in the exponential argument becomes a Riemann integral:

$$\sum_{i=1}^N \Delta t_i \left( \frac{\Delta x_i}{\Delta t_i} \right)^2 \xrightarrow{\Delta t \rightarrow 0} \int_0^t d\tau \underbrace{\left( \frac{dx_i}{d\tau} \right)^2}_{\dot{x}^2(\tau)} \quad t = t_N$$

where  $t = t_N$ . Substituting it back leads to:

$$dx_w(\tau) = \prod_{\tau=0^+}^t \frac{dx(\tau)}{\sqrt{4\pi D d\tau}} \exp\left(-\frac{1}{4D} \int_0^t \dot{x}^2(\tau) d\tau\right)$$

This expression has no rigorous meaning in this form ( $\dot{x}(\tau)$  *does not* exists!) but can be *formally manipulated* into other expressions that *have* a definite meaning, thus proving useful for the discussion.

## 1.17 Forces on the particle

We want now to generalize the framework we obtained to the case of a diffusing particle subject to *external forces*, e.g. a drop of ink diffusing through a water medium in the presence of gravity.

To do this, we first return to the beginning, deduce a Master Equation for a more general *evolution*, and then choose the right probability distribution reproducing the behaviour in presence of forces.

So, let's start by considering a particle moving on a *uniform* one-dimensional lattice ( $x_i = i \cdot l$ ,  $t_n = n \cdot \epsilon$ ), and satisfying the Markovian property, meaning that the probability  $W_i(t_{n+1})$  of being at the position labelled by  $i$  at the *next time-step*  $t_{n+1}$  depends only on the current state  $t_n$ , that is on the current probabilities  $W_j(t_n) \forall j$  and on the current transition probabilities  $W_{ij}(t_n)$  from  $j$  to  $i$ :

$$W_i(t_{n+1}) = \sum_{j=-\infty}^{+\infty} W_{ij}(t_n) W_j(t_n) \quad (1.89)$$

Previously, we assumed that:

$$W_{ij}(t_n) = \delta_{j,i-1} P_+ + \delta_{j,i+1} P_-$$

Which means that the particle only jumps from adjacent positions, one step at a time, and cannot remain at the same place. This Master Equation leads, in  $d = 3$  and in the continuum limit, to the usual Diffusion Equation:

$$\frac{\partial}{\partial t} W(\mathbf{x}, t | \mathbf{x}_0, t_0) = \nabla^2 W(\mathbf{x}, t | \mathbf{x}_0, t_0)$$

We now consider a more general case, where we drop the discretization of the space domain, allowing *jumps* of *any size* in  $\mathbb{R}$ . Then (1.89) becomes:

$$W(x, t_{n+1}) dx = \int_{-\infty}^{+\infty} dz W(x, t_{n+1} | x - z, t_n) W(x - z, t_n) \quad (1.90)$$

The integrand is the probability of the particle being in  $[x - z, x - z + dx]$  at time  $t_n$  and making a jump of size  $z$  to reach  $[x, x + dx]$  at time  $t_{n+1}$ . By summing over *all possible jump sizes* we compute the total probability of the particle being *near* the arrival position.

If we require *jumps* to be **independent** of each other<sup>3</sup>, as it is physically evident by the problem's symmetry, then the *jump* probabilities  $W(x, t_{n+1} | x - z, t_n)$  depend only on the *jump size*  $z$ .

Assuming a *isolate system*, as the particle cannot *escape*, **probability is con-**

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<sup>3</sup>^This is a stronger requirement than the Markovian property. In fact, *independent increments* imply a *Markov process*, but the converse is not true. See [http://statweb.stanford.edu/~adembo/math-136/Markov\\_note.pdf](http://statweb.stanford.edu/~adembo/math-136/Markov_note.pdf)

served:

$$\begin{aligned}
\int_{\mathbb{R}} dx W(x, t_{n+1}) &\stackrel{!}{=} \int_{\mathbb{R}} dy W(y, t_n) \\
&\stackrel{(1.90)}{=} \int_{\mathbb{R}} dz \int_{\mathbb{R}} dx W(x, t_{n+1}|x-z, t_n) W(x-z, t_n) = \\
&\stackrel{(a)}{=} \int_{\mathbb{R}} dz \int_{\mathbb{R}} dy W(y+z, t_{n+1}|y, t_n) W(y, t_n) = \\
&\stackrel{(b)}{=} \left( \int_{\mathbb{R}} dz W(\bar{y}+z, t_{n+1}|\bar{y}, t_n) \right) \left( \int_{\mathbb{R}} dy W(y, t_n) \right) \quad \forall \bar{y} \in \mathbb{R}
\end{aligned}$$

where in (a) we changed variables  $x \mapsto y = x - z$ , with  $dy = dx$ , and in (b) we used the *independent increments* property ( $\bar{y}$  is a arbitrary constant). Comparing the first and last lines leads to:

$$\int_{\mathbb{R}} dz W(y+z, t_{n+1}|y, t_n) = 1$$

Intuitively, if the particle *cannot disappear*, it *must make a jump*.

Here on, for notation simplicity, we denote:

$$W(y+z, t_{n+1}|y, t_n) \equiv W(+z|y, t_n)$$

Starting from (1.90) and taking the continuum limit in time we can write a *more general* diffusion equation. We start by constructing the difference quotient:

$$\begin{aligned}
W(x, t_{n+1}) - W(x, t_n) &= \int_{\mathbb{R}} dz W(+z|x-z, t_n) W(x-z, t_n) - W(x, t_n) = \\
&= \int_{\mathbb{R}} dz W(+z|x-z, t_n) W(x-z, t_n) - \underbrace{\int_{\mathbb{R}} dz W(+z|x, t_n) W(x, t_n)}_{=1} = \\
&= \int_{\mathbb{R}} dz \left[ \underbrace{W(+z|x-z, t_n) W(x-z, t_n)}_{F_z(x-z)} - \underbrace{W(+z|x, t_n) W(x, t_n)}_{F_z(x)} \right] = \\
&= \int_{\mathbb{R}} dz [F_z(x-z) - F_z(x)] = \\
&\stackrel{(a)}{=} \int_{\mathbb{R}} dz \left[ \cancel{F_z(x)} - z \frac{\partial}{\partial x} F_z(x) + \frac{z^2}{2} \frac{\partial^2}{\partial x^2} [F_z(x)] + \dots - \cancel{F_z(x)} \right] = \\
&= - \int_{\mathbb{R}} dz z \frac{\partial}{\partial x} [F_z(x)] + \frac{1}{2} \int_{\mathbb{R}} dz z^2 \frac{\partial^2}{\partial x^2} [F_z(x)] + \dots = \\
&\stackrel{(b)}{=} - \frac{\partial}{\partial x} \left[ \underbrace{\left( \int_{\mathbb{R}} dz z W(+z|x, t_n) \right)}_{\mu_1(x, t_n)} W(x, t_n) \right] + \\
&\quad + \frac{1}{2} \frac{\partial^2}{\partial x^2} \left[ \underbrace{\left( \int_{\mathbb{R}} dz z W(+z|x, t_n) \right)}_{\mu_2(x, t_n)} W(x, t_n) \right] + \dots
\end{aligned}$$

where  $F_z(x)$  is the probability of a *jump* of size  $z$  from the position  $x$ . In (a) we expanded  $F_z$  about  $x$ , and in (b) we exchanged the order of integrals and derivatives. Then we define the  $k$ -th moment of the *jump* pdf as follows:

$$\mu_k(x, t) = \int_{\mathbb{R}} dz z^k W(+z|x, t)$$

This allows us to rewrite the above difference in a more compact form:

$$W(x, t_{n+1}) - W(x, t_n) = \sum_{k=1}^{+\infty} \frac{(-1)^k}{k!} \frac{\partial^k}{\partial x^k} (\mu_k(x, t_n) W(x, t_n))$$

Physically, as probability is conserved, by the continuity equation, the *change* in probability density equals the divergence of a *flux*, which is just the  $x$  derivative in this one-dimensional case. So, if we *extract* a derivative, we can write the flux explicitly:

$$\begin{aligned} &= \frac{\partial}{\partial x} \left( \sum_{k=1}^{+\infty} \frac{(-1)^k}{k!} \frac{\partial^{k-1}}{\partial x^{k-1}} (\mu_k(x, t_n) W(x, t_n)) \right) \\ &\equiv -\frac{\partial}{\partial x} J(x, t_n) \end{aligned}$$

where  $J(x, t_n)$  is the *outward flux* at  $x$ , meaning that if  $J > 0$ , then  $W(x, t_{n+1}) < W(x, t_n)$  (the particle *escapes* from  $x$  to another place), and otherwise if  $J < 0$  we have  $W(x, t_{n+1}) > W(x, t_n)$  (the particle is *sucked in*  $x$ ).

If we integrate both sides over  $x$  and apply the probability conservation we get the boundary conditions for the flux:

$$\begin{aligned} \int_{\mathbb{R}} (W(x, t_{n+1}) - W(x, t_n)) dx &= \int_{\mathbb{R}} dx \left( -\frac{\partial}{\partial x} J(x, t_n) \right) \\ 1 - 1 &= -J(x, t_n) \Big|_{-\infty}^{+\infty} = J(-\infty, t_n) - J(+\infty, t_n) \end{aligned}$$

This means that, in a *isolate system*, the *flux* at  $\pm\infty$  must be the same.

Finally, normalizing by the time interval we get the complete difference quotient, which will become a time derivative in the continuum limit.

$$\frac{W(x, t_{n+1}) - W(x, t_n)}{t_{n+1} - t_n} = \frac{\partial}{\partial x} \left\{ \sum_{k=1}^{\infty} \frac{(-1)^k}{k!} \frac{\partial^{k-1}}{\partial x^{k-1}} \frac{\mu_k(x, t_n) W(x, t_n)}{t_{n+1} - t_n} \right\} \quad (1.91)$$

Letting  $t_{n+1} - t_n = \epsilon$ , in the limit  $\epsilon \rightarrow 0$  the left side will be  $\dot{W}(x, t)$ .

All that's left is to find an explicit definition for the *jump pdf*  $W(+z|x, t)$ . Previously, we assumed a **gaussian** pdf for the displacements:

$$z \sim \frac{1}{\sqrt{4\pi D\epsilon}} \exp \left( -\frac{(\Delta x)^2}{4D\epsilon} \right)$$

With this choice, the first two moments become:

$$\mu_1 = 0 \quad \mu_2 = 2D\epsilon$$

And the variance:

$$\text{Var}(z) = \mu_2 - \mu_1^2 = 2D\epsilon \propto \epsilon$$

However, for a particle subject to a force we would expect to have a *preferred jump direction*, leading to a *constant velocity motion* in the direction of the force. So we require a different  $\mu_1$ :

$$\langle z \rangle = \mu_1 = \int_{\mathbb{R}} z W(+z|x, t) \propto \epsilon f(x)$$

We still want to fix the variance to be proportional to  $\epsilon$ , as it is expected in a diffusion process.

An appropriate choice for such a distribution is given by:

$$W(+z|x, t) = F\left(\frac{z - \epsilon f(x, t)}{\sqrt{\epsilon \hat{D}(x, t)}} \frac{1}{\sqrt{\epsilon \hat{D}(x, t)}}\right) \quad (1.92)$$

with  $F, \hat{D}: \mathbb{R} \rightarrow \mathbb{R}$  functions, satisfying certain conditions, and with a physical meaning that we will now see.

First of all, we check the normalization:

$$1 \stackrel{!}{=} \int_{\mathbb{R}} dz W(+z|x, t) = \frac{1}{\sqrt{\epsilon \hat{D}(x, t)}} \int_{\mathbb{R}} dz F\left(\frac{z - \epsilon f(x, t)}{\sqrt{\epsilon \hat{D}(x, t)}}\right) \stackrel{(a)}{=} \int_{\mathbb{R}} dy F(y)$$

where in (a) we changed variables:

$$y = \frac{z - \epsilon f(x, t)}{\sqrt{\epsilon \hat{D}(x, t)}} \quad dz = \sqrt{\epsilon \hat{D}(x, t)} dy \quad (1.93)$$

Then we compute the first moment:

$$\begin{aligned} \langle z \rangle &= \mu_1(x, t) = \int_{\mathbb{R}} dz z F\left(\frac{z - \epsilon f(x, t)}{\sqrt{\epsilon \hat{D}(x, t)}}\right) \frac{1}{\sqrt{\epsilon \hat{D}(x, t)}} = \\ &\stackrel{(1.93)}{=} \int_{\mathbb{R}} dy \left( \epsilon f(x, t) + y \sqrt{\epsilon \hat{D}(x, t)} \right) F(y) = \\ &= \epsilon f(x, t) \underbrace{\int_{\mathbb{R}} F(y) dy}_{=1} + \sqrt{\epsilon \hat{D}(x, t)} \int_{\mathbb{R}} y F(y) dy \stackrel{!}{=} \epsilon f(x, t) \end{aligned}$$

So, in order to have the right normalization and the desired  $\langle z \rangle$  we need:

$$\begin{cases} \int_{\mathbb{R}} dy F(y) = 1 \\ \int_{\mathbb{R}} dy y F(y) = 0 \end{cases}$$

Both conditions are satisfied, for example, by all even normalized functions.

For the second moment:

$$\begin{aligned} \mu_2(x, t) &= \frac{1}{\sqrt{\epsilon \hat{D}(x, t)}} \int_{\mathbb{R}} dz z^2 F\left(\frac{z - \epsilon f(x, t)}{\sqrt{\epsilon \hat{D}(x, t)}}\right) = \\ &\stackrel{(1.93)}{=} \int_{\mathbb{R}} dy (\epsilon f(x, t) + y \sqrt{\epsilon \hat{D}(x, t)})^2 F(y) = \\ &= \int_{\mathbb{R}} dy F(y) [\epsilon^2 f^2 + y^2 \hat{D} \epsilon + 2\epsilon y \sqrt{\epsilon \hat{D}} f] = \\ &= \epsilon^2 f^2 + \hat{D} \epsilon \int_{\mathbb{R}} dy y^2 F(y) = \epsilon^2 f^2 + \hat{D} \epsilon \langle y^2 \rangle_{F(y)} \end{aligned}$$

And so the variance becomes:

$$\text{Var}(z) = \mu_2 - \mu_1^2 = \epsilon \hat{D} \langle y^2 \rangle_{F(y)} \propto \epsilon$$



which is proportional to  $\epsilon$  as desired. For notational simplicity, we introduce a new function  $D: \mathbb{R} \rightarrow \mathbb{R}$  such that:

$$\text{Var}(z) = \epsilon \hat{D} \langle y^2 \rangle_{F(y)} \equiv 2D(x, t) \epsilon \Rightarrow \mu_2(x, t) = \epsilon^2 f^2 + 2D(x, t)$$

We note that higher order moments are all of order  $O(\epsilon^{3/2})$ . For example, the third moment is:

$$\begin{aligned} \mu_3(x, t) &= \frac{1}{\sqrt{\epsilon \hat{D}(x, t)} \int_{\mathbb{R}} dz z^3 F\left(\frac{z - \epsilon f(x, t)}{\sqrt{\epsilon \hat{D}(x, t)}}\right)} = \\ &\stackrel{(1.93)}{=} \int_{\mathbb{R}} dy (\epsilon f(x, t) + y \sqrt{\epsilon \hat{D}(x, t)})^3 F(y) = \\ &= \int_{\mathbb{R}} dy \left( \epsilon^3 f^3 + y^3 (\epsilon \hat{D})^{3/2} + \cancel{3\epsilon^2 f^2 y \sqrt{\epsilon \hat{D}}} + 3\epsilon^2 f \hat{D} y^2 \right) F(y) = \\ &= \epsilon^3 f^3 + (\epsilon \hat{D})^{3/2} + 3\epsilon^2 f \hat{D} \langle y^2 \rangle_{F(y)} = O(\epsilon^{3/2}) \end{aligned}$$

Substituting back (1.92) in (1.91) we arrive to:

$$\begin{aligned} \frac{W(x, t_{n+1}) - W(x, t_n)}{\epsilon} &= -\frac{\partial}{\partial x} \left[ W(x, t_n) \underbrace{\frac{\mu_1(x, t_n)}{\epsilon}}_{f(x, t)} \right] + \frac{1}{2} \frac{\partial^2}{\partial x^2} \left[ \underbrace{\frac{\mu_2(x, t_n)}{\epsilon}}_{\epsilon f^2 + 2D(x, t)} W(x, t_n) \right] + \\ &\quad + \underbrace{\frac{1}{3!} \frac{\partial^3}{\partial x^3} \left[ W(x, t_n) \frac{\mu_3(x, t_n)}{\epsilon} \right]}_{O(\epsilon^{1/2})} + \dots \end{aligned}$$

Taking the limit  $\epsilon \rightarrow 0$ , we are left with:

$$\begin{aligned} \frac{\partial W(x, t)}{\partial t} &= -\frac{\partial}{\partial x} [f(x, t) W(x, t)] + \frac{1}{2} \frac{\partial^2}{\partial x^2} [2D(x, t) W(x, t)] = \\ &= -\frac{\partial}{\partial x} \left[ f(x, t) W(x, t) - \frac{\partial}{\partial x} (D(x, t) W(x, t)) \right] \end{aligned}$$

This is the **Fokker-Planck equation**, describing the diffusion process in the presence of a *force*  $f(x, t)$ , and a diffusion parameter  $D(x, t)$ .

Note that, in absence of forces  $f(x, t) \equiv 0$  and with a constant diffusion  $D(x, t) \equiv D$  we retrieve the usual *diffusion equation*:

$$\frac{\partial}{\partial t} W(x, t) = D \frac{\partial^2}{\partial x^2} W(x, t)$$

## 1.18 Langevin equation

The Fokker-Planck equation involves *probability distributions*, meaning that it describes the behaviour of *ensembles of trajectories* at once. However, we can find an equivalent description by focusing on a *single path*.

We start with a Wiener process, that is a stochastic process with *independent* and *gaussian* increments and *continuous* paths. Considering a time discretization  $\{t_i\}$ , the evolution of a single trajectory is described by:

$$x(t_{i+1}) = x(t_i) + \Delta x(t_i) \quad (1.94)$$

where each increment  $\Delta x(t_i)$  is sampled from a gaussian pdf:

$$\Delta x_i(t_i) \sim \frac{1}{\sqrt{4\pi D \Delta t_i}} \exp\left(-\frac{(\Delta x)^2}{4D \Delta t_i}\right)$$

To simplify notation, we change variables, so that:

$$\frac{\Delta B^2}{2} = \frac{\Delta x^2}{4D} \Rightarrow \Delta B = \frac{\Delta x}{\sqrt{2D}}$$

If  $x \sim p(x)$ , and  $y = y(x) \sim g(y)$ , then by the rule for a change of random variables we have:

$$g(y) = p(x(y)) \frac{dx(y)}{dy}$$

In this case:

$$\Delta B \sim \frac{1}{\sqrt{4\pi D \Delta t_i}} \exp\left(-\frac{(\Delta B)^2}{2\Delta t_i}\right) \underbrace{\frac{d\Delta x}{d\Delta B}}_{\sqrt{2D}} = \frac{1}{\sqrt{2\pi \Delta t_i}} \exp\left(-\frac{(\Delta B)^2}{2\Delta t_i}\right)$$

Note that now  $\langle \Delta B^2(t_i) \rangle = \Delta t_i$ , leaving out the  $D$ .

Substituting in (1.94) and rearranging we get:

$$x(t_{i+1}) - x(t_i) = \sqrt{2D} \Delta B(t_i) \quad (1.95)$$

We want now to form a time derivative in the left side, in order to arrive a (stochastic) differential equation for paths. To do this, we first extract a  $\Delta t_i$  factor from  $\Delta B(t_i)$  by performing another change of variables:

$$\Delta B(t_i) \equiv \Delta t_i \xi(t_i) \quad (1.96)$$

so that  $\Delta x_i = \sqrt{2D} \Delta t_i \xi_i$ , and all the *randomness* is now contained in the random variable  $\xi$ , which is distributed according to:

$$\xi(t_i) \sim \frac{1}{\sqrt{2\pi \Delta t_i}} \exp\left(-\frac{\Delta t_i^2 \xi_i^2}{2\Delta t_i}\right) \underbrace{\frac{d\Delta B_i}{d\xi(t_i)}}_{\Delta t_i} = \sqrt{\frac{\Delta t_i}{2\pi}} \exp\left(-\frac{\Delta t_i \xi_i^2}{2}\right) \quad \xi_i \equiv \xi(t_i)$$

Substituting back in (1.95) and dividing by  $\Delta t_i$  leads to:

$$\frac{x(t_{i+1}) - x(t_i)}{\Delta t_i} = \sqrt{2D} \xi(t_i)$$

And by taking the continuum limit  $\Delta t_i \rightarrow 0$  we get the **Langevin equation** for a Brownian particle:

$$\dot{x}(t) = \sqrt{2D} \xi(t) \quad (1.97)$$

We can see  $\xi(t)$  as a *highly irregular, quickly varying function*, which, in a certain sense, expresses the result of Brownian collisions at a certain instant. In particular, the following holds:

$$\langle \xi(t) \rangle = 0 \quad \langle \xi(t) \xi(t') \rangle = \delta(t - t')$$

meaning that the values of  $\xi(t)$  at different instants are completely *independent*.

Note that, as we saw previously, Brownian paths are not differentiable - and so  $\dot{x}(t)$  does not exist, and this is just a *formal* equation, with a definite meaning only in a given *discretization*. Also, note that  $\xi(t)$  is a random variable, and so this is an example of a **stochastic differential equation**. It is not clear how to find a solution to such an equation, or even how to *define* what a solution should be - and this will be the main topic of the next section.

We can rewrite (1.97) in a more *rigorous* form by “multiplying by  $dt$ ”, i.e. performing the change of variables (1.96), which - in the continuum limit - is  $dB = \xi dt$ , leading to:

$$dx(t) = \sqrt{2D} dB \quad dB \sim \frac{1}{\sqrt{2\pi dt}} \exp\left(-\frac{dB^2}{2 dt}\right)$$

Before moving on, we want to generalize this equation to the presence of *external forces*. As we saw previously, this just results in adding a *constant velocity motion* to the particle, leading to the full **Langevin equation**:

$$\begin{aligned} \dot{x}(t) &= f(x, t) + \sqrt{2D(x, t)}\xi(t) \\ dx(t) &= f(x, t) dt + \sqrt{2D(x, t)} dB \quad dB \sim \frac{1}{\sqrt{2\pi dt}} \exp\left(-\frac{dB^2}{2 dt}\right) \end{aligned} \quad (1.98)$$

The *physical* meaning of  $f(x, t)$  and  $D(x, t)$  can be more clearly seen by comparing (1.98) to the equation of motion of the Brownian particle.

Consider a particle of mass  $m$  immersed in a fluid, with a radius  $a$  that is much larger than the surrounding molecules (typically  $\sim 10^{-9}$  to  $10^{-7}$  m). The forces acting on it will be that of *viscous friction*  $-\gamma\dot{\mathbf{r}}$ , eventual *external forces*  $\mathbf{F}_{\text{ext}}$  (e.g. gravity), and a rapidly varying and *random* term  $\mathbf{F}_{\text{noise}}$ , encompassing the effect of the large number of collisions ( $\sim 10^{12}/\text{s}$ ) with the smaller fluid particles:

$$m\ddot{\mathbf{r}}(t) = -\gamma\dot{\mathbf{r}} + \mathbf{F}_{\text{ext}} + \mathbf{F}_{\text{noise}}(t)$$

Dividing both sides by  $\gamma$ :

$$\frac{m}{\gamma}\ddot{\mathbf{r}}(t) = -\dot{\mathbf{r}} + \frac{\mathbf{F}_{\text{ext}}(\mathbf{r}, t)}{\gamma} + \frac{\mathbf{F}_{\text{noise}}(t)}{\gamma} \quad (1.99)$$

Assuming a spherical particle,  $\gamma$  is given by Stokes law to be  $6\pi a\eta$ , where  $\eta$  is the viscosity of the surrounding fluid.

Note that, if we ignore the external force and the random term, the equation becomes:

$$\frac{d\dot{\mathbf{r}}(t)}{dt} = -\frac{\gamma}{m}\dot{\mathbf{r}}(t)$$

which has solution:

$$\dot{\mathbf{r}}(t) = \exp\left(-\frac{t}{\tau_B}\right)\dot{\mathbf{r}}(0) \quad \tau_B = \frac{m}{\gamma}$$

$\tau_B$  is in the scale of  $10^{-3}$  s, and represents the timescale of reaching equilibrium, i.e. 0 velocity. So, for Brownian motion to happen,  $\mathbf{F}_{\text{noise}}$  is necessary. Also, if we are interested in the motion on the scale of seconds, we can neglect the acceleration term. This is the **overdamped limit** (in analogy to a damped oscillator with high loss of energy due to attrition, so that it quickly reaches equilibrium without ever “overshooting”). Given that assumption, (1.99) becomes:

$$\dot{\mathbf{r}} = \frac{\mathbf{F}_{\text{ext}}}{\gamma} + \frac{\mathbf{F}_{\text{noise}}}{\gamma}$$

Which, for a particle moving in one dimension, reduces to:

$$x(t) = \underbrace{\frac{F_{\text{ext}}}{\gamma}}_{f(x,t)} + \underbrace{\frac{F_{\text{noise}}}{\gamma}}_{\sqrt{2D(x,t)}\xi(t)}$$

Comparing with (1.98) gives the physical meaning of  $f(x, t)$  and  $D(x, t)$ .

## 1.19 Summary

**Summary of the previous lectures.** We considered a more general stochastic process, a *Markov Process*, when the future only depends on the present. We wrote a Master Equation, and taking the continuum limit we get a second order partial differential equation, with two coefficients depending on the first two moments of the transition rate:  $f$  and  $D$ . We would want them to represent the *force* and *diffusion rate*, but we can't find their physical meaning. So we consider the Langevin equation, reaching the desired physical meaning. There, the increment depends on a *deterministic term*  $f$  and a *noise term*:

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$$dx(t) = f(x(t), t) dt + \sqrt{2D(x(t), t)} dB(t) \quad f = \frac{F_{\text{ext}}}{\gamma}$$

If we discretize this equation, passing to finite differences, we get:

$$\Delta x(t) = f(x(t), t)\Delta t + \sqrt{2D(x(t), t)}\Delta B(t) \quad \Delta B(t) \sim \frac{1}{\sqrt{2\pi\Delta t}} \exp\left(-\frac{\Delta B^2}{2\Delta t}\right)$$

This is needed because  $dx(t)/dt$  is ill-defined (as we saw in the previous lecture). Note that  $\Delta x(t) = x(t + \Delta t) - x(t)$ .

We want to show that this kind equation leads to the same Fokker-Planck equation that we saw previously, and that was derived from the Master Equation. Then we would like to examine how much the stochastic amplitude (coefficient of  $dB(t)$ ) is related to *temperature*. In fact, we know already that  $f$  depends on  $F_{\text{ext}}$ , with  $\mathbf{F}_{\text{ext}} = -\nabla V$ . We would like that, at constant temperature, the pdf of the stationary state will tend to the *Maxwell-Boltzmann distribution*:

$$\mathbb{P}(x, t) \xrightarrow[t \rightarrow \infty]{} \frac{1}{z} \exp\left(-\frac{V(x)}{k_B T}\right)$$

## 1.20 Stochastic integrals

We arrived at the Langevin equation:

$$\frac{dx}{dt} = f(x, t) + \sqrt{2D(x, t)}\xi(t) \quad (1.100)$$

where  $\xi(t)$  is a “rapidly varying, highly irregular function”, i.e. such that for  $t \neq t'$ ,  $\xi(t)$  and  $\xi(t')$  are statistically independent. As  $\langle \xi(t) \rangle = 0$ , this means that:

$$\langle \xi(t)\xi(t') \rangle = \delta(t - t')$$

Equation (1.100) does not make much sense, as  $\dot{x}(t)$  does not exist anywhere. Even changing variables to  $dB$  (i.e. “multiplying” both sides by  $dt$ ) and integrating, we are left with the following equation:

$$x(t) = x(0) + \int_0^t f(x(\tau), \tau) d\tau + \int_0^t \sqrt{2D(x(\tau), \tau)} dB(\tau)$$

It is not clear how the last integral is defined, as it involves a *stochastic term*  $dB$ .

So, before tackling the full problem, we take a step back and study the theory behind **stochastic calculus**. Let’s introduce a *generic* integral of that kind:

$$S_t = \int_0^t G(\tau) dB(\tau)$$

Intuitively, we could see this as an *infinite sum*, where each term  $G(\tau)$  is weighted by the outcome of a random variable  $B(\tau)$ .

So, to compute it, an idea is to first introduce a *time discretization*  $\{t_j\}_{j=0,\dots,n}$ , with  $t_n = t$ , leading to:

$$S_n = \sum_{i=0}^n G(\tau_i)[B(t_i) - B(t_{i-1})] \quad t_{i-1} \leq \tau_i \leq t_i \quad (1.101)$$

and then take the continuum limit for  $n \rightarrow \infty$ . This, however, proves to be more difficult than expected, for the following reasons:

- First of all, the increments  $B(t_i) - B(t_{i-1})$  are chosen *at random*. This means that  $S_n$  is a **random variable**. In fact, we could see  $S_t$  as the sum of points from  $G(\tau)$ , each *weighted* with a *randomly chosen weight*. So it is necessary to define what it means to take the limit of a sequence of random variables  $S_n$ . As we will see, there is no unique definition.
- It is not clear how to choose the *sampling instants*  $\tau_i$  for  $G(\tau)$  in the discretization (1.101). We could hope that in the limit of  $n \rightarrow \infty$ , any choice would lead to the same final result. This would be indeed true if  $B(\tau)$  were a differentiable function - except it is only *continuous* and *nowhere differentiable*. So we need to pay attention to the *specific* (and arbitrary) rule to be used in computing the discretization.

### 1.20.1 Limits of sequences of random variables

**Some basic definitions.** Recall that a probability space is defined by a triple  $(\Omega, \mathcal{F}, \mathbb{P})$ , where  $\Omega$  is a set of outcomes (*sample space*),  $\mathcal{F}$  is a  $\sigma$ -algebra on  $\Omega$ , containing all possible *events*, that is *sets of outcomes*, and  $\mathbb{P}: \mathcal{F} \rightarrow [0, 1]$  is the *probability measure*. Then, a **random variable** is a *measurable function*  $X: \Omega \rightarrow S$ , with  $S$  denoting a *state space*.

For example, let  $\Omega$  be the set of all possible results of rolling two dice, i.e. the set of ordered pairs  $(x_1, x_2)$  with  $x_1, x_2 \in \{1, 2, 3, 4, 5, 6\}$ . Then  $\mathcal{F}$  is the set of *all possible subsets* of  $\Omega$  (including both  $\Omega$  and  $\emptyset$ ) and  $\mathbb{P}: \mathcal{F} \ni f \mapsto \mathbb{P}(f)$  is given by:

$$\mathbb{P}(f) = \frac{|f|}{36}$$

where  $|f|$  is the cardinality of the set  $f$ .

A random variable can be, for example, the *sum* of the two dice:

$$X(\omega) = x_1 + x_2 \quad \forall \omega = (x_1, x_2) \in \Omega$$

Then, we can compute the probability of  $X$  assuming a certain value by measuring with  $\mathbb{P}$  the preimage set of  $X$ :

$$\mathbb{P}(X = 2) = \mathbb{P}(\omega \in \Omega | X(\omega) = 2) = \mathbb{P}(\{1, 1\}) = \frac{1}{36}$$

For discrete one-dimensional variables such as these all of this formalism does not lead to much gain, as there is an immediate and natural choice for  $(\Omega, \mathcal{F}, \mathbb{P})$ , which is usually denoted by the saying “random”. However, in more complex cases it becomes imperative to precisely define  $\Omega$ ,  $\mathcal{F}$  and  $\mathbb{P}$ , so to avoid ambiguous results (see Bertrand’s paradox).

Consider a sequence  $\{X_n\}_{n \in \mathbb{N}}$  of random variables in a certain probability space  $(\Omega, \mathcal{F}, \mathbb{P})$ . Suppose that  $X$  is another random variable, and we would like to give meaning to the concept of  $X_n$  “tending to”  $X$ :

$$X_n \xrightarrow[n \rightarrow \infty]{} X$$

There are several possibilities, here stated from the weakest to the strongest:

1. **Convergence in distribution.** In this case, we simply require that the distribution of  $S_n$  approaches that of  $S$  as  $n \rightarrow \infty$ . Let  $F_n$  and  $F$  be the cumulative distributions of  $S_n$  and  $S$ , respectively. Then:

$$X_n \xrightarrow[n \rightarrow \infty]{D} X \Leftrightarrow \lim_{n \rightarrow \infty} F_n(x) = F(x) \quad \forall x \in \mathbb{R} | F \text{ is continuous at } x$$

(The cumulative distribution, or cdf, is defined as  $F_X(x) = \mathbb{P}(X \leq x)$ ).

Note that, as we are merely comparing functions, there is no need for  $X_n$  or  $X$  to be defined on the *same probability space*. Also, here the focus is on *integral properties* of the random variables, so there is no guarantee that sampling  $X_n$  and  $X$  will lead to *close* results, even for a large  $n$ . For example, consider  $X_n$  to be a sequence of standard gaussians,

which obviously converges to a standard gaussian ( $X$ ) in the distribution sense. If we sample a number from  $X_{100}$  and one from  $X$ , they could be arbitrarily far away from each other with a non-zero probability, that remains the same for all  $n$ . If we want to *exclude* that possibility we need a *stronger requirement*, which leads to the next definition.

2. **Convergence in probability** (*Stochastic limit*). If the probability of values of  $X_n$  being *far* from values of  $X$  vanishes as  $n \rightarrow \infty$ , then  $X_n$  converges *in probability* to  $X$ :

$$X_n \xrightarrow{P} X \Leftrightarrow \lim_{n \rightarrow \infty} \mathbb{P}(|X_n - X| > \epsilon) = 0$$

Expanding the definition, this means that:

$$\forall \epsilon > 0, \forall \delta > 0, \exists N(\epsilon, \delta) \text{ s.t. } \forall n \geq N, \mathbb{P}(|X_n - X| > \epsilon) < \delta$$

In other words, the probability of “a significant discordance” between values sampled from  $X_n$  and  $X$  vanishes as  $n \rightarrow \infty$ . Intuitively,  $X_n$  and  $X$  are *strongly related*, i.e. they not only distribute similarly, but also come from *similar processes*. For example, let  $X$  be the *true length* of a stick chosen *at random* from a population of sticks, and  $X_n$  be a measurement of that length made with an instrument that is more and more precise as  $n \rightarrow \infty$ . Then, for large  $n$ , it is clear that  $X_n$  will have a value that is really close to that of  $X$ . In this case, we say that  $X_n$  converges *in probability* to  $X$ , as  $n \rightarrow \infty$ .

3. **Almost sure convergence**. An even stronger limit requires that:

$$X_n \xrightarrow{\text{a.s.}} X \Leftrightarrow \mathbb{P}\left(\liminf_{n \rightarrow \infty} \{\omega \in \Omega : |X_n(\omega) - X(\omega)| < \epsilon\}\right) = 1 \quad \forall \epsilon > 0$$

Here, the  $\liminf$  of a sequence of sets  $A_n$  is defined as:

$$\liminf_{n \rightarrow \infty} A_n = \bigcup_{N=1}^{\infty} \bigcap_{n \geq N} A_n$$

A member of  $\liminf A_n$  is a member of *all* sets  $A_n$ , *except* a *finite* number of them (i.e. it's *definitively* a member of the  $A_n$ , as it is  $\in A_n$  for all  $n \geq \bar{n}$ ). So the term inside the parentheses is the set of all outcomes  $\omega \in \Omega$  for which  $X_n(\omega)$  is *definitively* close to  $X(\omega)$ , i.e. it *covers* all events resulting in a sequence of  $X_n$  that *converges* to  $X$ .

If we take  $X_n$  and  $X$  to be *real-valued* random variables, then the definition is simpler:

$$X_n \xrightarrow{\text{a.s.}} X \Leftrightarrow \mathbb{P}\left(\omega \in \Omega : \lim_{n \rightarrow \infty} X_n(\omega) = X(\omega)\right) = 1$$

Or, in other words:

$$\lim_{n \rightarrow \infty} X_n(\omega) = X(\omega) \quad \forall \omega \in \Omega \setminus A$$

where  $A \subset \Omega$  has 0 measure.

**Almost sure convergence vs probability convergence.** The difference between the two definitions is subtle, and can be somewhat seen from the following example, taken from <http://bit.ly/2u2E9Rk> and <http://bit.ly/2Zy66v0>.

Consider a sequence  $\{X_n\}$  of *independent* random variables with only two possible values, 0 and 1, such that:

$$\mathbb{P}(X_n = 1) = \frac{1}{n} \quad \mathbb{P}(X_n = 0) = 1 - \frac{1}{n}$$

For  $\epsilon > 0$ :

$$\mathbb{P}(|X_n| \geq \epsilon) = \begin{cases} \frac{1}{n} & 0 < \epsilon \leq 1 \\ 0 & \text{otherwise} \end{cases}$$

As  $n \rightarrow \infty$ ,  $\mathbb{P}(|X_n| \geq \epsilon) \rightarrow 0$ , and so  $X_n \xrightarrow[n \rightarrow \infty]{P} 0$ .

However,  $X_n$  **does not** converge almost surely to 0. Consider a *realization* of the sequence  $X_n$ , i.e. the measured outcomes of all  $X_n$  during “one run” of the experiment. This will be a binary sequence, like 000101001... Now, consider an *ensemble* of such sequences. What is the average number of ones in them? We can estimate it by summing the probability to have a 1 in the first place, in the second, and so on:

$$\sum_{n=1}^{\infty} \frac{1}{n} = +\infty$$

This in fact implies, by the second Borel Cantelli theorem<sup>a</sup>, that the probability of getting  $X_n = 1$  *infinitely often* (i.o.) is 1, and so  $X_n$  *cannot* converge *almost surely* to 0.

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<sup>a</sup>See a proof at <http://bit.ly/2tcfZU4> The main idea is that, given a set of *independent* events ( $X_n = 1$ ), the sum of their probabilities diverges, then *surely* an infinite number of them *do indeed occur*. Formally: if  $\sum_{n=1}^{+\infty} \mathbb{P}(X_n = 1) = \infty$ , then  $\mathbb{P}(\limsup_{n \rightarrow \infty} \{X_n = 1\}) = \mathbb{P}(\cap_{N=1}^{\infty} \cup_{n \geq N} \{X_n = 1\}) = \mathbb{P}(\{X_n = 1\} \text{ i.o.}) = 1$

It can be proven that *almost sure convergence* implies *convergence in probability*, which implies *convergence in distribution*. However, for our purposes we are interested in *another kind of convergence*:

- **$L^q$  convergence:**

$$X_n \xrightarrow[n \rightarrow \infty]{L^q} X \Leftrightarrow \lim_{n \rightarrow \infty} \langle |X_n - X|^q \rangle = 0 \quad q \in \mathbb{N}$$

Note that this implies *convergence in probability*. In fact:

$$\mathbb{P}(|X - X_n| > \epsilon) = \langle \mathbb{I}_{|X - X_n| > \epsilon} \rangle \leq \underbrace{\langle \mathbb{I}_{|X - X_n| > \epsilon} \rangle}_{0 \leq \odot \leq 1} \underbrace{\left| \frac{X - X_n}{\epsilon} \right|^q}_{\geq 1} \quad (1.102)$$

where is a *characteristic function*, i.e. the random variable that is 1 when  $|X - X_n| > \epsilon$  and 0 otherwise - so that the second term is always  $\geq 1$



when it is not killed by the first one. Then, by substituting  $\mathbb{I}$  with its *maximum* 1 we get a *greater* term:

$$(1.102) \leq \langle |X - X_n|^q \rangle \frac{1}{\epsilon^q} \xrightarrow{n \rightarrow \infty} 0 \quad \forall \epsilon > 0$$

where we used the linearity of the average to extract the constant  $\epsilon^q$ , and then the  $L^q$  convergence (assumed by hypothesis).

Also,  $L^q$  convergence implies the convergence (in the usual sense) of the  $q$ -th moment:

$$X_n \xrightarrow[n \rightarrow \infty]{L^q} X \Rightarrow \lim_{n \rightarrow \infty} \langle |X_n|^q \rangle = \langle |X|^q \rangle \quad (1.103)$$

If we choose  $q = 2$ , we obtain **mean square convergence**:

$$X_n \xrightarrow[n \rightarrow \infty]{\text{m.s.}} X \Leftrightarrow \lim_{n \rightarrow \infty} \langle |X_n - X|^2 \rangle = 0$$

In this case it is easy to prove (1.103) by using the Cauchy-Schwarz inequality:

$$(\mathbb{E}(XY))^2 \leq \mathbb{E}(X^2)\mathbb{E}(Y^2)$$

If we let  $X = X_n - X$  and  $Y = 1$ , and assume that  $X_n$  converges to  $X$  in mean square, we obtain:

$$0 \leq (\mathbb{E}(X_n - X))^2 \leq \mathbb{E}((X_n - X)^2)\mathbb{E}(1) \xrightarrow{n \rightarrow \infty} 0$$

And so:

$$\mathbb{E}(X_n - X) = \mathbb{E}(X_n) - \mathbb{E}(X) \xrightarrow{n \rightarrow \infty} 0 \Rightarrow \lim_{n \rightarrow \infty} \mathbb{E}(X_n) = \mathbb{E}(X) \quad \square$$

**Hölder inequality.** Cauchy inequality is, in this case, a special case of the more general Hölder inequality. Consider a measure space  $(S, \Sigma, \mu)$  (where  $S$  is the space,  $\Sigma$  a  $\sigma$ -algebra and  $\mu$  a measure), and two measurable functions  $f, g: S \rightarrow \mathbb{R}$ :

$$\|fg\|_1 \leq \|f\|_p \|g\|_p \quad \|\cdot\|_p = \left( \int_S |\cdot|^p d\mu \right)^{1/p}$$

To compute a stochastic integral, we will proceed like the following:

- Discretize the integral as a finite (Riemann) sum, obtaining a sequence of *finer* and *finer* random variables  $\{S_n\}_{n \in \mathbb{N}}$
- Use a *mean square* limit to compute the limit  $S$  of the sequence  $\{S_n\}$

### 1.20.2 Prescriptions

All that's left is to choose a *rule* for the mid-points in the terms of the discretized sum. As we will see in the following example, there are several different possibilities, each leading to *different results*.

**Example 6** (A simple stochastic integral):

Suppose  $G(\tau) = B(\tau)$ , and consider the following integral:

$$S = \int_0^t B(\tau) dB(\tau)$$

If  $B(\tau)$  were differentiable, then we could simply change variables and solve:

$$S = \int_0^t B(\tau) \frac{dB(\tau)}{d\tau} d\tau = \frac{1}{2} B^2(\tau) \Big|_0^t = \frac{B^2(t) - B^2(0)}{2} \quad \text{if } \exists \frac{dB}{d\tau}$$

However, here  $B(\tau)$  is a *rapidly varying irregular function*, which is nowhere differentiable.

So, following our plan, we first discretize:

$$S_n = \sum_{i=1}^n B(\tau_i) [B(t_i) - B(t_{i-1})] \quad t_0 \equiv 0; t_n \equiv t; t_{i-1} \leq \tau_i \leq t_i \quad (1.104)$$

We now need a rule for choosing the  $\tau_i$ . The simplest possibility is to fix them in the “same relative position” in every interval  $[t_{i-1}, t_i]$ , that is:

$$\tau_i = \lambda t_i + (1 - \lambda) t_{i-1} \quad \lambda \in [0, 1] \quad (1.105)$$

Depending on the value of  $\lambda$ , the limit  $S$  will be different. We can quickly check this *before* computing  $S$ , by focusing on the *expected values*. In fact, we know that if  $S_n \xrightarrow[n \rightarrow \infty]{\text{m.s.}} S$ , then  $\langle S_n \rangle \xrightarrow[n \rightarrow \infty]{} S$  in the usual sense. So, we compute the average of  $S_n$ :

$$\langle S_n \rangle = \sum_{i=1}^n \langle B(\tau_i) (B(t_i) - B(t_{i-1})) \rangle = \sum_{i=1}^n (\langle B(\tau_i) B(t_i) \rangle - \langle B(\tau_i) B(t_{i-1}) \rangle)$$

We already computed the correlator function for the Brownian noise  $B(t)$ :

$$\langle B(t) B(t') \rangle = \min(t, t') \quad (1.106)$$

And so, as  $t_{i-1} \leq \tau_i \leq t_i$ , we get:

$$\langle S_n \rangle = \sum_{i=1}^n (\tau_i - t_{i-1})$$

Substituting the choice for  $\tau$  (1.105):

$$\langle S_n \rangle = \lambda \sum_{i=1}^n (t_i - t_{i-1}) = \lambda t_n = \lambda t$$

Which does not depend on  $n$ , making the limit trivial:

$$\langle S \rangle = \lim_{n \rightarrow \infty} \langle S_n \rangle = \lambda t$$

This dependence on the **prescription** of  $\tau_i$  is an important difference from ordinary calculus, meaning that many common results cannot be directly translated to stochastic calculus.

In practice, there are many possibilities for  $\lambda$ . The two most common are:

$$\lambda = \begin{cases} 0 & \text{Ito's prescription} \\ \frac{1}{2} & \text{Stratonovich's prescription (also called middle-point prescription)} \end{cases}$$

Leading to, as we will see:

$$S_n \xrightarrow[n \rightarrow \infty]{\text{m.s.}} S = \begin{cases} \frac{B^2(t) - B^2(0)}{2} - \frac{t}{2} & \lambda = 0 \\ \frac{B^2(t) - B^2(0)}{2} & \lambda = 1/2 \end{cases}$$

The Stratonovich prescription gives exactly the same result as ordinary calculus. However, note that it involves a dependence *on the future*, i.e. the next step of a path depends on the point that is a *half-step* later. This has no a real physical meaning (in a certain sense, it “violates causality”). That’s why many physicists prefer the Ito’s prescription.

Let’s explicitly compute both results.

**Ito’s prescription.** We want to prove the following result:

$$\sum_{i=1}^n B(t_{i-1})(B(t_i) - B(t_{i-1})) \xrightarrow[n \rightarrow \infty]{\text{m.s.}} \frac{B^2(t) - B^2(0)}{2} - \frac{t}{2} \quad (1.107)$$

Denoting:

$$B(t_i) = B_i; \quad \Delta B_i = B_i - B_{i-1}$$

we can rewrite (1.104) as:

$$S_n = \sum_{i=1}^n B_{i-1} \Delta B_i$$

First of all, we *split* that product in a sum of terms, with the double-product trick:

$$ab = \frac{1}{2}[(a+b)^2 - a^2 - b^2]$$

So that:

$$\begin{aligned} S_n &= \sum_{i=1}^n B_{i-1} \Delta B_i = \frac{1}{2} \sum_{i=1}^n \left[ \underbrace{(B_{i-1} + \Delta B_i)^2}_{B_i^2} - B_{i-1}^2 - (\Delta B_i)^2 \right] = \\ &= \frac{1}{2} \sum_{i=1}^n \left[ B_i^2 - B_{i-1}^2 - (\Delta B_i)^2 \right] = \frac{1}{2} (B_n^2 - B_0^2) - \frac{1}{2} \sum_{i=1}^n (\Delta B_i)^2 = \\ &= \frac{1}{2} (B^2(t) - B^2(0)) - \frac{1}{2} \sum_{i=1}^n (\Delta B_i)^2 \end{aligned}$$

Now (1.107) becomes:

$$\frac{B^2(t) - B^2(0)}{2} - \frac{1}{2} \sum_{i=1}^n (\Delta B_i)^2 \xrightarrow[n \rightarrow \infty]{\text{m.s.}} \frac{B^2(t) - B(0)}{2} - \frac{t}{2} \quad t_n = t; t_0 = 0$$

Applying the definition of *mean square limit*, this is equivalent to showing that:

$$\left\langle \left| \frac{B^2(t) - B^2(\theta)}{2} - \frac{1}{2} \sum_{i=1}^n (\Delta B_i)^2 - \left[ \frac{B^2(t) - B^2(\theta)}{2} - \frac{t}{2} \right] \right|^2 \right\rangle \xrightarrow[n \rightarrow \infty]{?} 0 \quad (1.108)$$

Expanding:

$$\begin{aligned} \frac{1}{4} \left\langle \left[ -\sum_{i=1}^n (\Delta B_i)^2 + t \right]^2 \right\rangle &= \frac{1}{4} \left\langle \left[ t - \sum_{i=1}^n (\Delta B_i)^2 \right]^2 \right\rangle \stackrel{(a)}{=} \frac{1}{4} \left\langle \left[ \sum_{i=1}^n (\Delta t_i - (\Delta B_i)^2) \right]^2 \right\rangle = \\ &\stackrel{(b)}{=} \frac{1}{4} \sum_{i,j=1}^n \langle [\Delta t_i - (\Delta B_i)^2][\Delta t_j - (\Delta B_j)^2] \rangle \end{aligned} \quad (1.109)$$

where in (a) we used  $t = \sum_{i=1}^n \Delta t_i$ , and in (b)  $(\sum_i a_i)^2 = \sum_{ij} a_i a_j$ . We can rewrite the sum highlighting the case where  $i = j$ :

$$(1.109) = \frac{1}{4} \left[ \sum_{i=1}^n \langle [\Delta t_i - (\Delta B_i)^2]^2 \rangle + \sum_{i \neq j} \langle [\Delta t_i - (\Delta B_i)^2][\Delta t_j - (\Delta B_j)^2] \rangle \right] \quad (1.110)$$

Noting that the  $\Delta B_i$  come from *independent gaussians*, we have that the expected values integrals factorize:

$$\langle A \rangle = \int d\Delta B_1 \dots d\Delta B_n A \prod_{i=1}^n \frac{1}{\sqrt{2\pi\Delta t_i}} \exp \left( -\frac{(\Delta B_i)^2}{2\Delta t_i} \right)$$

In other words, this means that the average of the product is just the product of the averages:

$$\begin{aligned} \langle (\Delta t_i - (\Delta B_i)^2)(\Delta t_j - (\Delta B_j)^2) \rangle &= \langle (\Delta t_i - (\Delta B_i)^2) \rangle \langle (\Delta t_j - (\Delta B_j)^2) \rangle = \\ &= [\Delta t_i - \langle (\Delta B_i)^2 \rangle][\Delta t_j - \langle (\Delta B_j)^2 \rangle] \end{aligned}$$

We already computed the second moment of that gaussian:

$$\langle (\Delta B_i)^2 \rangle = \int \frac{d\Delta B_i}{\sqrt{2\pi\Delta t_i}} \Delta B_i^2 \exp \left( -\frac{\Delta B_i^2}{2\Delta t_i} \right) = \Delta t_i$$

and so:

$$\langle (\Delta t_i - (\Delta B_i)^2) \rangle = 0$$

So we are left only with the first term of (1.110):

$$(1.110) = \frac{1}{4} \sum_{i=1}^n \langle [\Delta t_i - (\Delta B_i)^2]^2 \rangle = \frac{1}{4} \sum_{i=1}^n \left[ \Delta t_i^2 - 2\Delta t_i \underbrace{\langle (\Delta B_i)^2 \rangle}_{\Delta t_i} + \langle \Delta B_i^4 \rangle \right] \quad (1.111)$$

Recall that, for a random variable  $x$  sampled from a gaussian  $\mathcal{N}(0, \sigma)$ :

$$\langle x^{2n} \rangle = \sigma^{2n} \frac{(2n)!}{2^n n!} = \begin{cases} \sigma^2 & n = 1 \\ \sigma^4 \frac{4!}{4 \cdot 2!} = 3\sigma^4 & n = 2 \end{cases}$$

In our case, this means that  $\langle (\Delta B_i)^4 \rangle = \Delta t_i^2$ , leading to:

$$(1.111) = \frac{1}{2} \sum_{i=1}^n \Delta t_i^2$$

When taking the limit of the mesh ( $n \rightarrow \infty$ ), the number of summed terms become infinite, but also the size of each of them vanishes:

$$\max_i \Delta t_i \xrightarrow{n \rightarrow \infty} 0$$

To resolve that limit we need to use the fact that the end-point is fixed ( $t_n \equiv t$ ) and so:

$$\frac{1}{2} \sum_{i=1}^n \Delta t_i^2 \leq \frac{1}{2} \left( \sum_{i=1}^n \Delta t_i \right)^2 = \frac{1}{2} \left( \sum_{i=1}^n \Delta t_i \right) \underbrace{\left( \sum_{j=1}^n \Delta t_j \right)}_t \leq \frac{t}{2} \left( \max_i \Delta t_i \right) \xrightarrow{n \rightarrow \infty} 0$$

This proves (1.108), and so the desired result (1.107).

**Stratonovich's prescription.** In this case, we want to show that:

$$S_n = \sum_{i=1}^n B\left(\frac{t_i + t_{i-1}}{2}\right) [B(t_i) - B(t_{i-1})] \xrightarrow[n \rightarrow \infty]{\text{m.s.}} \frac{B^2(t) - B^2(0)}{2}$$

Note that now we need a set of *middle points* in the mesh, which leads to some complications.

One trick is to simply *double* the “resolution” of the discretization, and choose the *middle points* to be the *odd* indices. We then define:

$$S'_{2n} = \sum_{i=1}^{2n} B_{2i-1} (B_{2i} - B_{2(i-1)})$$

with  $t_{2i-1} \equiv (t_{2i} + t_{2(i-1)})/2$ , while the  $t_{2i}$  may be distributed arbitrarily. The full computation is very long and tedious, and not much enlightening, and is therefore omitted.

A shorter way to compute that, but not as rigorous, is by stating that:

$$S_n = \sum_{i=1}^n \frac{B(t_i) + B(t_{i-1})}{2} (B(t_i) - B(t_{i-1}))$$

However it is not obvious that is possible to *approximate* a midpoint of  $B$  with an average, as  $B(t_i)$  are all random variables. In fact, it is possible to show that the two expressions *have the same distribution*, but they are *not the same random variable*! In any way, if we do this, the thesis immediately follows:

$$= \frac{1}{2} \sum_{i=1}^n (B^2(t_i) - B^2(t_{i-1}))$$

### 1.20.3 Ito's calculus

In our calculations, we will be usually concerned with the following kinds of stochastic integrals  $G(t)$ :

1.  $\int_0^t F(B(\tau)) dB(\tau)$
2.  $\int_0^t g(\tau) dB(\tau)$
3.  $\int_0^t g(\tau) d\tau$  (usual integrals)

These  $G(t)$  are called **non-anticipating functions**, because they are independent of  $B(t') - B(t)$  for  $t' > t$ , meaning that they do not depend on what happens in the Brownian motion at times later than  $t$  (i.e. they do not depend on the future). So, by using Ito's prescription (I.p.) in the discretization and *mean square* (m.s.) for the continuum limit we get:

$$\int_0^t F(B(\tau)) dB(\tau) \stackrel{\text{I.p.}}{\underset{\text{m.s.}}{=}} \sum_{i=1}^n F(B_{i-1}) \Delta B_i$$

Note how  $F(B_{i-1})$  and  $\Delta B_i$  are independent of each other, simplifying the calculations. (Note that the Stratonovich prescription here causes *troubles* during evaluation, as it introduces some interdependence between different terms).

## 1.21 Stochastic Differential Calculus

### 1.21.1 Ito's rules of integration

We now consider a more general stochastic integral, and show that, using Ito's prescription:

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$$\begin{aligned} \int_0^t H(B(\tau), \tau) (dB(\tau))^k &\stackrel{\text{I.p.}}{\underset{\text{m.s.}}{=}} \sum_{i=1}^n H(B_{i-1}, \tau_{i-1}) (\Delta B_i)^k = \\ &= \begin{cases} \int_0^t H(B, \tau) dB(\tau) & k = 1 \\ \int_0^t H(B(\tau), \tau) d\tau & k = 2 \\ 0 & k > 2 \end{cases} \end{aligned}$$

This leads to the following “rules” for *Ito integrals*:

$$(dB)^n = \begin{cases} dB & n = 1 \\ dt & n = 2 \\ 0 & n > 2 \end{cases} \quad (1.112)$$

We already showed an example for  $k = 1$ , and we now proceed with the other two cases.

**Example 7** (Integral in  $dB^2$ ):

Consider a *non-anticipating* function  $G(\tau)$ , and the following stochastic integral:

$$I = \int_0^t G(\tau)(dB(\tau))^2$$

With *non-anticipating* we mean that  $G(\tau)$  does not depend on  $B(s) - B(\tau) \forall s > \tau$ , i.e. it does not depend on the *future*. Discretizing:

$$I = \lim_{n \rightarrow \infty}^{\text{m.s.}} I_n = \lim_{n \rightarrow \infty}^{\text{m.s.}} \sum_{i=1}^n G(t_{i-1}) \Delta B_i^2$$

For simplicity, denote:

$$G_i \equiv G_i \quad \Delta B_i \equiv B_i - B_{i-1} \quad \Delta t_i = t_i - t_{i-1}$$

We want to prove that:

$$\int_0^t G(\tau)(dB(\tau))^2 \stackrel{?}{=} \int_0^t G(\tau) d\tau = \lim_{n \rightarrow \infty} \sum_{i=1}^n G_{i-1} \Delta t_i$$

Applying the definition of a *mean square* limit, this is equivalent to:

$$\left\langle \left( \sum_{i=1}^n G_{i-1} \Delta B_i^2 - \sum_{i=1}^n G_{i-1} \Delta t_i \right)^2 \right\rangle \xrightarrow[n \rightarrow \infty]{?} 0$$

Expanding the square as a product of two sums over  $i$  and  $j$ , and then highlighting the case with  $i = j$ :

$$\begin{aligned} \left\langle \left[ \sum_{i=1}^n G_{i-1} [(\Delta B_i)^2 - \Delta t_i] \right]^2 \right\rangle &= \sum_{i,j=1}^n \langle G_{i-1} [(\Delta B_i)^2 - \Delta t_i] G_{j-1} [(\Delta B_j)^2 - \Delta t_j] \rangle = \\ &= \sum_{i=1}^n \langle G_{i-1}^2 [(\Delta B_i)^2 - \Delta t_i]^2 \rangle + 2 \sum_{i < j} \langle \underbrace{G_{i-1} [(\Delta B_i)^2 - \Delta t_i]}_{\text{yellow}} \underbrace{G_{j-1} [(\Delta B_j)^2 - \Delta t_j]}_{\text{blue}} \rangle \end{aligned} \quad (1.113)$$

As  $i < j$ , note that the yellow term *does not depend* on  $\Delta B_j = B_j - B_{j-1} = B(t_j) - B(t_{j-1})$ . In fact, as  $G$  is *non-anticipating*,  $G_{j-1}$  depends only on the previous steps. Thus, the yellow and blue terms are *independent* of each other, and so we can factorize the average:

$$(1.113) = \sum_{i=1}^n \langle G_{i-1}^2 [(\Delta B_i)^2 - \Delta t_i]^2 \rangle + 2 \sum_{i < j} \langle \underbrace{G_{i-1} [(\Delta B_i)^2 - \Delta t_i]}_{\text{yellow}} \rangle \langle \underbrace{G_{j-1} [(\Delta B_j)^2 - \Delta t_j]}_{\text{blue}} \rangle$$

Recall that:

$$\langle (\Delta B_j)^2 - \Delta t_j \rangle = \langle (\Delta B_j)^2 \rangle - \Delta t_j = 0$$

and so only the first term of (1.113) remains. Again, noting that  $G_{i-1}$  does not depend on  $\Delta B_i$ , as it is *non-anticipating*, can factorize the average:

$$(1.113) = \left\langle \sum_{i=1}^n G_{i-1}^2 [(\Delta B_i)^2 - \Delta t_i]^2 \right\rangle = \sum_{i=1}^n \underbrace{\langle G_{i-1}^2 \rangle}_{G_{i-1}^2} \langle [(\Delta B_i)^2 - \Delta t_i]^2 \rangle \quad (1.114)$$

Expanding the stochastic term:

$$\begin{aligned}\langle [(\Delta B_i)^2 - \Delta t_i]^2 \rangle &= \langle (\Delta B_i)^4 - 2\Delta t_i(\Delta B_i)^2 \rangle + \Delta t_i^2 = \\ &= \underbrace{\langle (\Delta B_i)^4 \rangle}_{3(\Delta t_i)^2} - 2\Delta t_i \underbrace{\langle (\Delta B_i)^2 \rangle}_{\Delta t_i} + \Delta t_i^2 = 2\Delta t_i^2\end{aligned}$$

And substituting back into the sum and taking the limit completes the proof:

$$(1.114) = 2 \sum_{i=1}^n G_{i-1}^2 \Delta t_i^2 \leq 2 \left( \max_{i \leq j \leq n} \Delta t_j \right) \sum_{i=1}^n G_{i-1}^2 \Delta t_i \xrightarrow{n \rightarrow \infty} 2 \cdot 0 \cdot \int_0^t G^2(\tau) d\tau = 0$$

This proves that  $(dB)^2 = dt$ .

**Example 8** (The case with  $n > 2$ ):

We want now to show that:

$$\int_0^t G(\tau) (dB(\tau))^n = \lim_{n \rightarrow \infty} \sum_{i=1}^n G_{i-1} (\Delta B_i)^n = 0$$

By definition, we want to show that:

$$\left\langle \left( \sum_{i=1}^n G_{i-1} (\Delta B_i)^n \right)^2 \right\rangle \xrightarrow{n \rightarrow \infty} 0$$

Expanding the square, and factorizing the averages (as  $G$  is *non-anticipating*) leads to:

$$\begin{aligned}\left\langle \left( \sum_{i=1}^n G_{i-1} (\Delta B_i)^n \right)^2 \right\rangle &= \sum_{i=1}^n \langle G_{i-1}^2 (\Delta B_i)^{2n} \rangle + 2 \sum_{i < j} \langle G_{i-1} G_{j-1} (\Delta B_i)^n (\Delta B_j)^n \rangle = \\ &= \sum_{i=1}^n G_{i-1}^2 \langle (\Delta B_i)^{2n} \rangle + 2 \sum_{i < j} \langle G_{i-1} G_{j-1} (\Delta B_i)^n \rangle \langle (\Delta B_j)^n \rangle\end{aligned}\tag{1.115}$$

Now, recall that the  $p$ -th central moment of  $X \sim \mathcal{N}(\mu, \sigma)$  can be computed with Isserlis theorem, resulting in:

$$\mathbb{E}[(X - \mu)^p] = \begin{cases} 0 & p \text{ is odd} \\ \sigma^p (p-1)!! & p \text{ is even} \end{cases}$$

where  $p!! = p \cdot (p-2) \cdot \dots \cdot 1$  is a *double factorial*, that can be rewritten in terms of factorials as follows:

$$p!! = \begin{cases} 2^k k! & p = 2k \text{ even} \\ \frac{(2k)!}{2^k k!} & p = 2k-1 \text{ odd} \end{cases}\tag{1.116}$$



So, if  **$n$  is odd**, the blue term in (1.115) vanishes. Let's suppose, for simplicity, that  $G$  is bounded, i.e.  $|G(\tau)| < K \forall \tau \in \mathbb{R}$ . Then:

$$(1.115) = \sum_{i=1}^n G_{i-1}^2 (\Delta t_i)^n \textcolor{blue}{(2n-1)!!} = \sum_{i=1}^n G_{i-1}^2 (\Delta t_i)^n \frac{(2n)!}{2^n n!} \leq \frac{K^2 (2n)!}{2^n n!} \sum_{i=1}^n (\Delta t_i)^n$$

$$\leq \frac{K^2 (2n)!}{2^n n!} \left( \max_{i \leq j \leq n} (\Delta t)^{n-1} \right) \underbrace{\sum_{i=1}^n \Delta t_i}_t \xrightarrow{n \rightarrow \infty} 0$$

On the other hand, if  **$n$  is even**, the blue term in (1.115) is not null. However, the same argument for  $n$  odd can be applied to the first term, which vanishes in the limit. So we only need to study the blue term:

$$(1.115) = 2 \sum_{i < j} \underbrace{G_{i-1} G_{j-1}}_{\leq K^2} (\Delta B_i)^n \langle (\Delta B_j)^n \rangle \quad (1.117)$$

Here, as  $n$  is even:

$$\langle (\Delta B_i)^n \rangle = (\Delta t_i)^{n/2} (n-1)!! = (\Delta t_i)^{n/2} \left( \textcolor{red}{2}^{\frac{n}{2}} - 1 \right)!! \stackrel{(1.116)}{=} (\Delta t_i)^{n/2} \frac{n!}{2^{n/2} (n/2)!}$$

And so:

$$(1.117) \leq 2K^2 \left( \frac{n!}{2^{n/2} (n/2)!} \right)^2 \sum_{i < j}^n \Delta t_i^{n/2} \Delta t_j^{n/2}$$

$$\leq 2K^2 \left( \frac{n!}{2^{n/2} (n/2)!} \right)^2 \left( \max_{i \leq l \leq n} \Delta t_l \right)^{2(n/2-1)} \underbrace{\sum_{i < j}^n \Delta t_i \Delta t_j}_{\leq t^2} \xrightarrow{n \rightarrow \infty} 0 \quad \square$$

#### Example 9 (Other cases):

Ito's rules allow us to consider even more general integrals. For example:

$$\int_0^t G(\tau) dB(\tau) d\tau = 0$$

In fact, as  $(dB)^2 = d\tau$ ,  $dB d\tau = 0$  because  $(dB)^n = 0 \forall n > 2$ .

#### Example 10 (Integration of polynomials):

By using Ito's rules we can find a formula for integrating *powers* of the Brownian motion:

$$\int_0^t (B(\tau))^n dB(\tau)$$

We first differentiate a polynomial, and then recover the rule for integration by performing the inverse operation.

Recall that, in general, a differential is *the increment* of a function after a small *nudge* of its argument:

$$df(t) = f(t + dt) - f(t)$$

The same holds in the stochastic case. In particular:

$$\begin{aligned} d(B(t))^n &= [B(t + dt)]^n - (B(t))^n = [B(t) + dB(t)]^n - (B(t))^n = \\ &\stackrel{(a)}{=} \sum_{k=0}^n \binom{n}{k} (dB(t))^k (B(t))^{n-k} - (B(t))^n = \\ &= \cancel{(B(t))^n} + \sum_{k=1}^n \binom{n}{k} (dB(t))^k (B(t))^{n-k} - \cancel{(B(t))^n} = \\ &\stackrel{(b)}{=} \underbrace{n(dB(t))(B(t))^{n-1}}_{k=1} + \underbrace{\frac{n(n-1)}{2} \overbrace{(dB(t))^2}^{dt} (B(t))^{n-2}}_{k=2} + \underbrace{0}_{k>2} \end{aligned}$$

where in (a) we used Newton's binomial formula, and in (b) the previously found Ito's rules for integration (1.112). Letting  $m = n - 1$  and isolating  $dB(t)$  leads to:

$$(m+1)(B(t))^m dB(t) = (dB(t))^{m+1} - \frac{m(m+1)}{2} (B(t))^{m-1} dt$$

Finally, dividing by  $m+1$  and integrating leads to the desired formula:

$$\begin{aligned} \int_0^\tau (B(t))^m dB(t) &= \frac{1}{m+1} \int_0^\tau d(B(t))^{m+1} - \frac{m}{2} \int_0^\tau (B(t))^{m-1} dt = \\ &= \frac{1}{m+1} (B(t))^{m+1} \Big|_0^\tau - \frac{m}{2} \int_0^\tau (B(t))^{m-1} dt = \\ &= \frac{(B(\tau))^{m+1} - (B(0))^{m+1}}{m+1} - \frac{m}{2} \int_0^\tau (B(t))^{m-1} dt \end{aligned}$$

And in the case  $m = 1$  we retrieve the previously obtained result:

$$\int_0^\tau B(t) dB(t) = \frac{B^2(\tau) - B^2(0)}{2} - \frac{\tau}{2}$$

**Example 11** (General differentiation rule):

Because  $(dB)^2 = dt$ , when computing differentials from a Taylor expansion up to  $O(dt^2)$  one must compute even the terms of order  $dB^2$ . For example,

consider a generic function  $f(B(t), t)$ :

$$\begin{aligned} df(B(t), t) &= \frac{\partial f}{\partial t} dt + \frac{\partial f}{\partial B} dB(t) + \underbrace{\frac{1}{2} \frac{\partial^2 f}{\partial t^2}}_{O([dt]^2)} + \frac{1}{2} \frac{\partial^2 f}{\partial B^2} \underbrace{[dB(t)]^2}_{dt} + \\ &\quad + \frac{\partial^2 f}{\partial B(t) \partial t} \underbrace{dt dB(t)}_0 + O([dt]^2) = \\ &= \frac{\partial f}{\partial t} dt + \frac{\partial f}{\partial B} dB(t) + \frac{1}{2} \frac{\partial^2 f}{\partial B^2} dt + O([dt]^2) \end{aligned}$$

## 1.22 Derivation of the Fokker-Planck equation

Starting from the Master Equation and taking the continuum limit we arrived at the Fokker-Planck equation:

$$\dot{W}(x, t) = -\frac{\partial}{\partial x} \left[ f(x, t) W(x, t) - \frac{\partial}{\partial x} W(x, t) D(x, t) \right] \quad (1.118)$$

At the same time, if we consider the dynamics of a *single path*, adding a *stochastic term* to the second law of motion, we arrive at the Langevin equation (in the overdamped limit):

$$dx(t) = f(x(t), t) dt + \sqrt{2D(x(t), t)} dB(t) \quad (1.119)$$

We want now to show that these two formulations are equivalent, by deriving (1.118) from (1.119). The main idea is to introduce a *test function*  $h(x(t))$ , and compute its expected value at the instant  $t$  over *all possible points* that can be reached by the trajectory  $x(t)$ , thus obtaining a value that will depend on the *global* probability distribution  $W(x, t)$ . Then, we can use Langevin equation to describe the dynamics of each *single path*. In this way, we will obtain a relation between a quantity involving  $W(x, t)$  and the parameters  $f(x, t)$  and  $D(x, t)$  appearing in (1.119), which will hopefully be (1.118).

So, let's start by computing the average of  $h(x(t))$  at a fixed time:

$$\langle h(x(t)) \rangle = \int_{\mathbb{R}} dx W(x, t) h(x)$$

As we seek to construct a *time derivative*, we start by differentiating:

$$d\langle h(x(t)) \rangle = \left( \frac{\partial}{\partial t} \int_{\mathbb{R}} dx W(x, t) h(x) \right) dt = dt \int_{\mathbb{R}} dx \dot{W}(x, t) h(x) \quad (1.120)$$

And then dividing by  $dt$  leads to:

$$\frac{d}{dt} \langle h(x(t)) \rangle = \int_{\mathbb{R}} dx \dot{W}(x, t) h(x) \quad (1.121)$$

However, we could also start by differentiating  $h(x(t))$ :

$$dh(x(t)) = h(x(t) + dx(t)) - h(x(t)) = \quad (1.122)$$

$$\stackrel{(a)}{=} h'(x(t)) dx(t) + \frac{1}{2} h''(x(t)) [dx(t)]^2 + O([dx(t)]^2) \quad (1.123)$$

where in (a) we used a Taylor expansion for the first term. From (1.119), and applying Ito's rules, we can obtain explicit expressions for the  $[dx(t)]^n$ :

$$\begin{aligned} [dx(t)]^2 &= f^2 [dt]^2 + 2D \overbrace{[dB(t)]^2}^{dt} + f\sqrt{2D} \overbrace{dB(t) dt}^0 \\ [dx(t)]^3 &= O([dt]^2) \end{aligned}$$

And substituting in (1.123) leads to:

$$\begin{aligned} dh(x(t)) &= h'[f dt + \sqrt{2D} dB] + \frac{1}{2} h'' 2D dt + O([dt]^2) = \\ &= dt [h' f + h'' D] + h' \sqrt{2D} dB \end{aligned}$$

Taking the expected value:

$$\begin{aligned} d\langle h(x(t)) \rangle &= \langle dt [h' f + h'' D] \rangle + \langle h' \sqrt{2D} dB \rangle = \\ &\stackrel{(a)}{=} \langle dt [h' f + h'' D] \rangle + \underbrace{\langle \sqrt{2D} h' \rangle \langle dB \rangle}_0 = \\ &= \langle dt [h' f + h'' D] \rangle \end{aligned}$$

where in (a) we used the fact that  $D(x(t), t)$  is *non-anticipating*, allowing to factor the average.

Dividing by  $dt$  and expanding the average leads to:

$$\begin{aligned} \frac{d}{dt} \langle h(x(t)) \rangle &= \int_{\mathbb{R}} dx W(x, t) [h'(x) f(x, t) + h''(x) D(x, t)] = \\ &= \int_{\mathbb{R}} dx W(x, t) f(x, t) h'(x) + \int_{\mathbb{R}} dx W(x, t) D(x, t) h''(x) = \\ &\stackrel{(a)}{=} \cancel{W h f \Big|_{-\infty}^{+\infty}} - \int_{\mathbb{R}} dx h \frac{\partial}{\partial x} (W f) + \\ &\quad + \cancel{W D h' \Big|_{-\infty}^{+\infty}} - \cancel{h \frac{\partial}{\partial x} (D W) \Big|_{-\infty}^{+\infty}} + \int_{\mathbb{R}} dx h \frac{\partial^2}{\partial x^2} (W D) = \\ &= \int_{\mathbb{R}} dx h(x) \left[ \frac{\partial^2}{\partial x^2} (W(x, t) D(x, t)) - \frac{\partial}{\partial x} (W(x, t) f(x, t)) \right] \end{aligned} \quad (1.124)$$

where in (a) we integrated by parts the first integral once, and the second one twice.

Finally, equating (1.121) and (1.124) leads to:

$$\frac{d}{dt} \langle h(x(t)) \rangle = \int_{\mathbb{R}} dx \frac{\partial}{\partial t} W(x, t) h(x) = \int_{\mathbb{R}} dx h(x) \left[ \frac{\partial^2}{\partial x^2} (W(x, t) D(x, t)) - \frac{\partial}{\partial x} (W(x, t) f(x, t)) \right]$$

As this relation holds for *any* test function  $h(x)$ , it means that the *integrands* are equal. So, by collecting a derivative, we retrieve the the Fokker-Planck equation (1.118):

$$\frac{\partial}{\partial t} W(x, t) = -\frac{\partial}{\partial x} \left[ f(x, t) W(x, t) - \frac{\partial}{\partial x} (W(x, t) D(x, t)) \right]$$

## 1.23 The role of temperature

From physical observations, we expect the amplitude of stochastic oscillations in Brownian motion to be dependent on temperature - as it is a direct effect of collisions with molecules in thermal equilibrium. So, we want to derive an explicit relation between the diffusion parameter  $D$  and  $T$ .

We start by assuming that, for  $t \rightarrow \infty$ , the particle will be *at equilibrium*, meaning that its distribution will be given by the Maxwell-Boltzmann:

$$W(x, t) \xrightarrow{t \rightarrow \infty} P_{\text{eq}}(x) = \frac{e^{-\beta V(x)}}{Z} \quad Z = \int_{\mathbb{R}} dx e^{-\beta V(x)}; \quad \beta = \frac{1}{k_B T}$$

Recall the Fokker-Planck equation:

$$\frac{\partial}{\partial t} W(x, t) = -\frac{\partial}{\partial x} \left[ f(x, t) W(x, t) - \frac{\partial}{\partial x} (D(x, t) W(x, t)) \right]$$

From the Langevin equivalence, and some physical reasoning, we found that:

$$f(x, t) = \frac{F_{\text{ext}}}{\gamma} = -\frac{1}{\gamma} \frac{\partial V(x)}{\partial x} \quad \gamma = 6\pi\eta a$$

Where  $F_{\text{ext}}$  is an external conservative force with potential  $V(x)$  acting on the Brownian particle, assumed to be a sphere of radius  $a$  moving through a medium of viscosity  $\eta$ . Assuming  $D(x, t) \equiv D$  for simplicity, the Fokker-Planck equation becomes:

$$\frac{\partial W^*}{\partial t} = \frac{\partial}{\partial x} \left[ \frac{W^*}{\gamma} \frac{\partial V}{\partial x} + D \frac{\partial W^*}{\partial x} \right]$$

Here we are interested in the *particular solution*  $W^*(x)$  that will be reached at the equilibrium, as it *does not* depend on time. So:

$$\frac{\partial W^*}{\partial t} \stackrel{!}{=} 0$$

Meaning that:

$$\left[ \frac{W^*(x)}{\gamma} \frac{\partial V}{\partial x} + D \frac{\partial W^*}{\partial x} \right] = \text{constant} \quad \forall x \quad (1.125)$$

As this relation holds for *any*  $x$ , we can examine it in the limit  $x \rightarrow \infty$  to find the value of the constant. In fact, as  $W^*(x)$  is a normalized pdf, we expect:

$$W^*, \frac{\partial W^*}{\partial x} \xrightarrow{x \rightarrow \infty} 0$$

And so the constant in (1.125) must be 0, leading to:

$$\frac{\partial W^*}{\partial x} = -\frac{1}{\gamma D} W^* \frac{\partial V}{\partial x} \Rightarrow \frac{1}{W^*} \frac{\partial W^*}{\partial x} = \ln(W^*) = -\frac{1}{\gamma D} \frac{\partial V}{\partial x}$$

Integrating, we find:

$$\ln W^*(x) = -\frac{1}{\gamma D} V(x) + c \Rightarrow W^*(x) = K \exp\left(-\frac{1}{\gamma D} V(x)\right) \stackrel{!}{=} \frac{1}{Z} \exp(-\beta V(x))$$

And by comparing the two functions we obtain the desired relation:

$$\beta = \frac{1}{\gamma D} = \frac{1}{k_B T} \Rightarrow D = \frac{k_B T}{\gamma} = \frac{k_B T}{6\pi\eta a}$$

This is indeed the same relation that Einstein found when examining Brownian motion (*fluctuation-dissipation relationship*, 1905). As  $D(x, t) \propto T$ , the amplitude of stochastic oscillations (from Langevin equation) is proportional  $\sqrt{2D} \propto \sqrt{T}$ .

## 1.24 Harmonic overdamped oscillator

(Lesson 9 of  
14/11/19)  
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Using the framework developed in the previous sections, we now tackle a more general setting, that of a particle moving in a *harmonic potential* and subject to thermal noise. This will be useful to model the local behaviour about the minima of *any* potential - as they are approximately harmonic.

So, consider a particle of mass  $m$  moving in one dimension through a *viscous* medium and immersed in a *harmonic* potential. To model the random collisions with the other (much smaller) particles in the fluid we add a *stochastic term*  $\sqrt{2D}\gamma\xi$ . The equation of motion becomes:

$$m\ddot{x} = -\gamma\dot{x} - m\omega^2 x + \sqrt{2D}\gamma\xi \quad (1.126)$$

As  $m/\gamma$  is much smaller than the timescale we are interested in, we can neglect it, reaching the *overdamped limit*:

$$\dot{x} = -\underbrace{\frac{m\omega^2}{\gamma}}_k x + \sqrt{2D}\xi$$

And multiplying by  $dt$ :

$$dx(t) = -kx(t) dt + \sqrt{2D} dB(t) \quad (1.127)$$

As usual, we introduce a time discretization  $\{t_j\}_{j=1,\dots,n}$ . Letting:

$$x(t_i) \equiv x_i; \quad \Delta x_i \equiv x_i - x_{i-1}; \quad B(t_i) \equiv B_i; \quad \Delta t_i = t_i - t_{i-1}$$

we arrive to:

$$\Delta x_i = -kx_{i-1}\Delta t_i + \sqrt{2D}\Delta B_i \quad (1.128)$$

Note that we evaluated the potential term  $-kx(\tau)$  at the *left extremum* of the discretized interval  $[t_{i-1}, t_i]$ , following Ito's prescription.

To solve (1.127) the plan will be the following:

1. Use the discretization to find the *infinitesimal probability*  $\mathbb{P}(\{\Delta x_i\}_{i=1,\dots,n})$  of a *discretized path*, i.e. of a path traversing all *gates*  $[x_i, x_i + dx_i]$  at successive instants  $0 \equiv t_1 < \dots < t_n \equiv t$ .
2. Find the probability for a continuous path  $dP \equiv \mathbb{P}(\{x(\tau)_{\tau \in [0,t]}\})$  by taking the limit  $n \rightarrow \infty$ .

3. Find the transition probabilities that solve (1.127) by using a *path integral* to evaluate:

$$W(x_t, t; x_0, 0) = \langle \delta(x_t - x(\tau)) \rangle_W \equiv \int_{\mathbb{R}^T} \delta(x_t - x(\tau)) dP$$

In other words, this is the *fraction* of paths (from the set  $\mathbb{R}^T$  of all continuous paths happening in the timeframe  $[0, t]$ ) that start in  $x_0$  at instant 0, and reach  $x_t$  at instant  $t$ .

To find  $\mathbb{P}(\{\Delta x_i\}_{i=1, \dots, n})$  we start from the joint pdf  $\mathbb{P}(\{\Delta B_i\}_{i=1, \dots, n})$  that we already know, and perform a change of random variables according to (1.128). In practice, start from:

$$\mathbb{P}(\Delta B_1, \dots, \Delta B_n) = \prod_{i=1}^n \frac{d\Delta B_i}{\sqrt{2\pi\Delta t_i}} \exp\left(-\sum_{i=1}^n \frac{\Delta B_i^2}{2\Delta t_i}\right)$$

Then insert  $\Delta B_i$  in terms of  $\Delta x_i$  from (1.128):

$$\Delta B_i = \frac{\Delta x_i + kx_{i-1}\Delta t_i}{\sqrt{2D}}$$

and then multiply by the determinant  $J$  of the jacobian of the change of variables to find the desired new pdf:

$$\begin{aligned} \mathbb{P}(x_1, x_2, \dots, x_n) &= \mathbb{P}(\Delta x_1) \mathbb{P}(\Delta x_2 | \Delta x_1) \mathbb{P}(\Delta x_3 | \Delta x_1, \Delta x_2) \cdots = \\ &= \prod_{i=1}^n \frac{d\Delta x_i}{\sqrt{2\pi\Delta t_i}} \exp\left(-\sum_{i=1}^n \frac{1}{2\Delta t_i} \left(\frac{\Delta x_i + kx_{i-1}\Delta t_i}{\sqrt{2D}}\right)^2\right) J \\ J &= \det \left| \frac{\partial(\Delta B_1, \dots, \Delta B_n)}{\partial(\Delta x_1, \dots, \Delta x_n)} \right| = \det \left| \frac{\partial(\Delta x_1, \dots, \Delta x_n)}{\partial(\Delta B_1, \dots, \Delta B_n)} \right|^{-1} = \begin{vmatrix} \sqrt{2D} & 0 & \cdots & 0 \\ 0 & \sqrt{2D} & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & \sqrt{2D} \end{vmatrix}_{n \times n}^{-1} = (2D)^{-n/2} \end{aligned}$$

And so:

$$\mathbb{P}(\Delta x_1, \dots, \Delta x_n) = \prod_{i=1}^n \left( \frac{d\Delta x_i}{\sqrt{4\pi D \Delta t_i}} \right) \exp\left(-\sum_{i=1}^n \frac{1}{2\Delta t_i} \left(\frac{\Delta x_i + kx_{i-1}\Delta t_i}{\sqrt{2D}}\right)^2\right) \quad (1.129)$$

Taking the limit  $n \rightarrow \infty$ :

$$dP \equiv \mathbb{P}(x(\tau)) = \left( \prod_{\tau=0^+}^t \frac{dx(\tau)}{\sqrt{4\pi D d\tau}} \right) \exp\left(-\frac{1}{4D} \int_0^t (\dot{x} + kx)^2 d\tau\right)$$

where we used:

$$\frac{1}{\Delta t_i} (\Delta x_i + kx_{i-1}\Delta t_i)^2 = \frac{\Delta t_i^2}{\Delta t_i} \left( \frac{\Delta x_i}{\Delta t_i} + kx_{i-1} \frac{\Delta t_i}{\Delta t_i} \right)^2 \xrightarrow{n \rightarrow \infty} (\dot{x} + kx)^2 dt$$

Expanding the square in (1.129):

$$dP = \prod_{i=1}^n \underbrace{\frac{d\Delta x_i}{\sqrt{4\pi D \Delta t_i}} \exp\left(-\sum_{i=1}^n \frac{\Delta x_i^2}{4D \Delta t_i}\right)}_{\text{Wiener measure } (dx_W)} \underbrace{\exp\left(-\frac{k}{2D} \sum_{i=1}^n x_{i-1} \Delta x_i\right)}_{\text{stochastic integral}} \underbrace{\exp\left(-\frac{k^2}{4D} \sum_{i=1}^n \Delta t_i x_{i-1}^2\right)}_{\text{normal integral}} \quad (1.130)$$

Let's focus on the stochastic integral. We already know that, for Ito's integrals, the usual rules of calculus do not apply. In particular, we can't just do:

$$\sum_{i=1}^n x_{i-1} \Delta x_i \xrightarrow{n \rightarrow \infty} \int_0^t x(\tau) dx(\tau) \neq \frac{x^2(t) - x^2(0)}{2}$$

So, more in general for a differentiable function  $h(x)$ :

$$\int_0^t h'(\tau) dx(\tau) \neq h(x(t)) - h(x(0)) \quad (1.131)$$

The idea is now to start from the right side and use Ito's rules to *correct* the left side, so to have a usable identity for integration. As always, we start by discretizing time  $\{t_i\}_{i=1, \dots, n}$ :

$$h(x(t)) - h(x(0)) = \sum_{i=1}^n [h(x(t_i)) - h(x(t_{i-1}))] \equiv \sum_{i=1}^n \Delta h_i$$

In the limit,  $t_i = t_{i-1} + dt$ , and so the  $\Delta h_i$  are *differentials* of  $h$ :

$$\Delta h_i = \frac{dh}{dx_i} \Delta x_i + \frac{1}{2} \frac{d^2 h}{dx_i^2} \Delta x_i^2 + O(\Delta x_i^3)$$

Now:

$$\Delta x_i = \frac{d\Delta B_i}{d\Delta x_i} \Delta B_i + O(\Delta B_i^2) \approx \sqrt{2D} \Delta B_i$$

And by Ito's rules,  $\Delta B_i^2 = \Delta t_i$  and  $\Delta B_i^n = 0$  for  $n \geq 3$ . So:

$$\Delta h_i = h' \Delta x_i + \frac{1}{2} h'' \underbrace{\Delta x_i^2}_{2D \Delta t_i}$$

And substituting back in (1.131) leads to:

$$h(x(t)) - h(x(0)) = \sum_{i=1}^n (h'_i \Delta x_i + h''_i D \Delta t_i)$$

Rearranging:

$$\sum_{i=1}^n h'_i \Delta x_i = h(x(t)) - h(x(0)) - D \sum_{i=1}^n h''_i \Delta t_i$$

In the limit  $n \rightarrow \infty$ , the sums become integrals:

$$\int_0^t h' dx(\tau) = h(x(t)) - h(x(0)) - D \int_0^t h'' d\tau \quad (1.132)$$



We can finally apply the result (1.132) to our case, by setting  $h'(x(\tau)) = x(\tau)$ , so that:

$$h(x(t)) = \int x(\tau) = \frac{x(t)^2}{2}; \quad h''(x(\tau)) = 1$$

Substituting in (1.132) leads to:

$$\sum_{i=1}^n x_{i-1} \Delta x_i \xrightarrow{n \rightarrow \infty} \int_0^t x(\tau) dx(\tau) = \frac{x^2(t) - x^2(0)}{2} - D \underbrace{\int_0^t d\tau}_t = \frac{x^2(t) - x^2(0)}{2} - Dt$$

And substituting this result back in (1.130) leads to:

$$dP \underset{n \rightarrow \infty}{=} dx_W \exp \left( -\frac{k}{2D} \left[ \frac{x_t^2 - x_0^2}{2} - Dt \right] \right) \exp \left( -\frac{k^2}{4D} \int_0^t x^2(\tau) d\tau \right)$$

From this expression we can compute *transition probabilities*. Let  $T = [0, t]$  and  $\mathbb{R}^T$  be the space of continuous functions  $T \rightarrow \mathbb{R}$ , then:

$$\begin{aligned} W(x_t, t | x_0, 0) &= \langle \delta(x_t - x) \rangle_W = \int_{\mathbb{R}^T} \delta(x_t - x) dP = \\ &= \int_{\mathbb{R}^T} dx_W \delta(x(t) - x) \exp \left( -\frac{k}{2D} \left[ \frac{x_t^2 - x_0^2}{2} - Dt \right] \right) \exp \left( -\frac{k^2}{4D} \int_0^t x^2(\tau) d\tau \right) = \\ &= \exp \left( -\frac{k}{2D} \left[ \frac{x_t^2 - x_0^2}{2} - Dt \right] \right) \underbrace{\int_{\mathbb{R}^T} dx_W \delta(x(t) - x) \exp \left( -\frac{k^2}{4D} \int_0^t x^2(\tau) d\tau \right)}_{\text{CFR } I_4 \text{ on 28/10}} = \\ &= \exp \left( -\frac{k}{2D} \left[ \frac{x_t^2 - x_0^2}{2} - Dt \right] \right) \sqrt{\frac{k}{4\pi D \sinh(kt)}} \exp \left( -\frac{kx_t^2}{4D} \coth(kt) \right) \end{aligned} \quad (1.133)$$

**Exercise 1.24.1** (Some more integrals):

Check that:

$$W(x, 0 | x_0, 0) = \delta(x - x_0)$$

**Hint.** Start from the case  $x_0 = 0$ . Using (1.133), after some algebra:

$$W(x, t | 0, 0) = \sqrt{\frac{k}{2\pi D(1 - e^{-2kt})}} \exp \left( -\frac{k}{2D} \frac{x^2}{1 - e^{-2kt}} \right) \quad (1.134)$$

And then show  $W(x, t | 0, 0) \xrightarrow{t \rightarrow 0} \delta(x)$ . The general case follows by translating that solution.

**Alternative derivation** The same result for the transition probabilities  $W(x, t | x_0, 0)$  can be found solving the Fokker-Planck equation:

$$\dot{W}(x, t | x_0, 0) = \frac{\partial}{\partial x} \left( kxW + D \frac{\partial}{\partial x} W \right) \quad (1.135)$$

A quick way to solve this differential equation is to note that  $\{\Delta B_i\}$  are all i.i.d.

gaussian variables, and so  $x$ , which is a sum of  $\Delta B_i$  must have a *gaussian* pdf. So we can make an *ansatz* for the solution:

$$W(x, t|x_0, 0) = \frac{1}{Z(t)} \exp(-a(t)x^2 + b(t)x) \quad (1.136)$$

Where  $a(t)$  and  $b(t)$  are the gaussian parameters, and  $Z(t)$  the normalization factor. All that's left is to substitute (1.136) in (1.135) and solve for  $a, b, Z$ .

### 1.24.1 Equilibrium distribution

As before, we expect the equilibrium distribution to follow Maxwell-Boltzmann formula:

$$W_{\text{eq}}(x) = \frac{1}{Z} \exp(-\beta V(x)) = \frac{1}{Z} \exp\left(-\frac{m\omega^2 x^2}{2k_B T}\right) \quad Z = \int_{\mathbb{R}} \exp(-\beta V(x)) \quad (1.137)$$

Starting from (1.134) and taking the limit  $t \rightarrow \infty$ :

$$\lim_{t \rightarrow \infty} W(x, t|0, 0) = \sqrt{\frac{k}{2\pi D}} \exp\left(-\frac{k}{2D} x^2\right) \quad (1.138)$$

Comparing (1.137) with (1.138) we find:

$$\frac{m\omega^2}{2k_B T} = \frac{k}{2D} = \frac{m\omega^2}{2\gamma D} \Rightarrow k_B T = \gamma D$$

So we obtain the same relation between  $D$  and  $T$  that we found in the general case.

### 1.24.2 High dimensional generalization

We can generalize the previous results to the case where  $\Delta \mathbf{B}_i = (\Delta B_i^1, \dots, \Delta B_i^d)^T$  are  $d$ -dimensional vectors, following a *multivariate gaussian distribution*:

$$\mathbb{P}(\Delta \mathbf{B}_1, \dots, \Delta \mathbf{B}_n) = \prod_{i=1}^n \prod_{\alpha=1}^d \frac{dB_i^\alpha}{\sqrt{2\pi\Delta t_i}} \exp\left(-\frac{\Delta B_i^\alpha}{2\Delta t_i}\right)$$

As different components of the same  $\Delta \mathbf{B}_i$  are independent, by Ito's rules of integration:

$$dB_i^\alpha dB_i^\beta = \delta_{\alpha\beta} dt_i \quad dB_i^\alpha dB_i^\beta dB_i^\gamma = 0$$

We then need to write  $d$  different Langevin equations, one for each component:

$$dx^\alpha(t) = f^\alpha(x(t), t) dt + \sqrt{2D_\alpha(x(t), t)} dB^\alpha(t)$$

More in general, the stochastic term could be:

$$\sum_{\beta=1}^d g_{\alpha\beta}(x(t), t) dB^\beta(t)$$

and in our case  $g_{\alpha\beta} = 2\sqrt{2D_\alpha}\delta_{\alpha\beta}$ .

The Fokker-Planck equation then becomes:

$$\dot{W}(\mathbf{x}, t) = \sum_{\alpha=1}^d \frac{\partial}{\partial x^\alpha} \left( -f_\alpha(\mathbf{x}, t)W(\mathbf{x}, t) + \frac{\partial}{\partial x^\alpha} D_\alpha(\mathbf{x}, t)W(\mathbf{x}, t) \right)$$

And the joint probability for a *discretized* path:

$$\mathbb{P}(\Delta\mathbf{x}_1, \dots, \Delta\mathbf{x}_n) = \prod_{i=1}^n \prod_{\alpha=1}^d \frac{d\Delta x_i^\alpha}{\sqrt{4\pi D_\alpha \Delta t_i}} \exp \left( - \sum_{i=1}^n \sum_{\alpha=1}^d \frac{(\Delta x_i^\alpha - f_{i-1}^\alpha \Delta t_i)^2}{4D_\alpha \Delta t_i} \right)$$

And taking the limit  $n \rightarrow \infty$ :

$$\mathbb{P}(\mathbf{x}(\tau)) = \prod_{\tau=0^+}^t \left( \frac{d^d \mathbf{x}(\tau)}{\sqrt{4\pi} d\tau \prod_{\alpha=1}^d \sqrt{D_\alpha}} \right) \exp \left( - \sum_{\alpha=1}^d \frac{1}{4D_\alpha} \int_0^t (\dot{x}^\alpha - f^\alpha)^2 d\tau \right)$$

### 1.24.3 Underdamped Harmonic Oscillator

If we do not ignore the inertia term in (1.126) we are left with:

$$m\ddot{\mathbf{x}} = m\dot{\mathbf{v}} = -\gamma\dot{\mathbf{x}} + \mathbf{F}(\mathbf{x}) + \sqrt{2D}\boldsymbol{\xi}$$

This second order (stochastic) differential equation can be written as a system of two first order equations:

$$\begin{cases} d\mathbf{x} = \mathbf{v} dt \\ d\mathbf{v} = \left( -\frac{\gamma}{m}\mathbf{v} + \frac{\mathbf{F}(\mathbf{x})}{m} \right) dt + \frac{\sqrt{2D}}{m} d\mathbf{B} \end{cases}$$

This leads to a *generalization* of the Fokker-Planck equation, named **Kramer equation**:

$$\dot{W}(\mathbf{x}, \mathbf{v}, t) = \nabla_{\mathbf{v}} \left[ \left( \frac{\gamma\mathbf{v}}{m} - \frac{\mathbf{F}}{m} \right) W(\mathbf{x}, \mathbf{v}, t) + \frac{\gamma^2 D}{m^2} \nabla_{\mathbf{v}} W(\mathbf{x}, \mathbf{v}, t) \right] + \nabla_{\mathbf{x}} (-\mathbf{v}W(\mathbf{x}, \mathbf{v}, t))$$

In the limit  $t \rightarrow \infty$ , the distribution at equilibrium will be:

$$W(\mathbf{x}, \mathbf{v}) = \frac{1}{Z} \exp \left( -\beta \left[ \frac{m\|\mathbf{v}\|^2}{2} + V(\mathbf{x}) \right] \right) \quad D = \frac{k_B T}{\gamma}$$

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## 1.25 Particle in a conservative force-field

In last section, we examined a particle of radius  $a$  immersed in a harmonic potential  $U(x) = m\omega^2 x^2/2$ , moving through a medium with viscosity  $\eta$  and subject to thermal fluctuations of amplitude proportional to  $\sqrt{2D}$ , so that its dynamics are described by the following *stochastic differential equation*:

$$dx = -kx dt + \sqrt{2D} dB \quad k = \frac{m\omega^2}{\gamma} \quad \gamma = 6\pi\eta a$$

The solution, expressed as the *transition probability* between any two given points, is a path integral:

$$W(x_t, t | x_0, 0) = \exp \left( -\frac{x_t^2 - x_0^2}{4D} k + \frac{kt}{2} \right) \langle \exp \left( -\int_0^t V(x(\tau)) d\tau \right) \delta(x(t) - x_t) \rangle_W \quad (1.139)$$

with  $V(x(\tau)) = k^2 x^2(\tau)/(4D)$ . The average is computed with the Wiener measure:

$$\langle f(x(\tau)) \rangle_W \equiv \int_{\mathbb{R}^T} \left( \prod_{\tau=0^+}^t \frac{dx(\tau)}{\sqrt{4\pi D d\tau}} \right) \exp \left( -\frac{1}{4D} \int_0^t \dot{x}^2(\tau) d\tau \right) f(x(\tau))$$

with  $\mathbb{R}^T$  being the set of continuous functions  $T \rightarrow \mathbb{R}$ , and  $T = [0, t]$ .

We want now to show that, in the more general case of a particle immersed in a generic potential  $U(x)$ , a path integral similar to the highlighted term in (1.139) will appear. Of course, the function  $V(x(\tau))$  will be different, but it will be proportional to  $U(x)$  - as it is evident in the harmonic case.

So, let's consider a particle in a 3D space  $\mathbf{r} = (x_1, x_2, x_3)^T$ , immersed in a conservative force-field  $\mathbf{F}(\mathbf{r}) = -\nabla U(\mathbf{r})$  with potential  $U(\mathbf{r})$ , and subject to thermal noise. The Langevin equation becomes:

$$d\mathbf{r} = \mathbf{f}(\mathbf{r}) dt + \sqrt{2D} d\mathbf{B} \quad \mathbf{f}(\mathbf{r}) = \frac{\mathbf{F}(\mathbf{r})}{\gamma} \quad \gamma = 6\pi\eta a \quad (1.140)$$

with  $\mathbf{B} = (B_1, B_2, B_3)^T$  being a  $d = 3$  vector with gaussian components:

$$\Delta B_\alpha \sim \frac{1}{\sqrt{2\pi\Delta t}} \exp \left( -\frac{\Delta B_\alpha^2}{2\Delta t} \right) \quad \alpha = 1, 2, 3 \quad (1.141)$$

As different components are independent, the joint pdf for the vector  $\Delta\mathbf{B}$  is just the product of the three terms in (1.141):

$$\Delta\mathbf{B} \sim \frac{1}{(2\pi\Delta t)^{3/2}} \exp \left( -\frac{\|\Delta\mathbf{B}\|^2}{2\Delta t} \right)$$

As before, we introduce a time discretization  $\{t_j\}_{j=0,\dots,n}$  with  $t_0 \equiv 0$  and  $t_n \equiv t$  fixed, so that (1.140) becomes:

$$\Delta\mathbf{r}_i = \mathbf{r}(t_i) - \mathbf{r}(t_{i-1}) = \mathbf{f}_{i-1} \Delta t_i + \sqrt{2D} \Delta\mathbf{B}_i$$

where the force  $\mathbf{f}(\mathbf{r})$  is evaluated at the left side  $t_{i-1}$  of each discrete interval  $[t_{i-1}, t_i]$ , following Ito's prescription.

Then, starting from the joint pdf of the  $\{\Delta\mathbf{B}_i\}$ :

$$dP(\Delta\mathbf{B}_1, \dots, \Delta\mathbf{B}_n) = \prod_{i=1}^n \frac{d^3\Delta\mathbf{B}_i}{(2\pi\Delta t)^{3/2}} \exp \left( -\sum_{i=1}^n \frac{\|\Delta\mathbf{B}_i\|^2}{2\Delta t_i} \right)$$

we perform a change of variables by inverting (1.140):

$$\Delta \mathbf{B}_i = \frac{\Delta \mathbf{r}_i - \mathbf{f}_{i-1} \Delta t_i}{\sqrt{2D}} \Rightarrow \left| \frac{\partial \{\Delta B_i^\alpha\}}{\partial \{\Delta r_j^\beta\}} \right| = \left| \frac{\partial \{\Delta r_j^\beta\}}{\partial \{\Delta B_i^\alpha\}} \right|^{-1} = (2D)^{3/2}$$

This leads to the joint pdf for the increments  $\{\Delta \mathbf{r}_i\}$ :

$$dP(\Delta \mathbf{r}_1, \dots, \Delta \mathbf{r}_n) = \left( \prod_{i=1}^n \frac{d^3 \Delta \mathbf{r}_i}{(4\pi D \Delta t_i)^{3/2}} \right) \exp \left[ -\frac{1}{4D} \sum_{i=1}^n \frac{\|\Delta \mathbf{r}_i - \mathbf{f}_{i-1} \Delta t_i\|^2}{\Delta t_i} \right] \quad (1.142)$$

Expanding the square in the exponential:

$$-\frac{1}{4D} \sum_{i=1}^n \left[ \frac{\|\Delta \mathbf{r}_i\|^2}{\Delta t_i} + \|\mathbf{f}_{i-1}\|^2 \Delta t_i - 2\Delta \mathbf{r}_i \cdot \mathbf{f}_{i-1} \right]$$

allows to recognize the  $d = 3$  Wiener measure in (1.142):

$$\begin{aligned} dP(\{\Delta \mathbf{r}_i\}) &= \underbrace{\left( \prod_{i=1}^n \frac{d^3 \Delta \mathbf{r}_i}{(4\pi D \Delta t_i)^{3/2}} \exp \left[ -\frac{1}{4D} \sum_{i=1}^n \frac{\|\Delta \mathbf{r}_i\|^2}{\Delta t_i} \right] \right)}_{d_W^3 \mathbf{r}} \\ &\quad \cdot \exp \left( -\frac{1}{4D} \underbrace{\sum_{i=1}^n \|\mathbf{f}_{i-1}\|^2 \Delta t_i}_{\int_0^t \|\mathbf{f}(\mathbf{r}(\tau))\|^2 d\tau} + \frac{1}{2D} \underbrace{\sum_{i=1}^n \mathbf{f}_{i-1} \cdot \Delta \mathbf{r}_i}_{\int_0^t \mathbf{f}(\mathbf{r}(\tau)) \cdot d\mathbf{r}(\tau)} \right) \end{aligned} \quad (1.143)$$

Let's focus on the *stochastic integral* (the one in  $d\mathbf{r}(\tau)$ ). For this we need to generalize to  $d = 3$  the integration formula we found in the previous section. Consider a multi-variable scalar function  $h(\mathbf{r}): \mathbb{R}^3 \rightarrow \mathbb{R}$ ,  $\mathbf{r} \mapsto h(\mathbf{r})$ . As before, we start from the difference:

$$\begin{aligned} h(\mathbf{r}_n) - h(\mathbf{r}_0) &= h(\mathbf{r}_n) - h(\mathbf{r}_{n-1}) + h(\mathbf{r}_{n-1}) - h(\mathbf{r}_{n-2}) + \dots + h(\mathbf{r}_1) - h(\mathbf{r}_0) = \\ &= \sum_{i=1}^n (h(\mathbf{r}_i) - h(\mathbf{r}_{i-1})) = \sum_{i=1}^n \Delta h_i \end{aligned} \quad (1.144)$$

In the discretization,  $\mathbf{r}_i = \mathbf{r}_{i-1} + \Delta \mathbf{x}$ , with  $\Delta \mathbf{x} = (\Delta x_i^1, \Delta x_i^2, \Delta x_i^3)$ . Each differential  $\Delta h_i$  is then:

$$\begin{aligned} \Delta h_i &= h(\mathbf{r}_i) - h(\mathbf{r}_{i-1}) \equiv h_i - h_{i-1} = \\ &\stackrel{(a)}{=} \cancel{h(\mathbf{r}_{i-1})} + \sum_{\alpha=1}^3 \left[ \frac{\partial}{\partial x^\alpha} h(\mathbf{r}_{i-1}) \right] \Delta x_i^\alpha + \frac{1}{2} \sum_{\alpha, \beta=1}^3 \left[ \frac{\partial^2}{\partial x^\alpha \partial x^\beta} h(\mathbf{r}_{i-1}) \right] \Delta x_i^\alpha \Delta x_i^\beta + \dots - \cancel{h(\mathbf{r}_{i-1})} = \\ &\stackrel{(b)}{=} \sum_{\alpha=1}^3 \left[ \frac{\partial}{\partial x^\alpha} h(\mathbf{r}_{i-1}) \right] \Delta x_i^\alpha + D \sum_{\alpha, \beta=1}^3 \left[ \frac{\partial^2}{\partial x^\alpha \partial x^\beta} h(\mathbf{r}_{i-1}) \right] \Delta t_i \end{aligned} \quad (1.145)$$

where in (a) we expanded the first term in Taylor series about  $\mathbf{r}_{i-1}$ , and in (b) we used Ito's rules, and in particular the fact that:

$$\Delta x_i^\alpha \Delta x_i^\beta = \Delta t_i 2D \delta_{\alpha\beta}$$

Substituting (1.145) back in (1.144) leads to:

$$h(\mathbf{r}_n) - h(\mathbf{r}_0) = \sum_{i=1}^n \Delta h_i = \sum_{i=1}^n \sum_{\alpha=1}^3 \frac{\partial}{\partial x^\alpha} h_{i-1} \Delta x_i^\alpha + D \sum_{\alpha=1}^3 \frac{\partial^2}{\partial x^{\alpha 2}} h_{i-1} \Delta t_i$$

and then, in the continuum limit:

$$h(\mathbf{r}(t)) - h(\mathbf{r}(0)) = \int_0^t \nabla h(\mathbf{r}) \cdot d^3 \mathbf{r} + D \int_0^t \nabla^2 h(\mathbf{r}(\tau)) d\tau$$

Rearranging we arrive at the desired formula for integration:

$$\int_0^t \nabla h(\mathbf{r}) \cdot d^3 \mathbf{r} = h(\mathbf{r}(t)) - h(\mathbf{r}(0)) - D \int_0^t \nabla^2 h(\mathbf{r}(\tau)) d\tau \quad (1.146)$$

Thanks to (1.146) we can solve the stochastic integral in (1.143):

$$\int_0^t \mathbf{f}(\mathbf{r}(\tau)) \cdot d^3 \mathbf{r}(\tau)$$

Inserting  $\mathbf{f}(\mathbf{r}) = -\nabla U(\mathbf{r})/\gamma$  and applying the formula leads to:

$$\int_0^t \mathbf{f}(\mathbf{r}(\tau)) \cdot d^3 \mathbf{r}(\tau) = -\frac{1}{\gamma} \int_0^t \nabla U(\mathbf{r}(\tau)) \cdot d^3 \mathbf{r}(\tau) = -\frac{1}{\gamma} \left[ U(\mathbf{r}(t)) - U(\mathbf{r}(0)) - D \int_0^t \nabla^2 U(\mathbf{r}(\tau)) d\tau \right]$$

Substituting back in (1.143):

$$\begin{aligned} dP &= d_W^3 \mathbf{r} \exp \left( -\frac{1}{4D} \int_0^t \|\mathbf{f}\|^2 d\tau + \frac{1}{2D} \left[ -\frac{1}{\gamma} [U(\mathbf{r}(t)) - U(\mathbf{r}(0))] + \frac{D}{\gamma} \int_0^t \nabla^2 U(\mathbf{r}(\tau)) d\tau \right] \right) = \\ &= d_W^3 \mathbf{r} \exp \left( -\frac{1}{4D} \int_0^t d\tau \underbrace{\left[ \|\mathbf{f}\|^2 - \frac{2D}{\gamma} \nabla^2 U \right]}_{V(\mathbf{r})} \right) \exp \left( -\frac{1}{2D\gamma} [U(\mathbf{r}(t)) - U(\mathbf{r}(0))] \right) \end{aligned} \quad (1.147)$$

where:

$$V = \mathbf{f}^2 - \frac{2D}{\gamma} \nabla^2 U = \mathbf{f}^2 - 2D \nabla \cdot \mathbf{f}$$

Using the just found measure  $dP$  we can compute path integrals, and in particular *transition probabilities*:

$$\begin{aligned} W(\mathbf{r}, t | \mathbf{r}_0, 0) &= \int_{\mathbb{R}^T} dP \delta(\mathbf{r}(t) - \mathbf{r}) \equiv \langle \delta(\mathbf{r}(t) - \mathbf{r}(0)) \rangle_W = \\ &= \int_{\mathbb{R}^T} d_W^3 \mathbf{r} \exp \left( -\frac{1}{4D} \int_0^t V(\mathbf{r}(\tau)) d\tau \right) \delta(\mathbf{r}(t) - \mathbf{r}) \exp \left( -\frac{1}{2D\gamma} (U(\mathbf{r}) - U(\mathbf{r}_0)) \right) = \\ &= \langle \exp \left( -\frac{1}{4D} \int_0^t V(\mathbf{r}(\tau)) d\tau \right) \delta(\mathbf{r}(t) - \mathbf{r}) \rangle_W \exp \left( -\frac{1}{2D\gamma} (U(\mathbf{r}) - U(\mathbf{r}_0)) \right) \end{aligned}$$

This expression is indeed similar to that derived in the specific case of the harmonic oscillator (1.139), meaning that the techniques we used to evaluate previous path integrals can be useful in much more general cases.

This observation has indeed a deeper meaning, as we found a way to describe the dynamics of conservative systems with a path integral. We already know that the behaviour of these systems can be also described with partial differential equations (e.g. the Fokker-Planck equation). So, there should be a link between path integrals and PDEs, that will be explored in the next section.

## 1.26 Feynman-Kac formula

It is possible to use the machinery of stochastic processes and path integrals to solve certain partial differential equations, which - as we will see - are of fundamental importance in Quantum Mechanics.

In this regard, a very important result is offered by the **Feynman-Kac formula**. The main idea is to use a Brownian process to *simulate many paths*, and express the solution of the differential equation as the *average* of a certain functional computed over all these paths.

More precisely, consider the following *partial differential equation* (Bloch's equation):

$$\partial_t W_B(x, t) = D \partial_x^2 W_B(x, t) - V(x) W_B(x, t) \quad D \in \mathbb{R}, V: \mathbb{R} \rightarrow \mathbb{R} \quad (1.148)$$

The **Feynman-Kac** formula states that the function  $W_B(x, t)$  that solves (1.148) can be found by computing a Wiener path integral:

$$W_B(x, t) \equiv \langle \exp \left( - \int_0^t V(x(\tau)) d\tau \right) \delta(x(t) - x) \rangle_W \quad (1.149)$$

Note that this result can be generalized to more dimensions - but we will limit ourselves to the  $d = 1$  case for simplicity.

**Proof.** We now show that (1.149) indeed satisfies (1.148). As usual, we start by defining a time discretization,  $\{t_i\}_{i=0, \dots, n+1}$ , so that  $t_0 \equiv 0$  and  $t_{n+1} \equiv \bar{t}$  is the instant at which we wish to evaluate the solution  $W_B(x, t)$ . Then (1.149) at that instant will be obtained by the *continuum limit* of the discretized average  $\psi_{n+1}(x)$ :

$$W_B(x, \bar{t}) = \lim_{n \rightarrow \infty} \psi_{n+1}(x)$$

$$\psi_{n+1}(x) = \int_{\mathbb{R}^{n+1}} \left( \prod_{i=1}^{n+1} \frac{dx_i}{\sqrt{4\pi D \Delta t_i}} \right) \exp \left( - \sum_{i=1}^{n+1} \frac{(x_i - x_{i-1})^2}{4D \Delta t_i} - \sum_{i=1}^{n+1} \Delta t_i V(x_i) \right) \delta(x_{n+1} - x) \quad (1.150)$$

Note that  $\psi_{n+1}(x)$  is the average of a functional over *all paths* that arrive in  $x$  at the instant  $\bar{t}$ , making exactly  $n + 1$  steps from their starting point 0. In the following, the intuition is to see these paths as *being generated*, i.e. evolving *step* after *step* from 0 to  $x$ . For example, suppose we want to approximate (1.150). We would start by choosing an *ensemble* of paths arriving to  $x$  after  $n + 1$

timesteps, compute the functional on each of them, and average the results. However, we could also do it in another - a bit stranger - way. Consider the same ensemble of paths we already (supposedly) generated. From each of them, remove the last step. We now have a set of paths that arrive *close* to  $x$ , and will arrive exactly there if we let another timestep pass. However, we decide to compute the functional on each of these paths and then average the results, before letting them arrive at their destination. So, in a certain sense, we will estimate the value of the functional “a timestep in the past”. Of course, we can repeat this process, removing more and more timesteps at every iteration. At the end, we will have a sequence of numbers detailing the “evolution” of the functional from the start to the end. Turns out that the *rule* for such an evolution is exactly (1.148). So, to prove Feynman-Kac, we just have to find that rule - meaning how to relate  $\psi_{n+1}$  to its “past”  $\psi_n$  (in the continuum limit  $n \rightarrow \infty$ ).

This is just an informal intuition, that will only be useful as a guide for the rest of the proof. So, let's go on.

For simplicity, we choose the time discretization as **uniform**, so that  $\Delta t_i \equiv \epsilon \forall i$ , and:

$$t_{n+1} = (n+1)\epsilon \equiv \bar{t} \Rightarrow \epsilon = \frac{\bar{t}}{n+1}$$

We then rewrite (1.150), highlight the last term (the one with the  $x_{n+1}$ ) and integrate to remove the  $\delta$ :

$$\begin{aligned} \psi_{n+1}(x) &= \int_{\mathbb{R}^n} \left( \prod_{i=1}^n \frac{dx_i}{\sqrt{4\pi D\epsilon}} \right) \exp \left( - \sum_{i=1}^n \frac{(x_i - x_{i-1})^2}{4D\epsilon} - \sum_{i=1}^n \epsilon V(x_i) \right) \cdot \\ &\quad \cdot \int_{\mathbb{R}} \frac{dx_{n+1}}{\sqrt{4\pi D\epsilon}} \exp \left( - \frac{(x_{n+1} - x_n)^2}{4D\epsilon} - \epsilon V(x_{n+1}) \right) \delta(x_{n+1} - x) = \\ &= \int_{\mathbb{R}^n} \left( \prod_{i=1}^n \frac{dx_i}{\sqrt{4\pi D\epsilon}} \right) \exp \left( - \sum_{i=1}^n \frac{(x_i - x_{i-1})^2}{4D\epsilon} - \sum_{i=1}^n \epsilon V(x_i) \right) \cdot \\ &\quad \cdot \frac{1}{\sqrt{4\pi D\epsilon}} \exp \left( - \frac{(x - x_n)^2}{4D\epsilon} - \epsilon V(x) \right) \end{aligned} \quad (1.151)$$

Now, with some algebra, we recognize in these integrals a term  $\psi_n(x_n)$ , indicating the expected value of the functional over all paths reaching  $x_n$  (which is close to the end-point  $x$ ) at timestep  $t_n = t - \epsilon$ . We start by rearranging, putting the integration over  $dx_n$  at the front:

$$\begin{aligned} (1.151) &= \int_{\mathbb{R}} \frac{dx_n}{\sqrt{4\pi D\epsilon}} \exp \left( - \frac{(x - x_n)^2}{4D\epsilon} - \epsilon V(x) \right) \cdot \\ &\quad \cdot \frac{1}{\sqrt{4\pi D\epsilon}} \int_{\mathbb{R}^{n-1}} \left( \prod_{i=1}^{n-1} \frac{dx_i}{\sqrt{4\pi D\epsilon}} \right) \exp \left( - \sum_{i=1}^{\textcolor{red}{n}} \frac{(x_i - x_{i-1})^2}{4D\epsilon} - \epsilon \sum_{i=1}^{\textcolor{red}{n}} V(x_i) \right) \end{aligned} \quad (1.152)$$

Now we *change* all the  $x_i$  in the second line to  $y_i$ , and then add a  $\delta$  (with its integral) to *connect*  $y_n$  to  $x_n$ , which appears in the integral in the first line. In



this way we will highlight the desired  $\psi_n(x_n)$ :

$$(1.152) = \int_{\mathbb{R}} \frac{dx_n}{\sqrt{4\pi D\epsilon}} \exp\left(-\frac{(x-x_n)^2}{4D\epsilon} - \epsilon V(x)\right) \cdot \underbrace{\int_{\mathbb{R}^n} \left(\prod_{i=1}^n \frac{dy_i}{\sqrt{4\pi D\epsilon}}\right) \exp\left(-\sum_{i=1}^n \frac{(y_i - y_{i-1})^2}{4D\epsilon} - \epsilon \sum_{i=1}^n V(y_i)\right) \delta(x_n - y_n)}_{\psi_n(x_n)} \quad (1.153)$$

And so:

$$\psi_{n+1}(x) = e^{-\epsilon V(x)} \int_{\mathbb{R}} \frac{dx_n}{\sqrt{4\pi D\epsilon}} \exp\left(-\frac{(x-x_n)^2}{4D\epsilon}\right) \psi_n(x_n) \quad (1.154)$$

This is relation between  $\psi_{n+1}(x)$  and its “past”  $\psi_n(x)$  that we were searching for. Now, to retrieve (1.148), all that’s left is to put (1.154) in differential form. We start by simplifying the integral, making it similar to a gaussian with a change of variables:

$$-\frac{(x-x_n)^2}{4D\epsilon} \stackrel{!}{=} -\frac{z^2}{2} \Rightarrow z = -\frac{x-x_n}{\sqrt{2D\epsilon}}; \quad x_n = x + \sqrt{2D\epsilon}z; \quad dx_n = \sqrt{2D\epsilon}dz$$

which leads to:

$$\psi_{n+1}(x) = e^{-\epsilon V(x)} \int_{-\infty}^{+\infty} \frac{dz}{\sqrt{2\pi}} \exp\left(-\frac{z^2}{2}\right) \psi_n(x_n + z\sqrt{2D\epsilon}) \quad (1.155)$$

As  $n \rightarrow \infty$ ,  $z \rightarrow 0$ . We will not prove this, but note that:

$$z = -\frac{x-x_n}{\epsilon} \frac{\sqrt{\epsilon}}{\sqrt{2D}}$$

where the first factor is a *velocity*, which must be physically limited, and so  $n \rightarrow \infty \Rightarrow \epsilon \rightarrow 0 \Rightarrow z \rightarrow 0$ .

This means that we can expand  $\psi_n$  in Taylor series about  $x$ :

$$\psi_n(x_n + z\sqrt{2D\epsilon}) = \psi_n(x) + z\sqrt{2D\epsilon}\psi'_n(x) + z^2 D\epsilon\psi''_n(x) + O(z^3\epsilon^{3/2})$$

Substituting back in (1.155):

$$\begin{aligned} \psi_{n+1}(x) = e^{-\epsilon V(x)} & \left[ \underbrace{\psi_n(x) \int_{\mathbb{R}} \frac{dz}{\sqrt{2\pi}} \exp\left(-\frac{z^2}{2}\right)}_1 + \underbrace{\sqrt{2D\epsilon}\psi'_n(x) \int_{\mathbb{R}} \frac{dz}{\sqrt{2\pi}} z \exp\left(-\frac{z^2}{2}\right)}_0 + \right. \\ & \left. + D\epsilon\psi''_n(x) \underbrace{\int_{\mathbb{R}} \frac{dz}{\sqrt{2\pi}} z^2 \exp\left(-\frac{z^2}{2}\right)}_1 + O(\epsilon^2) \right] \quad (1.156) \end{aligned}$$

as the integrand is just a standard gaussian ( $\mu = 0$ ,  $\sigma = 1$ ). Note how the error term is of order  $\epsilon^2$ , as the first non-null integral in the series will be that with  $z^4$ :

$$\int_{\mathbb{R}} \frac{dz}{\sqrt{2\pi}} z^k \frac{(2D\epsilon)^{k/2}}{k!} \psi_n^{(k)} = \begin{cases} 0 & k \text{ odd} \\ 1^k (k-1)!! & k \text{ even} \end{cases}$$

Expanding also the  $e^{-\epsilon V(x)}$  term:

$$e^{-\epsilon V(x)} = 1 - \epsilon V(x) + \frac{\epsilon^2 V^2(x)}{2} + O(\epsilon^3)$$

Finally, substituting back in (1.156), expanding the product and ignoring all terms of order 2 or higher in  $\epsilon$ :

$$\psi_{n+1}(x) = \psi_n(x) + D\epsilon\psi_n''(x) - \epsilon V(x)\psi_n(x) + O(\epsilon^2)$$

Rearranging:

$$\frac{\psi_{n+1} - \psi_n}{\epsilon} = D\psi_n'' - V\psi_n$$

And when  $\epsilon \rightarrow 0$  the first term becomes a time derivative, leading to Bloch's equation, and proving Feynman-Kac formula:

$$\partial_t W_B(x, t) = D\partial_x^2 W_B(x, t) - V(x)W_B(x, t)$$

### 1.26.1 Application to Quantum Mechanics

It is possible to map the Schrödinger equation to the Bloch equation (1.148), and then use Feynman-Kac formula to solve it.

Recall the time-dependent Schrödinger equation for a particle immersed in a  $d = 1$  potential  $v(x)$  and described by a wavefunction  $\psi(x, t)$ :

$$i\hbar\partial_t\psi(x, t) = -\frac{\hbar^2}{2m}\partial_x^2\psi(x, t) + v(x)\psi(x, t)$$

This is already similar to (1.148), except for the presence of a complex coefficient  $i$ . We can remove it with a change of variable  $t \mapsto it$ , leading to:

$$i\hbar(i)\frac{\partial}{\partial t}\psi(x, it) = -\hbar\frac{\partial}{\partial t}\psi(x, it) = -\frac{\hbar^2}{2m}\partial_x^2\psi(x, it) + v(x)\psi(x, it)$$

Defining  $\psi(x, it) \equiv \hat{\psi}(x, t)$  and multiplying both sides by  $-\hbar^{-1}$  leads to:

$$\frac{\partial}{\partial t}\hat{\psi}(x, t) = \frac{\hbar}{2m}\frac{\partial^2}{\partial x^2}\hat{\psi}(x, t) - \frac{v(x)}{\hbar}\hat{\psi}(x, t)$$

which has the form of Bloch's equation:

$$\frac{\partial}{\partial t}\hat{\psi}(x, t) = D\frac{\partial^2}{\partial x^2}\hat{\psi}(x, t) - V(x)\hat{\psi}(x, t) \quad D = \frac{\hbar}{2m}; \quad V(x) = \frac{v(x)}{\hbar}$$

## 1.27 Variational methods

Consider a particle subject to an external conservative force  $\mathbf{F}(\mathbf{r}) = -\nabla U(\mathbf{r})$ , moving through a viscous medium and subject to thermal noise. The probability density for a path  $x(\tau)$  can be derived from (1.147), after “dividing by the

volume element” and taking the limit  $n \rightarrow \infty$ :

$$\begin{aligned}
\Omega[\mathbf{r}(\tau)] &\equiv \frac{dP}{dV} = \\
&= \exp \left( -\frac{1}{4D} \int_0^t d\tau \dot{\mathbf{r}}^2(\tau) + \underbrace{\int_0^t d\tau \left( -\frac{1}{4D} \right) \left[ \|\mathbf{f}\|^2 - \frac{2D}{\gamma} \nabla^2 U \right]}_{V(\mathbf{r})} - \frac{1}{2D\gamma} [U(\mathbf{r}(t)) - U(\mathbf{r}(0))] \right) = \\
&= \exp \left( -\frac{1}{4D} \int_0^t d\tau \dot{\mathbf{r}}^2(\tau) - \underbrace{\frac{1}{4D} \int_0^t d\tau \left[ \left\| \frac{\mathbf{F}}{\gamma} \right\|^2 + \frac{2D}{\gamma} \nabla \cdot \mathbf{F} \right]}_{V(\mathbf{r})} + \frac{1}{2D\gamma} \int_{\mathbf{r}(0)}^{\mathbf{r}(t)} d^3\mathbf{r} \cdot \mathbf{F}(\mathbf{r}) \right)
\end{aligned} \tag{1.157}$$

with  $\mathbf{f}(\mathbf{r}) = \mathbf{F}/\gamma$ , and  $\gamma = 6\pi\eta a$  ( $\eta$  being the medium viscosity, and  $a$  the particle radius). If we change variables in the last integral:

$$\int_{\mathbf{r}(0)}^{\mathbf{r}(t)} d^3\mathbf{r} \cdot \mathbf{F}(\mathbf{r}) = \int_0^t d\tau \mathbf{F}(\mathbf{r}) \cdot \frac{d\mathbf{r}(\tau)}{d\tau}$$

we can rewrite (1.157) as a single integral:

$$\Omega[\mathbf{r}(\tau)] = \exp \left( -\frac{1}{4D} \int_0^t d\tau L(\mathbf{r}(\tau)) \right) \tag{1.158}$$

with the function  $L: \mathbb{R} \rightarrow \mathbb{R}$ ,  $\mathbf{r}(\tau) \mapsto L(\mathbf{r}(\tau))$  defined as:

$$\begin{aligned}
L(\mathbf{r}(\tau)) &\equiv \dot{\mathbf{r}}^2(\tau) + \left\| \frac{\mathbf{F}(\mathbf{r}(\tau))}{\gamma} \right\|^2 + \frac{2D}{\gamma} \nabla \cdot \mathbf{F}(\mathbf{r}(\tau)) - \frac{2}{\gamma} \mathbf{F}(\mathbf{r}(\tau)) \cdot \dot{\mathbf{r}}(\tau) = \\
&= \left\| \dot{\mathbf{r}}(\tau) - \frac{\mathbf{F}(\mathbf{r}(\tau))}{\gamma} \right\|^2 + \frac{2D}{\gamma} \nabla \cdot \mathbf{F}(\mathbf{r}(\tau))
\end{aligned} \tag{1.159}$$

### Classical path.

Consider the **classical limit**  $D \rightarrow 0$ . Then the  $\nabla \cdot \mathbf{F}$  term in (1.159) vanishes, and as  $-1/(4D) \rightarrow \infty$ , there will be only *one path* with *non-zero* probability, i.e. the one  $\mathbf{r}_c(\tau)$  for which the functional vanishes:

$$\int_0^t d\tau L(\mathbf{r}_c(\tau)) = 0 \Rightarrow \int_0^t d\tau \left\| \dot{\mathbf{r}}_c(\tau) - \frac{\mathbf{F}(\mathbf{r}_c(\tau))}{\gamma} \right\|^2 = 0$$

We can then compute that path. As the integrand is a non-negative function, for its integral to be 0 it must be 0  $\forall t$ , leading to:

$$\frac{d\mathbf{r}_c}{d\tau} = \frac{\mathbf{F}(\mathbf{r}_c)}{\gamma}$$

which is just the equation of motion from classical mechanics.

Let's now use the form (1.158) to compute path integrals. For example, consider a transition probability:

$$W(\mathbf{r}_t, t | \mathbf{r}_0, 0) = \int_{\mathcal{C}\{\mathbf{r}_0, 0; \mathbf{r}_t, t\}} d\mathbf{r}(\tau) \underbrace{\exp \left( -\frac{1}{4D} \int_0^t d\tau L(\mathbf{r}(\tau)) \right)}_{\Omega[\mathbf{r}(\tau)]} \tag{1.160}$$

Let's define the functional:

$$S[\mathbf{r}(\tau)] = \int_0^t d\tau L(\mathbf{r}(\tau))$$

Given the form of (1.160), the path  $\mathbf{r}_c(\tau)$  that *minimizes*  $S[\mathbf{r}(\tau)]$  will give the greatest contribution to the path integral. The parameter  $D$  *modulates* the relative contributions of paths. If  $D \rightarrow 0$ ,  $\mathbf{r}_c(\tau)$  will be the only contributing path, but if  $D \gg 1$ , many different paths will have a significant contribution. Suppose that  $\mathbf{r}_c(\tau)$  is indeed important, meaning that  $D$  is sufficiently small (more precisely, that  $S[\mathbf{r}_c(\tau)]/D \gg 1$ ). Then, we write any generic path  $\mathbf{x}(\tau)$  as the most important one  $\mathbf{x}_c(\tau)$  plus a “deviation”  $\mathbf{y}(\tau)$ :

$$\mathbf{x}(\tau) = \mathbf{x}_c(\tau) + \underbrace{(\mathbf{x}(\tau) - \mathbf{x}_c(\tau))}_{\mathbf{y}(\tau)}$$

Note that as the end-points of every path are fixed,  $\mathbf{y}(0) = \mathbf{y}(t) = 0$ . Then, we expand in series the functional:

$$S[\mathbf{x}(\tau)] = S[\mathbf{x}_c(\tau) + \mathbf{y}(\tau)] = S[\mathbf{x}_c] + \delta S[\mathbf{x}_c, \mathbf{y}] + \frac{1}{2!} \delta^2 S[\mathbf{x}_c, \mathbf{y}] + \dots$$

where the  $\delta$  terms are the *variations* of the functional<sup>4</sup>. For example, the first variation  $\delta S[\mathbf{x}_c, \mathbf{y}]$  is given by, measures how much  $S$  *varies* to first order when changing  $\mathbf{y}(\tau)$ . As  $\mathbf{x}_c$  is a minimum of  $S$ , it is also a *stationary point*, meaning that paths close to  $\mathbf{x}_c$  do not change the value  $S[\mathbf{x}_c]$  to first order. Applying the definition of the first variation, this leads to the Euler-Lagrange equations for determining  $\mathbf{x}_c$ :

$$\delta S[\mathbf{x}_c, \mathbf{y}] = \frac{\partial L(\mathbf{r}(\tau))}{\partial x_i} - \frac{d}{d\tau} \frac{\partial L(\mathbf{r}(\tau))}{\partial \dot{x}_i} \stackrel{!}{=} 0 \quad i = 1, 2, 3$$

Then, note how all other terms of the series involve integrals of  $\mathbf{y}(\tau)$ , which do not depend on  $x$  - as  $\mathbf{y}(\tau)$  starts from 0 and returns to 0 at  $t$ . So:

$$S[\mathbf{x}(\tau)] = S[\mathbf{x}_c] + \underbrace{\frac{1}{2!} \delta^2 S[\mathbf{x}_c, \mathbf{y}] + \dots}_{h(t)}$$

Substituting back in (1.160):

$$W(\mathbf{r}_t, t | \mathbf{r}_0, 0) = \underbrace{-\frac{1}{4D} \exp(h(t))}_{\Phi(t)} \exp\left(-\frac{1}{4D} S[\mathbf{x}_c]\right) = \Phi(t) \exp\left(-\frac{1}{4D} \int_0^t d\tau L[\mathbf{r}_c(\tau)]\right)$$

The function  $\Phi(t)$  is called *fluctuation factor*, and its computation is not trivial in the general case. However, if we are dealing with transition probabilities, we can use the *normalization condition* to find it:

$$\int_{\mathbb{R}^3} d^3 \mathbf{r} W(\mathbf{r}, t | \mathbf{r}, 0) \equiv 1$$

**Example 12** (Simple integral with variational methods):

<sup>4</sup>^See [www2.math.uconn.edu/~gordina/NelsonAaronHonorsThesis2012.pdf](http://www2.math.uconn.edu/~gordina/NelsonAaronHonorsThesis2012.pdf) for a refresher

An example will hopefully clarify the essence of the variational method. Let's start with a already known integral, in the  $d = 1$  case:

$$\begin{aligned} W(x, t|x_0, 0) &= \int_{\mathbb{R}^T} \left( \prod_{\tau=0^+}^t \frac{dx(\tau)}{\sqrt{4\pi D d\tau}} \right) \exp \left( -\frac{1}{4D} \int_0^t \dot{x}^2(\tau) d\tau \right) \delta(x - x(t)) = \\ &= \frac{1}{\sqrt{4\pi Dt}} \exp \left( -\frac{(x - x_0)^2}{4Dt} \right) \end{aligned} \quad (1.161)$$

Let's compute it again, this time using variations. In this case we are interested in the functional:

$$S[x(\tau)] = \int_0^t \dot{x}^2(\tau) d\tau \quad (1.162)$$

To minimize it, we solve the Euler-Lagrange equations:

$$\frac{d}{d\tau} \frac{\partial S(x_c)}{\partial \dot{x}} - \frac{\partial S(x_c)}{\partial x} = 0 \Rightarrow 0 - 2\ddot{x}_c = 0 \Rightarrow \ddot{x}_c(\tau) = 0$$

Integrating two times:

$$\dot{x}_c(\tau) = a \Rightarrow x_c(\tau) = a\tau + b$$

The boundary conditions are path's two extrema:

$$x_c(0) = b \stackrel{!}{=} 0; \quad x_c(t) = at + x_0 \stackrel{!}{=} x \Rightarrow a = \frac{x - x_0}{t}$$

leading to:

$$x_c(\tau) = x_0 + \frac{x - x_0}{t} \tau$$

So the path minimizing  $S$  is just the straight line joining  $x_0$  to  $x$ . We can now express any path  $x(\tau)$  as a *deviation* from the  $x_c(\tau)$ :

$$x(\tau) = x_c(\tau) + y(\tau) \quad y(0) = y(t) = 0 \quad (1.163)$$

This is a change of variables for (1.161), from  $x(\tau)$  to  $y(\tau)$  ( $x_c(\tau)$  is a *fixed* path). As this is just a translation,  $dx(\tau) = dy(\tau)$  and the path integral becomes:

$$\begin{aligned} W(x, t|x_0, 0) &= \int_{\mathbb{R}^T} \left( \prod_{\tau=0^+}^t \frac{dy(\tau)}{\sqrt{4\pi D d\tau}} \right) \delta(y(t) - 0) S[x_c(\tau) + y(\tau)] = \\ &= \int_{\mathcal{C}\{0,0;0,t\}} \left( \prod_{\tau=0^+}^t \frac{dy(\tau)}{\sqrt{4\pi D d\tau}} \right) S[x_c(\tau) + y(\tau)] \end{aligned} \quad (1.164)$$

To compute  $S$ , first we differentiate (1.163):

$$\dot{x}(\tau) = \dot{x}_c(\tau) + \dot{y}(\tau)$$

and substitute in (1.162), leading to:

$$S[x(\tau)] = \int_0^t d\tau (\dot{x}_c + \dot{y})^2 = \int_0^t \dot{x}_c^2(\tau) d\tau + 2 \int_0^t \dot{x}_c(\tau) \dot{y}(\tau) d\tau + \int_0^t \dot{y}^2(\tau) d\tau$$

Note that the middle term vanishes. We can see it by integrating by parts:

$$\int_0^t \dot{x}_c(\tau) \dot{y}(\tau) d\tau = \dot{x}_c(\tau) y(\tau) \Big|_0^t - \int_0^t \ddot{x}_c(\tau) y(\tau) d\tau = 0$$

as  $y(0) = y(t) = 0$  and  $\ddot{x}_c(\tau) \equiv 0$ . Going back to (1.164):

$$W(x, t|x_0, 0) = \int_{\mathbb{R}^T} \left( \prod_{\tau=0^+}^t \frac{dy(\tau)}{\sqrt{4\pi D d\tau}} \right) \delta(y(t) - 0) \exp \left( -\frac{1}{4D} \left[ \int_0^t \dot{x}_c^2(\tau) d\tau + \int_0^t \dot{y}^2(\tau) d\tau \right] \right)$$

As  $x_c(\tau)$  is fixed, we can bring it outside the integral:

$$= \exp \left( -\int_0^t \dot{x}_c^2(\tau) d\tau \right) \underbrace{\int_{\mathbb{R}^T} \left( \prod_{\tau=0^+}^t \frac{dy(\tau)}{\sqrt{4\pi D d\tau}} \right) \delta(y(t) - 0) \exp \left( -\frac{1}{4D} \int_0^t \dot{y}^2(\tau) d\tau \right)}_{\Phi(t)}$$

We recognize the remaining path integral as a function  $\Phi(t)$  of time only, and finally:

$$\begin{aligned} W(x, t|x_0, 0) &= \Phi(t) \int_0^t d\tau \dot{x}_c^2(\tau) = \Phi(t) \exp \left[ -\frac{1}{4D} \left( \frac{x^2 - x_0^2}{t^2} \right) \underbrace{\int_0^t d\tau}_t \right] = \\ &= \Phi(t) \exp \left( -\frac{(x - x_0)^2}{4Dt} \right) \end{aligned}$$

To find the remaining  $\Phi(t)$  we can now use the normalization condition:

$$\int_{-\infty}^{+\infty} dx W(x, t|x_0, 0) \stackrel{!}{=} 1$$

In this case, this is just a gaussian integral:

$$\int_{\mathbb{R}} dx \Phi(t) \exp \left( -\frac{(x - x_0)^2}{4Dt} \right) = \Phi(t) \sqrt{4\pi Dt} \stackrel{!}{=} 1 \Rightarrow \Phi(t) = \frac{1}{\sqrt{4\pi Dt}}$$

And so we retrieve the correct result:

$$W(x, t|x_0, 0) = \frac{1}{\sqrt{4\pi Dt}} \exp \left( -\frac{(x - x_0)^2}{4Dt} \right)$$

**Gaussian integrals.** There is another, more specific, way to interpret the results we discussed in this section. Instead of working in the continuum, we could use a discretization, and see path integrals as (1.161) as integrals of a

highly dimensional gaussian. For example, in the case just examined, we have:

$$W(x, t | x_0, 0) = \lim_{n \rightarrow \infty} I_N$$

$$I_n = \int_{\mathbb{R}^n} \left( \prod_{i=1}^n \frac{dx_i}{\sqrt{4\pi D \Delta t_i}} \right) \exp \left( - \sum_{i=1}^n \frac{(x_i - x_{i-1})^2}{4D \Delta t_i} \right) \delta(x - x_n)$$

Performing the integration over the  $dx_n$  we can remove the  $\delta$ , leaving only a multivariate gaussian:

$$I_n = \int_{\mathbb{R}^{n-1}} \frac{1}{\sqrt{4\pi D \Delta t_i}} \left( \prod_{i=1}^n \frac{dx_i}{\sqrt{4\pi D \Delta t_i}} \right) \exp \left( - \sum_{i=1}^n \frac{(x_i - x_{i-1})^2}{4D \Delta t_i} \right) \Big|_{x_n=x}$$

This is a gaussian in the form of:

$$\int_{\mathbb{R}^n} d^n \mathbf{x} \exp \left( -\frac{1}{2} \mathbf{x}^T A \mathbf{x} + \mathbf{b}^T \mathbf{x} \right) \quad (1.165)$$

Note that removing the  $\delta$  inserts a linear term in the exponential, here highlighted:

$$\sum_{i=1}^n \frac{(x_i - x_{i-1})^2}{4D \Delta t_i} \Big|_{x=x_n} = \sum_{i=1}^{n-1} \frac{(x_i - x_{i-1})^2}{4D \Delta t_i} + \frac{x_n^2 + 2x_n x_{n-1} + x_{n-1}^2}{4D \Delta t_n}$$

and so  $\mathbf{b} \neq \mathbf{0}$ .

Recall that to solve (1.165) we proceeded with a change of variables,  $\mathbf{x} = \mathbf{x}_c + \mathbf{y}$ , where  $\mathbf{x}_c$  is the *minimum* of the gaussian (see 10/10 notes). This leads to a result that is proportional to the exponential evaluated at  $\mathbf{x}_c$ :

$$\begin{aligned} \int_{\mathbb{R}^n} d^n \mathbf{x} \exp \left( -\frac{1}{2} \mathbf{x}^T A \mathbf{x} + \mathbf{b}^T \mathbf{x} \right) &= \frac{(2\pi)^{n/2}}{\sqrt{\det(A)}} \exp \left( \frac{1}{2} \mathbf{b}^T A^{-1} \mathbf{b} \right) = \\ &= \frac{(2\pi)^{n/2}}{\sqrt{\det(A)}} \exp \left( \text{Stat}_{\mathbf{x}} \left[ -\frac{1}{2} \mathbf{x}^T A \mathbf{x} + \mathbf{b} \cdot \mathbf{x} \right] \right) \\ \text{Stat}_{\mathbf{x}} F(\mathbf{x}) &= F(\mathbf{x}_c); \quad \mathbf{x}_c \text{ such that } \frac{\partial F(\mathbf{x})}{\partial x_i} \Big|_{\mathbf{x}=\mathbf{x}_c} = 0 \quad \forall i = 1, \dots, n \end{aligned}$$

So, in the discrete case, the same *variational result* just derives from choosing the best set of coordinates to describe the multivariate gaussian.

## 1.28 Variational methods

**Example 13** (Overdamped harmonic oscillator with variational methods):

Consider a particle immersed in a harmonic potential  $U(x) = m\omega^2 x^2/2$  and subject to thermal noise, moving in a viscous medium. In the **overdamped limit**  $m/\gamma \rightarrow 0$  (where  $\gamma = 6\pi\eta a$ , with  $\eta$  the medium's viscosity and  $a$  the particle's radius), the equation of motion becomes:

$$dx(t) = -kx(t) dt + \sqrt{2D} dB(t) \quad k = \frac{m\omega^2}{\gamma}$$

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A path  $\{x(\tau)\}$  solving that equation has a *infinitesimal* probability given by:

$$dP = \left( \prod_{\tau=0^+}^t \frac{dx(\tau)}{\sqrt{4\pi D d\tau}} \right) \exp \left( -\frac{1}{4D} \int_0^t (\dot{x} + kx)^2 d\tau \right)$$

as we already derived. We are now interested in computing the transition probabilities:

$$W(x, t|x_0, 0) = \int_{\mathbb{R}^T} \delta(x(t) - x) dP$$

Following the variational method, we arrive to:

$$W(x, t|x_0, 0) = \Phi(t) \exp \left( -\frac{1}{4D} S[x_c(\tau)] \right) \quad (1.166)$$

where  $S$  is the *action functional* for the harmonic potential:

$$S[x(\tau)] = \int_0^t L(\dot{x}, x) d\tau \quad L(\dot{x}, x) = (\dot{x} + kx)^2$$

and  $x_c(\tau)$  is the path that *stationarizes*  $S[x(\tau)]$ , meaning that  $\delta S[x_c(\tau)] = 0$  and so it satisfies the Euler-Lagrange equation:

$$0 \stackrel{!}{=} \frac{\partial L}{\partial x} \Big|_{x_c} - \frac{d}{dt} \frac{\partial L}{\partial \dot{x}} \Big|_{x_c} = 2k(\dot{x}_c + kx_c) - 2(\ddot{x}_c + k\dot{x}_c) = 2(k^2 x_c - \ddot{x}_c)$$

as:

$$\begin{aligned} \frac{\partial L}{\partial x} &= 2k(\dot{x} + kx) \\ \frac{\partial L}{\partial \dot{x}} &= 2(\dot{x} + kx) \end{aligned}$$

So, to find  $x_c(\tau)$  we need to solve:

$$\begin{cases} \ddot{x}_c = k^2 x_c \\ x_c(0) = x_0 \\ x_c(t) = x \end{cases}$$

This is the second order ordinary differential equation for an *harmonic repulsor*, which has the following general integral:

$$x_c(\tau) = Ae^{k\tau} + Be^{-k\tau}$$

Imposing the boundary conditions leads to:

$$\begin{aligned} \begin{cases} x_0 \stackrel{!}{=} A + B \\ x \stackrel{!}{=} Ae^{kt} + Be^{-kt} \end{cases} &\Rightarrow \begin{cases} B = x_0 - A \\ xe^{kt} = Ae^{2kt} + B \end{cases} \Rightarrow xe^{kt} - x_0 = A[e^{2kt} - 1] \\ \Rightarrow A &= \frac{xe^{kt} - x_0}{e^{2kt} - 1} \frac{e^{-kt}}{e^{-kt}} = \frac{(xe^{kt} - x_0)e^{-kt}}{\frac{e^{kt} - e^{-kt}}{2}} = \frac{x - x_0 e^{-kt}}{2 \sinh(kt)} \\ B &= x_0 - A = -\frac{x - x_0 e^{kt}}{2 \sinh(kt)} = 2 \end{aligned}$$



Then we evaluate the action at the stationary path  $x_c(\tau)$ :

$$\begin{aligned}
S[x_c(\tau)] &= \int_0^t (\dot{x} + kx)^2 d\tau = \int_0^t [2kAe^{k\tau}]^2 d\tau = 4k^2 A^2 \frac{1}{2k} e^{2k\tau} \Big|_0^t = \\
&= 4kA^2 \frac{e^{2kt} - 1}{2} \frac{e^{-kt}}{e^{-kt}} = 4kA^2 \sinh(kt) e^{kt} = \\
&= 4k \frac{(x - x_0 e^{-kt})^2}{4 \sinh(kt)} e^{kt} = \frac{k(x - x_0 e^{-kt})^2}{e^{kt} - e^{-kt}} \frac{2}{e^{-kt}} = \frac{2k(x - x_0 e^{-kt})^2}{1 - e^{-2kt}}
\end{aligned}$$

Substituting back in (1.166):

$$W(x, t|x_0, 0) = \Phi(t) \exp \left( -\frac{k}{2D(1 - e^{-2kt})} [x - x_0 e^{-kt}]^2 \right)$$

All that's left to find  $\Phi(t)$  is to use the normalization condition:

$$\begin{aligned}
1 &\stackrel{!}{=} \int_{\mathbb{R}} dx W(x, t|x_0, 0) = \Phi(t) \int_{\mathbb{R}} dx \exp \left( -\overbrace{\frac{k}{2D(1 - e^{-2kt})}}^{\alpha} [x - x_0 e^{-kt}]^2 \right) = \\
&= \Phi(t) \sqrt{\frac{\pi}{\alpha}} = \Phi(t) \sqrt{\frac{2\pi D(1 - e^{-2kt})}{k}} \Rightarrow \Phi(t) = \sqrt{\frac{k}{2\pi D}} \frac{1}{\sqrt{1 - e^{-2kt}}}
\end{aligned}$$

And so the full solution is:

$$\begin{aligned}
W(x, t|x_0, 0) &= \sqrt{\frac{k}{2\pi D}} \frac{1}{\sqrt{1 - e^{-2kt}}} \exp \left( -\frac{k}{2D} \frac{(x - x_0 e^{-kt})^2}{(1 - e^{-2kt})} \right) \\
&\xrightarrow{t \rightarrow \infty} \sqrt{\frac{k}{2\pi D}} \exp \left( -\frac{k}{2Dx^2} \right)
\end{aligned}$$

As before, we can compute the  $t \rightarrow \infty$  with a Maxwell-Boltzmann distribution  $e^{-\beta U(x)}$ , obtaining:

$$\frac{1}{2} \beta m \omega^2 x^2 = \frac{k}{2D} x^2 \Rightarrow D = \frac{k}{\beta m \omega^2} = \frac{1}{\beta \gamma} = \frac{k_B T}{\gamma} \Rightarrow D \gamma = k_B T$$

as we previously derived.

If we do not consider the overdamped limit, however, the equation of motion is given by:

$$m\ddot{x} = -\gamma\dot{x} - m\omega^2 x + \sqrt{2D\gamma}\xi$$

This can be rewritten as a system of two first order (stochastic) differential equations:

$$\begin{cases} dx(\tau) = v(\tau) d\tau \\ dv(\tau) = -\frac{\gamma}{m} v(\tau) d\tau + \frac{\gamma\sqrt{2D}}{m} dB \end{cases}$$

It is convenient to “symmetrize” the system, by adding a stochastic term also in the first equation:

$$\begin{cases} dx(\tau) = v(\tau) d\tau + 2\hat{D}\sqrt{d\hat{B}} \\ dv(\tau) = -\frac{\gamma}{m}v(\tau) d\tau + \frac{\gamma\sqrt{2D}}{m} dB \end{cases}$$

and then we'll consider the limit  $\hat{D} \rightarrow 0$ .

First, as usual, we discretize, with  $\{t_i\}_{i=0,\dots,n}$  and  $t_0 \equiv 0$ ,  $t_n \equiv t$ , arriving to:

$$\begin{cases} \Delta x_i = v_{i-1}\Delta t_i + \sqrt{2\hat{D}}\Delta\hat{B}_i \\ \Delta v_i = -\frac{\gamma}{m}v_{i-1}\Delta t_i + \frac{\gamma}{m}\sqrt{2D}\Delta B_i \end{cases}$$

Where the velocity is evaluated at  $t_{i-1}$  as per Ito's prescription. As  $\Delta B_i$  and  $\Delta\hat{B}_i$  are **independent** gaussian increments, their joint distribution is just a product:

$$dP(\Delta B_1, \Delta\hat{B}_1, \dots, \Delta B_n, \Delta\hat{B}_n) = \left( \prod_{i=1}^n \frac{d\Delta B_i}{\sqrt{2\pi\Delta t_i}} \frac{d\Delta\hat{B}_i}{\sqrt{2\pi\Delta t_i}} \right) \exp\left(-\frac{1}{2} \sum_{i=1}^n \frac{\Delta B_i^2}{\Delta t_i} - \frac{1}{2} \sum_{i=1}^n \frac{\Delta\hat{B}_i^2}{\Delta t_i}\right)$$

As done previously (see 14/11 notes), to get the distribution for  $\Delta x_i$  and  $\Delta v_i$  we make a change of random variables:

$$\begin{aligned} \Delta\hat{B}_i &= \frac{\Delta x_i - v_{i-1}\Delta t_i}{\sqrt{2\hat{D}}} \\ \Delta B_i &= \left(\Delta v_i + \frac{\gamma}{m}v_{i-1}\Delta t_i\right) \frac{m}{\gamma\sqrt{2D}} \end{aligned}$$

with jacobian:

$$\begin{aligned} \det \left| \frac{\partial\{\Delta\hat{B}_i\}}{\partial\{\Delta x_i\}} \right| &= (2\hat{D})^{-n/2} \\ \det \left| \frac{\partial\{\Delta B_i\}}{\partial\{\Delta x_i\}} \right| &= \det \left| \frac{\partial\{\Delta x_i\}}{\partial\{\Delta B_i\}} \right|^{-1} = \left(\frac{\gamma}{m}\sqrt{2D}\right)^{-n} = \left(\frac{\gamma^2}{m^2}2D\right)^{-n/2} \end{aligned}$$

leading to:

$$\begin{aligned} dP(\{\Delta x_i\}, \{\Delta v_i\}) &= \left( \prod_{i=1}^n \frac{d\Delta x_i}{\sqrt{4\pi D\Delta t_i}} \frac{d\Delta v_i}{\sqrt{4\pi D\Delta t_i\gamma^2/m^2}} \right) \cdot \\ &\cdot \exp\left(-\frac{1}{2} \sum_{i=1}^n \frac{m^2}{2\gamma^2 D} \left[ \left( \frac{\Delta v_i + \gamma/mv_{i-1}\Delta t_i}{\Delta t_i} \right)^2 \Delta t_i \right] \right) \cdot \\ &\cdot \exp\left(-\frac{1}{2} \sum_{i=1}^n \frac{1}{2\hat{D}} \left[ \left( \frac{\Delta x_i - v_{i-1}\Delta t_i}{\Delta t_i} \right)^2 \Delta t_i \right] \right) = \\ &= \left( \prod_{i=1}^n \frac{d\Delta x_i}{\sqrt{4\pi D\Delta t_i}} \frac{d\Delta v_i}{\sqrt{4\pi D\Delta t_i\gamma^2/m^2}} \right) \cdot \\ &\cdot \exp\left(-\frac{m^2}{4D\gamma^2} \sum_{i=1}^n \left[ \left( \frac{\Delta v_i}{\Delta t_i} + \frac{\gamma}{m}v_{i-1} \right)^2 \Delta t_i \right] \right) \cdot \\ &\cdot \exp\left(-\frac{1}{4\hat{D}} \sum_{i=1}^n \left[ \left( \frac{\Delta x_i}{\Delta t_i} - v_{i-1} \right)^2 \Delta t_i \right] \right) \quad (1.167) \end{aligned}$$

Taking the continuum limit  $n \rightarrow \infty$  leads to:

$$dP(\{x(\tau), v(\tau)\}) = \left( \prod_{\tau=0^+}^t \frac{dx(\tau)}{\sqrt{4\pi\hat{D}d\tau}} \frac{dv(\tau)}{\sqrt{4\pi D d\tau \gamma^2/m^2}} \right) \cdot \exp \left( -\frac{m^2}{4D\gamma^2} \int_0^t d\tau \left[ \dot{v}(\tau) + \frac{\gamma}{m} v(\tau) \right]^2 - \frac{1}{4\hat{D}} \int_0^t d\tau [\dot{x}(\tau) - v(\tau)]^2 \right)$$

In the limit  $\hat{D} \rightarrow 0^+$ ,  $1/(4\hat{D}) \rightarrow +\infty$ , and so the gaussian pdf for the  $\Delta\hat{B}_i$  becomes *infinitely thin*, and the only path with a non-vanishing probability will be the one where:

$$\int_0^t d\tau [\dot{x} - v(\tau)]^2 = 0$$

As any  $> 0$  value will lead to  $\exp(-\infty) = 0$ . In particular, the  $i$ -th factor of the discretization becomes:

$$\begin{aligned} & \frac{1}{\sqrt{4\pi\hat{D}\Delta t_i}} \exp \left[ -\frac{1}{4\hat{D}} \left( \frac{\Delta x_i}{\Delta t_i} - v_0^2 \right) \Delta t_i \right] = \\ & = \frac{1}{\sqrt{4\pi\hat{D}\Delta t_i}} \exp \left( -\frac{1}{4\hat{D}\Delta t_i} (\Delta x_i - v_{i-1}\Delta t_i)^2 \right) \xrightarrow{\hat{D} \rightarrow 0} \delta(\Delta x_i - v_{i-1}\Delta t_i) \end{aligned}$$

where we used a limit definition for the  $\delta$ :

$$\lim_{\epsilon \rightarrow 0} \frac{1}{\sqrt{4\pi\epsilon}} \exp \left( -\frac{x^2}{4\epsilon} \right) = \delta(x)$$

with  $\epsilon = \hat{D}\Delta t_i$  and  $x = \Delta x_i - v_{i-1}\Delta t_i$ .

Substituting back in (1.167):

$$\begin{aligned} dP(\{\Delta x_i\}, \{\Delta v_i\}) &= \left( \prod_{i=1}^n d\Delta x_i \delta(\Delta x_i - v_{i-1}\Delta t_i) \frac{d\Delta v_i}{\sqrt{4\pi D \Delta t_i \gamma^2/m^2}} \right) \cdot \\ &\cdot \exp \left( -\frac{m^2}{4D\gamma^2} \sum_{i=1}^n \left[ \left( \frac{\Delta v_i}{\Delta t_i} + \frac{\gamma}{m} v_{i-1} \right)^2 \Delta t_i \right] \right) \end{aligned}$$

Now consider the discretized transition probability:

$$\begin{aligned} W(x_n, v_n, t_n | x_0, v_0, 0) &= \int_{\mathbb{R}^n \times \mathbb{R}^n} dP(\{x_i, v_i\}) \delta(x_n - x) \delta(v_n - v) = \quad (1.168) \\ &= \int_{\mathbb{R}^n \times \mathbb{R}^n} \left( \prod_{i=1}^n d\Delta x_i \delta(\Delta x_i - v_{i-1}\Delta t_i) \frac{d\Delta v_i}{\sqrt{4\pi D \Delta t_i \gamma^2/m^2}} \right) \cdot \\ &\cdot \exp \left( -\frac{m^2}{4D\gamma^2} \sum_{i=1}^n \left[ \left( \frac{\Delta v_i}{\Delta t_i} + \frac{\gamma}{m} v_{i-1} \right)^2 \Delta t_i \right] \right) \delta(v_n - v) \delta(x_n - x) \end{aligned}$$

Let's focus on the integrations over  $x_i$ :

$$\begin{aligned} & \int_{\mathbb{R}^n} \left( \prod_{i=1}^n d\Delta x_i \delta(\Delta x_i - v_{i-1}\Delta t_i) \right) \delta(x_n - x) = \\ & = \int_{\mathbb{R}^n} d\Delta x_1 \dots d\Delta x_n \delta(\Delta x_1 - v_0\Delta t_1) \dots \delta(\Delta x_n - v_{n-1}\Delta t_n) \delta(x_n - x) \end{aligned}$$

We then perform the change of variables  $\Delta x_1 = x_1 - x_0$ , with  $x_0$  constant, so that  $d\Delta x_1 = dx_1$ . Then we integrate over  $dx_1$ , eliminating the first  $\delta$  and setting  $x_1 = x_0 - v_0\Delta t_1$ :

$$\int_{\mathbb{R}^n} dx_1 d\Delta x_2 \dots d\Delta x_n \delta(x_1 - x_0 - v_0\Delta t_1) \delta(\Delta x_2 - v_1\Delta t_2) \dots \delta(\Delta x_n - v_{n-1}\Delta t_n) \delta(x_n - x) = \int_{\mathbb{R}^{n-1}} d\Delta x_2 \dots d\Delta x_n \delta(x_2 - x_0 - v_0\Delta t_1 - v_1\Delta t_2) \dots \delta(\Delta x_n - v_{n-1}\Delta t_n) \delta(x_n - x)$$

Repeating these steps for all the other variables except the last one, we arrive to:

$$= \int_{\mathbb{R}} dx_n \delta\left(x_n - x_0 - \sum_{i=1}^n v_{i-1}\Delta t_i\right) \delta(x_n - x) = \delta\left(x - x_0 - \sum_{i=1}^n v_{i-1}\Delta t_i\right)$$

In the continuum limit, this becomes:

$$\delta\left(x - x_0 - \int_0^t v(\tau) d\tau\right)$$

Substituting back in (1.168) and finally taking the limit  $n \rightarrow \infty$ :

$$W(x, v, t | x_0, v_0, 0) = \int_{\mathbb{R}^T} \left( \prod_{\tau=0^+}^t \frac{dv(\tau)}{\sqrt{4\pi D d\tau \gamma/m^2}} \right) \exp\left(-\frac{m^2}{4D\gamma} \int_0^t \left(\dot{v}(\tau) + \frac{\gamma}{m}v(\tau)\right)^2 d\tau\right) \cdot \delta(v(t) - v) \delta\left(x - x_0 - \int_0^t v(\tau) d\tau\right)$$

We can now use the variational method to compute that integral. So, let  $v_c(\tau)$  be the path, starting at  $v(0) = v_0$  that *stationarizes* the action functional:

$$S[v(\tau)] = \int_0^t \left(\dot{v}(\tau) + \frac{\gamma}{m}v(\tau)\right)^2 d\tau$$

so that  $\delta S[v_c(\tau)] = 0$ , and also satisfies the constraints imposed by the  $\delta$ :

$$v(t) \stackrel{!}{=} v \quad x - x_0 \stackrel{!}{=} \int_0^t v(\tau) d\tau$$

Then, the path integral is given by:

$$W(x, v, t | x_0, v_0, 0) = \Phi(t) \exp\left(-\frac{m^2}{4D\gamma} \int_0^t \left(\dot{v}_c(\tau) + \frac{\gamma}{m}v_c(\tau)\right)^2 d\tau\right) \quad (1.169)$$

All that's left is to compute  $v_c(\tau)$  and evaluate the integral. This is a problem of *constrained optimization*, for which we use the method of Lagrange multipliers.

**Brief refresher of Lagrange multipliers.** Suppose we have two functions  $F, g: \mathbb{R}^2 \rightarrow \mathbb{R}$ , with  $F(x, y)$  being the function to maximize, and  $g(x, y) = c \in \mathbb{R}$  a constraint. A stationary point  $(x_0, y_0)$  of  $F$  subject to the constraint  $g(x, y) = c$  is such that if we move slightly from  $(x_0, y_0)$  along the contour  $g(x, y) = c$ , the value of  $F(x, y)$  does not change (to first order). This happens if the contour of  $F$  passing through the stationary point  $F(x, y) = F(x_0, y_0)$  is parallel at  $(x_0, y_0)$  to that of  $g(x, y) = c$ , meaning that at  $(x_0, y_0)$  the gradients of  $F$  and  $g$  are parallel:

$$\nabla_{x,y} F = \lambda \nabla_{x,y} g \quad \lambda \in \mathbb{R}$$

(Here we assume that  $\nabla_{x,y}g(x_0, y_0) \neq \mathbf{0}$ ). Rearranging:

$$\nabla_{x,y}(F(x, y) - \lambda g(x, y)) = \mathbf{0}$$

Together with the constraint equation  $g(x, y) = c$ , we have now 3 equations in 3 unknowns  $(x, y, \lambda)$  that can be solve to yield the desired stationary point  $(x_0, y_0)$ .

In this case, we have *functionals* instead of functions, and *functionals derivatives* (i.e. variations) instead of derivatives. So, to find the stationary points of:

$$\int_0^t \left( \dot{v}(\tau) + \frac{\gamma}{m} v(\tau) \right)^2 d\tau \quad (a)$$

subject to the constraint:

$$\int_0^t v(\tau) d\tau = x - x_0 \quad (b)$$

we need to solve:

$$\delta \int_0^t \underbrace{\left[ \left( \dot{v}(\tau) + \frac{\gamma}{m} v(\tau) \right)^2 - \lambda v(\tau) \right]}_{L(v, \dot{v})} d\tau = 0$$

And applying the definition of first variation (the  $\delta$  above) leads to solving the Euler-Lagrange equations:

$$\frac{\partial L}{\partial v} - \frac{d}{d\tau} \frac{\partial L}{\partial \dot{v}} \Big|_{v=v_c} \stackrel{!}{=} 0$$

Expanding the computations:

$$2 \left( \dot{v}_c + \frac{\gamma}{m} v_c \right) \frac{\gamma}{m} - \lambda - \frac{d}{d\tau} \left[ 2 \left( \dot{v}_c + \frac{\gamma}{m} v_c \right) \right] = 0 \Rightarrow \ddot{v}_c(\tau) = v_c(\tau) \left( \frac{\gamma}{m} \right)^2 - \frac{\lambda}{2}$$

The homogeneous solution is again a combination of exponentials:

$$v_c(\tau) = A \exp \left( -\frac{\gamma}{m} \tau \right) + B \exp \left( \frac{\gamma}{m} \tau \right)$$

And for the inhomogeneous general integral we just need to add a particular solution, for example the one with constant velocity  $\dot{v}(\tau) = \text{const} \Rightarrow \ddot{v}_c(\tau) = 0$ , given by:

$$v_c(\tau) = \frac{\lambda}{2} \left( \frac{m}{\gamma} \right)^2$$

Then, we need to impose the boundary conditions:

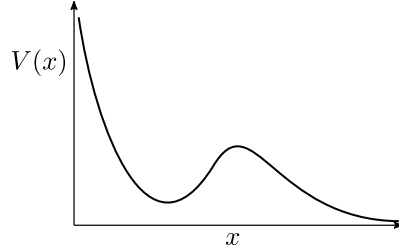
$$v_c(0) = v_0 \quad v_c(t) = v \quad \int_0^t v(\tau) d\tau = (x - x_0)$$

So we have 3 parameters (the two constants of integration  $A, B$  and  $\lambda$ ) and 3 equations. After finding all of them, we just need to evaluate the integral (1.169) (computations omitted).

## 1.29 Diffusion with obstacles

(Lesson 15 of  
21/11/19)  
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Consider a particle in a potential  $U(x)$  (fig. 1.4), with a local minimum separated by a *barrier*. In the classical case, if the particle's energy is sufficiently low, it can become *forever* trapped inside the minimum. However, in the presence of *thermal fluctuations* there may be a possibility of escape - a sort of classical tunnelling.



**Figure (1.4)** – Potential graph

We first consider an easier problem, that of the diffusion process on a compact domain  $[a, b]$ , representing the *boundaries* of the potential well of fig. 1.4. We then suppose that the particle cannot escape from the left side  $a$ , but it can do so - and always does - from the right one  $b$ . This means that  $a$  is a “reflecting” boundary - i.e. if the particle hits  $x = a$  it “bounces back”), while  $x = b$  is an *absorbing* boundary, that is a particle reaching  $b$  can be “absorbed by the environment” and disappear from the system. In the more general case, the probability of reflection at  $x = a$  or absorption at  $x = b$  will not be certain, but will depend on the particle's energy.

Recall the Langevin equation:

$$dx(t) = \underbrace{\frac{F(x, t)}{\gamma}}_{f(x, t)} dt + \sqrt{2D(x, t)} dB \quad F(x) = -U'(x); x \in [a, b]$$

This is equivalent to the Fokker-Planck equation:

$$\begin{aligned} \frac{\partial}{\partial t} W(x, t|x_0, 0) &= -\frac{\partial}{\partial x} \left[ \overbrace{f(x, t)W(x, t|x_0, 0) - \frac{\partial}{\partial x}(D(x, t)W(x, t|x_0, 0))}^{J(x, t)} \right] = \\ &= -\frac{\partial}{\partial x} \left[ \underbrace{-\frac{U'(x)}{\gamma}}_{A(x)} W(x, t|x_0, 0) - \frac{\partial}{\partial x} \left( \underbrace{\frac{k_B T}{\gamma}}_D W(x, t|x_0, 0) \right) \right] = \end{aligned} \quad (1.170)$$

$$= -\partial_x [A(x)W(x, t|x_0, 0)] + \partial_x^2 [D(x)W(x, t|x_0, 0)] \quad (1.171)$$

where we inserted  $D(x, t) \equiv D = k_B T / \gamma$  (derived from the equilibrium limit).  $J(x, t)$  is the probability flux coming out from  $x$  at instant  $t$ .

To solve (1.170) we need a precise mathematical description for the *reflecting* and *absorbing* boundaries:

- In  $x = a$ , the *reflecting* boundary condition means that:

$$J(a, t) = A(a)W(a, t|x_0, 0) - [\partial_x D(x)W(x, t|x_0, 0)]|_{x=a} \stackrel{!}{=} 0 \quad \forall t \quad (1.172)$$

As every particle that goes in  $a$  immediately comes out after being reflected, the *inward* flux and *outward* one are the same, and so their sum is 0.

- In  $b$ , however, the *absorbing* boundary condition means that the probability to find the particle here is exactly 0:

$$W(b, t|x_0, 0) \stackrel{!}{=} 0 \quad (1.173)$$

As  $x \in [a, b]$ , the domain of equation (1.170) is not isotropic anymore - meaning that the solution  $W(x, t|x_0, 0)$  will depend on  $x_0$ , making the problem much difficult. The idea is then to translate the problem from finding the full transition probability  $W(x, t|x_0, 0)$  to finding a simpler, but still interesting, function, that depends on less parameters.

One possible choice is given by the **survival probability**, i.e. the probability that a particle starting at a given point  $x$  will still be inside the interval  $[a, b]$  at a later time  $t$ :

$$G(x, t) = \int_a^b dy W(y, t|x, 0)$$

Note that we keep the starting time fixed at 0, and integrate over all the possible *destinations* of the particle - reducing the number of variables from 4 to 2.

Note that generally  $G(x, t) \neq 1$ , as the boundary in  $b$  offers a possibility of escape, leading to a *violation* of the conservation of probability. In fact the condition (1.173)  $W(b, t|x_0, t_0) = 0$  does not mean that the flux here is null. Recalling the definition of  $J(x, t)$  from (1.170):

$$\begin{aligned} J(b, t) &= \overline{A(b)W(b, t|x_0, t_0)} - \partial_x(D(x)W(x, t|x_0, t_0))|_{x=b} = \\ &= -(\overline{\partial_x D(x)W(b, t|x_0, t_0)}) - D(b)\partial_x W(x, t|x_0, t_0)|_{x=b} \neq 0 \end{aligned}$$

Now, we need to translate (1.170) to a differential equation for  $G(x, t)$ . We can start by evaluating the time derivative of  $G(x, t)$ :

$$\frac{\partial}{\partial t} G(x, t) = \int_a^b dx' \frac{\partial}{\partial t} W(x', t|x, 0) \quad (1.174)$$

We could use (1.171) to expand the  $\partial_t W(x', t|x, 0)$  term - but this does not really work:

$$\frac{\partial}{\partial t} G(x, t) = \int_a^b dx' [-\partial_{x'}(A(x')W(x', t|x, 0)) + \partial_{x'}^2(D(x')W(x', t|x, 0))]$$

To reconstruct derivatives of  $G(x, t)$  in the right side, we would need to bring the  $\partial_{x'}$  out of the integrals - but this is not possible, as  $x'$  is the variable of integration. One way to solve this would be to somehow move the derivative from  $\partial_{x'}$  to  $\partial_x$ .

To do this, we start from the ESCK relation:

$$\int_a^b dx_1 W(x_2, t_2 | x_1, t_1) W(x_1, t_1 | x_0, t_0) = W(x_2, t_2 | x_0, t_0) \quad t_0 < t_1 < t_2$$

Differentiating with respect to the middle time  $t_1$ :

$$\int_a^b dx_1 [W(x_1, t_1 | x_0, t_0) \partial_{t_1} W(x_2, t_2 | x_1, t_1) + W(x_2, t_2 | x_1, t_1) \partial_{t_1} W(x_1, t_1 | x_0, t_0)] = 0$$

We then use (1.171) to expand the highlighted term:

$$\begin{aligned} & \int_a^b dx_1 W(x_1, t_1 | x_0, t_0) \partial_{t_1} W(x_2, t_2 | x_1, t_1) + \\ & + \int_a^b dx_1 W(x_2, t_2 | x_1, t_1) [-\partial_{x_1} A(x_1) W(x_1, t_1 | x_0, t_0) + \partial_{x_1}^2 D(x_1) W(x_1, t_1 | x_0, t_0)] = 0 \end{aligned}$$

And then we integrate by parts the second term, to move the  $\partial_{x_1}$  and  $\partial_{x_1}^2$  derivatives:

$$\begin{aligned} & \int_a^b dx_1 W(x_1, t_1 | x_0, t_0) \partial_{t_1} W(x_2, t_2 | x_1, t_1) + \\ & - A(x_1) W(x_1, t_1 | x_0, t_0) W(x_2, t_2 | x_1, t_1) \Big|_{x_1=a}^{x_1=b} + W(x_2, t_2 | x_1, t_1) [\partial_{x_1} D(x_1) W(x_1, t_1 | x_0, t_0)] \Big|_{x_1=a}^{x_1=b} \\ & - D(x_1) W(x_1, t_1 | x_0, t_0) [\partial_{x_1} W(x_2, t_2 | x_1, t_1)] \Big|_{x_1=a}^{x_1=b} \\ & + \int_a^b dx_1 [A(x_1) W(x_1, t_1 | x_0, t_0) \partial_{x_1} W(x_2, t_2 | x_1, t_1) + D(x_1) W(x_1, t_1 | x_0, t_0)] \partial_{x_1}^2 W(x_2, t_2 | x_1, t_1) = 0 \end{aligned}$$

In the limit  $t_1 \rightarrow 0$ ,  $W(x_1, t_1 | x_0, t_0) = \delta(x_1 - x_0) \delta(t_1 - t_0)$ . This makes all the boundary terms vanish (given that  $x_0 \neq a, b$ ), and allows to compute the other integrals (with  $x_1 = x_0$  and  $t_1 = t_0$ ), leading to:

$$\frac{\partial}{\partial t_0} W(x_2, t_2 | x_0, t_0) + A(x_0) \frac{\partial}{\partial x_0} W(x_2, t_2 | x_0, t_0) + D(x_0) \frac{\partial^2}{\partial x_0^2} W(x_2, t_2 | x_0, t_0) = 0$$

Rearranging, and dropping some subscripts:

$$\partial_{t_0} W(x, t | x_0, t_0) = -A(x_0) \partial_{x_0} W(x, t | x_0, t_0) - D(x_0) \partial_{x_0}^2 W(x, t | x_0, t_0) \quad (1.175)$$

This is the **backward Fokker-Planck equation**, as all derivatives are with respect to the starting time or position - meaning that it can be used to “retrodict” the past given the future. This could be used for computing  $\partial_t G(x, t)$  - but first we need to express the derivative  $\partial_{t_0}$  in terms of the derivative  $\partial_t$  that appears in  $\partial_t G(x, t)$ .

Supposing that  $A(x)$  and  $D(x)$  are time-independent (as we implicitly did in the previous notation), then (1.171) is an *autonomous* differential equation, meaning that the solution does not change after a time translation:

$$W(x, t | x_0, t_0) = W(x, t - t_0 | x_0, 0)$$

Differentiating with respect to  $t_0$ :

$$\partial_{t_0} W(x, t | x_0, t_0) = \partial_{t'} W(x, t' | x_0, 0) \Big|_{t'=t-t_0} \partial_{t_0} (t - t_0) = -\partial_t W(x, t - t_0 | x_0, 0) = -\partial_t W(x, t | x_0, t_0)$$



Substituting this relation in (1.175) we get:

$$\partial_t W(x, t|x_0, t_0) = A(x_0)\partial_{x_0} W(x, t|x_0, t_0) + D(x_0)\partial_{x_0}^2 W(x, t|x_0, t_0) \quad (1.176)$$

Finally, we can use (1.176) in (1.174):

$$\frac{\partial}{\partial t} G(x, t) = \int_a^b dx' \partial_t W(x', t|x, 0) = \quad (1.177)$$

$$\begin{aligned} &= \stackrel{(1.176)}{=} \int_a^b dx' [A(x)\partial_x W(x', t|x, 0) + D(x)\partial_x^2 W(x', t|x, 0)] = \\ &= A(x)\partial_x \underbrace{\int_a^b dx' W(x', t|x, 0)}_{G(x, t)} + D(x)\partial_x^2 \underbrace{\int_a^b dx' W(x', t|x, 0)}_{G(x, t)} = \\ &= A(x)\partial_x G(x, t) + D(x)\partial_x^2 G(x, t) \end{aligned} \quad (1.178)$$

We have now a differential equation for  $G(x, t)$ , and we need to translate the appropriate boundary conditions (1.172) and (1.173). The latter is immediate:

$$W(b, t|x_0, 0) = 0 \quad \forall t \forall x_0 \in [a, b] \Rightarrow G(x, t)|_{x=b} = 0 \quad (1.179)$$

However, the analogous of (1.172) requires a bit more work. So we start again from the ESCK relation, and differentiate with respect to the mid-time:

$$\partial_\tau \int_a^b dy W(x', t|y, \tau) W(y, \tau|x, 0) = \partial_\tau W(x', t|x, 0) = 0$$

Expanding the left side:

$$\int_a^b dy [W(y, \tau|x, 0) \partial_\tau W(x', t|y, \tau) + W(x', t|y, \tau) \partial_\tau W(y, \tau|x, 0)] = 0$$

We can now use (1.175) for the term highlighted in yellow, and (1.171) (also called **forward Fokker-Planck equation**) for the term in green, leading to:

$$\begin{aligned} &\int_a^b dy [-A(y)\partial_y W(x', t|y, \tau) - D(y)\partial_y^2 W(x', t|y, \tau)] W(y, \tau|x, 0) + \\ &\int_a^b dy [-\partial_y A(y)W(y, \tau|x, 0) + \partial_y^2 D(y)W(y, \tau|x, 0)] W(x', t|y, \tau) \end{aligned}$$

We now integrate by parts the first term, moving the  $\partial_y$  and  $\partial_y^2$  derivatives away from  $W(x', t|y, \tau)$ :

$$\begin{aligned} &- A(y)W(x', t|y, \tau)W(y, \tau|x, 0) \Big|_{y=a}^{y=b} + \int_a^b dy [\partial_y A(y)W(y, \tau|x, 0)] W(x', t|y, \tau) + \\ &- D(y)W(y, \tau|x, 0)[\partial_y W(x', t|y, \tau)] \Big|_{y=a}^{y=b} + W(x', t|y, \tau)[\partial_y D(y)W(y, \tau|x, 0)] \Big|_{y=a}^{y=b} + \\ &- \int_a^b dy [\partial_y^2 D(y)W(y, \tau|x, 0)] W(x', t|y, \tau) - \int_a^b dy \partial_y [A(y)W(y, \tau|x, 0)] W(x', t|y, \tau) + \\ &+ \int_a^b dy \partial_y^2 [D(y)W(y, \tau|x, 0)] W(x', t|y, \tau) = 0 \end{aligned}$$

The highlighted terms cancel out, leaving only boundaries:

$$\begin{aligned} & -A(y)W(x', t|y, \tau)W(y, \tau|x, 0) \Big|_{y=a} - D(y)W(y, \tau|x, 0)[\partial_y W(x', t|y, \tau)] \Big|_{y=a}^{y=b} + \\ & + W(x', t|y, \tau)[\partial_y D(y)W(y, \tau|x, 0)] \Big|_{y=a}^{y=b} = 0 \end{aligned}$$

Now  $W(b, t|x_0, 0) = 0$  (1.173), and also  $W(x', t|b, \tau) = 0$ , as a particle starting in  $b$  escapes immediately from  $[a, b]$ . This makes all the boundary terms vanish at  $y = b$ , leaving only:

$$\begin{aligned} & +A(a)W(x', t|a, \tau)W(a, \tau|x, 0) + D(a)W(a, \tau|x, 0)[\partial_y W(x', t|y, \tau)] \Big|_{y=a} + \\ & -W(x', t|a, \tau)[\partial_y D(y)W(y, \tau|x, 0)] \Big|_{y=a} = 0 \end{aligned}$$

Collecting  $W(x', t|a, \tau)$  allows to recognize a  $J(x, t)$  term:

$$\begin{aligned} & D(a)W(a, \tau|x, 0)[\partial_y W(x', t|y, \tau)] \Big|_{y=a} + \\ & + W(x', t|a, \tau) \underbrace{\left[ A(a)W(a, \tau|x, 0) - [\partial_y D(y)W(y, \tau|x, 0)] \Big|_{y=a} \right]}_{J(a, \tau)} = 0 \end{aligned}$$

But recall that  $J(a, \tau) = 0 \forall \tau$  as per (1.173). So only a term remains:

$$D(a)W(a, \tau|x, 0)[\partial_y W(x', t|y, \tau)] \Big|_{y=a} = 0 \Rightarrow W(a, \tau|x, 0) = 0 \vee \partial_y W(x', t|y, \tau) \Big|_{y=a} = 0 \quad \forall \tau$$

Finally, by integrating the second term:

$$\int_a^b dx' \partial_y W(x', t|y, \tau) = \partial_y \int_a^b dx' W(x', t|y, \tau) = \partial_y G(y, \tau)$$

And evaluating at  $y = a$  leads to:

$$\partial_x G(x, t)|_{x=a} = 0 \tag{1.180}$$

which is the last boundary condition we needed for  $G(x, t)$ .

So, the problem now becomes:

$$\begin{cases} \partial_t G(x, t) = A(x)\partial_x G(x, t) + D(x)\partial_x^2 G(x, t) \\ \partial_x G(x, t)|_{x=a} = 0 \\ G(x, t)|_{x=b} = 0 \end{cases}$$

We can make one last simplification by *removing* the time coordinate. Let's introduce  $T(x)$  as being the *lifetime* of a particle starting at  $x$  - meaning the amount of time needed for that particle to “disappear” by reaching  $b$  (so, in this case,  $T(x)$  coincides with  $T_{\text{ftv}}(b, x)$ , i.e. the *time to the first visit* of  $b$ ). The exact value of  $T(x)$  will depend on the particle's path, making  $T(x)$  a random variable. Note that:

$$G(x, t) = \mathbb{P}(T(x) > t)$$

That is, the survival probability is the probability that the particle *has not yet reached*  $b$  during the time interval  $[0, t]$ , which is equivalent to saying that its lifetime is greater than  $t$ . Denoting with  $\mathbb{P}_{\text{ftv}}(T_b) dT_b$  the probability that a particle will visit  $b$  in the time range  $[T_b, T_b + dT_b]$ , we have:

$$G(x, t) = \mathbb{P}(T(x) > t) = \int_t^{+\infty} \mathbb{P}_{\text{ftv}}(T_b) dT_b = - \int_{+\infty}^t \mathbb{P}_{\text{ftv}}(T_b) dT_b$$

Differentiating with respect to  $t$ :

$$\partial_t G(x, t) = -\mathbb{P}_{\text{ftv}}(t)$$

As we need a function, and  $T(x)$  is a random variable, we consider its *average*, i.e. the *mean time of arrival at  $b$*   $T_b(x)$ :

$$\begin{aligned} T_b(x) &\equiv \langle T(x) \rangle \equiv \int_0^{+\infty} t \mathbb{P}_{\text{ftv}}(t) dt = - \int_0^{+\infty} t \partial_t G(x, t) dt = \\ &= -tG(x, t) \Big|_{t=0}^{t=+\infty} + \int_0^{+\infty} G(x, t) dt \stackrel{(a)}{=} \langle G(x) \rangle \end{aligned} \quad (1.181)$$

In (a) we used that  $tG(x, t)$  vanishes at  $t = 0$  and also at  $t = +\infty$ , because the particle will eventually reach  $x = b$  if given infinite time to do so. It is not clear if  $G(x, t) \xrightarrow[t \rightarrow \infty]{} 0$  *faster* than  $t \rightarrow \infty$ , so that  $tG(x, t) \xrightarrow[t \rightarrow \infty]{} 0$ . Here, we will just assume it, as it is physically reasonable.

Then, we need to translate once again everything to expressions involving  $T_b(x)$ . Fortunately, this time it is much quicker. To get the differential equation, we just integrate (1.178):

$$\int_0^{+\infty} dt \partial_t G(x, t) = A(x) \partial_x \int_0^{+\infty} G(x, t) dt + D(x) \partial_x^2 \int_0^{+\infty} G(x, t) dt$$

And applying (1.181) we get:

$$G(x, t) \Big|_{t=0}^{t=+\infty} = G(x, +\infty) - G(x, 0) = -1 = A(x) \partial_x T_b(x) + D(x) \partial_x^2 T_b(x)$$

as  $G(x, +\infty) = 0$  (no particle lives eternally) and  $G(x, 0) = 0$  (as a particle does not “disappear” immediately for  $x \neq b$ ). Similarly, integrating (1.180) and (1.179) leads to:

$$\begin{cases} A(x) \partial_x T_b(x) + D(x) \partial_x^2 T_b(x) = -1 \\ T_b(x)|_{x=b} = 0 \\ \partial_x T_b(x)|_{x=a} = 0 \end{cases}$$

This is a linear ordinary differential equation. We start by letting  $f(x) = \partial_x T_b(x)$ , leading to:

$$f'(x) = -\frac{A(x)}{D(x)} f(x) - \frac{1}{D(x)} \quad f(a) = 0$$

First consider the *homogeneous* equation:

$$A(x)\Phi(x) + D(x)\Phi'(x) = 0$$

This can be solved by separation of variables:

$$Af + D\frac{d\Phi}{dx} = 0 \Rightarrow \frac{d\Phi}{\Phi} = -\frac{A}{D} dx \Rightarrow \ln|\Phi(x)| = -\int_{x_0}^x \frac{A(y)}{D(y)} dy + c$$

where  $x_0$  is a fixed point  $\in [a, b]$  (it does not matter which one). Exponentiating:

$$\Phi(x) = \exp\left(-\int_{x_0}^x \frac{A(y)}{D(y)} dy\right) k$$

Where  $k = e^c$  will be fixed by the boundary condition  $f(a) = 0$ . First, we need to find the general integral of the inhomogeneous equation - for example by using the method of **variation of parameters**.

**Refresher of variation of parameters.** Consider the following Cauchy problem:

$$\begin{cases} y' = A(t)y + b(t) \\ y(t_0) = y_0 \end{cases}$$

Suppose we know a solution  $\Phi(t)$  of the homogeneous equation  $y' = A(t)y$ . Then  $\Phi' = A\Phi$ . We search for a particular solution for the full equation in the form  $\tilde{\varphi}(t) = \Phi(t)c(t)$ . Substituting in the equation:

$$\Phi'c + c'\Phi = A\Phi c + c'\Phi = A\Phi c + b \Rightarrow c' = \Phi^{-1}b$$

This can be integrated to find  $c$ , and then  $\tilde{\varphi}$ . Then, the general integral will be the sum of the homogeneous solution  $\Phi(t)$  and the particular one  $\tilde{\varphi}$ . Imposing the boundary condition will lead to the general integral:

$$\varphi(t) = \Phi(t)\Phi(t_0)^{-1}y_0 + \Phi(t) \int_{t_0}^t \Phi(\tau)^{-1}b(\tau) d\tau \quad (1.182)$$

Applying formula (1.182) leads to the desired  $f(x)$ :

$$\begin{aligned} f(x) &= \Phi(x)\Phi(a) \cdot 0 + \Phi(x) \int_a^x dz \Phi(z)^{-1} \left[ -\frac{1}{D(z)} \right] = \\ &= \exp\left(-\int_{x_0}^x \frac{A(y)}{D(y)} dy\right) \int_a^x -\frac{dz}{D(z)} \exp\left(+\int_{x_0}^z \frac{A(y)}{D(y)} dy\right) = \\ &= -\int_a^x \frac{dz}{D(z)} \exp\left(+\int_x^z \frac{A(y)}{D(y)} dy\right) \end{aligned}$$

Recall that  $f(x) = \partial_x T_b(x)$ , with  $T_b(b) = 0$ . So, to find  $T_b(x)$  we need one last integration:

$$T_b(x) = \int_{x_0}^x dy f(y) + c$$

Imposing  $T_b(b) = 0$  leads to:

$$T_b(b) = \int_{x_0}^b dy f(y) + c \stackrel{!}{=} 0 \Rightarrow c = - \int_{x_0}^b dy f(y)$$

Leading to:

$$T_b(x) = \int_b^x dy f(y) = \int_x^b dy \int_a^y \frac{dz}{D(z)} \exp \left( - \int_z^y dv \frac{A(v)}{D(v)} \right) \quad (1.183)$$

### 1.29.1 Escape from a potential well

Let's now use (1.183) to solve the problem we started from. So, suppose to have a potential  $U(x)$  with a local minimum at  $x = c$ , and a local maximum at  $x = d$ , with  $c < d$ . Consider a particle starting at  $x = c$ . We wish to compute the average first visit time of  $d$ , denoted with  $\langle T(c \rightarrow d) \rangle$ . This can be done by redefining the system as the half-line  $[-\infty, d]$ , with  $x = -\infty$  being a *reflective* boundary, and  $x = d$  an *absorbing* one. We can do this because we are not interested in the behaviour *after* passing  $d$ , but just in the mean arrival times. So  $A(x) = -\partial_x U(x)/\gamma$ . Supposing to be at equilibrium,  $D(x) \equiv D = 1/(\gamma B)$ . Letting  $a = -\infty$  and  $b = d$  leads to:

$$\begin{aligned} T_d(x) &= \int_x^d dy \int_{-\infty}^y \beta \gamma dz \exp \left( - \int_z^y -dv \frac{\partial_v U(v)}{\gamma} \gamma \beta \right) = \\ &= \beta \gamma \int_x^d dy \int_{-\infty}^y dz \exp(\beta[U(y) - U(z)]) = \\ &= \beta \gamma \int_x^d dy e^{\beta U(y)} \underbrace{\int_{-\infty}^y dz e^{-\beta U(z)}}_{e^{F(y)}} = \beta \gamma \int_x^d dy e^{\beta U(y) + F(y)} \end{aligned}$$

It is not possible to evaluate this integral in the general case. However, in the limit  $\beta \rightarrow \infty$  ( $T \rightarrow 0$ ) we can use the saddle-point approximation.

Recall Laplace's formula:

$$\int_a^b e^{Mf(x)} dx \underset{M \rightarrow +\infty}{\approx} \sqrt{\frac{2\pi}{M|f''(x_0)|}} e^{Mf(x_0)}$$

where  $f'(x_0) = 0$  and  $f''(x_0) < 0$ .

For the integral in  $dz$ ,  $f(z) = -U(z)$ . We search for a maximum of  $f(z)$ , i.e. a minimum of  $U(z)$ , which is  $z = c$ . So:

$$\int_{-\infty}^y e^{-\beta U(z)} dz = \sqrt{\frac{2\pi}{\beta U''(c)}} e^{-\beta U(c)}$$

This is a constant, and can be brought outside the integral over  $dy$ . Then, by applying Laplace's formula once again:

$$\int_c^d dy e^{\beta U(y)} = \sqrt{\frac{2\pi}{\beta |U''(d)|}} e^{\beta U(d)}$$

as now  $f(y) = U(y)$ , and  $U$  has a local maximum in  $y = d$ . Finally, this leads to:

$$T_d(c) \underset{T \rightarrow 0}{\approx} \frac{2\pi\gamma}{\sqrt{U''(c)|U''(d)|}} \exp(\beta[U(d) - U(c)])$$

Note that the mean transition time from  $c$  to  $d$  diverges exponentially as the barrier's height  $U(d) - U(c)$  rises. Equivalently, the *escape transition rate*  $1/T_d(c) \rightarrow 0$ .

## 1.30 Feynman Path Integral

We finish our discussion about the diffusion formalism noting several correspondences with quantum processes.

Recall the Schrödinger equation:

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} \psi(x, t) &= -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x, t) + V(x) \psi(x, t) = \\ &= H(x, \partial_x^2, t) \psi(x, t) \end{aligned}$$

where  $H$  is the *Hamiltonian* operator:

$$H(x, \partial_x^2, t) \equiv -\frac{\hbar^2}{2m} \partial_x^2 + V(x, t)$$

If we consider a free particle ( $V(x, t) \equiv 0$ ), the Schrödinger equation becomes:

$$\partial_t \psi = i \frac{\hbar}{2m} \partial_x^2 \psi \quad \psi(x, 0) = \delta(x - x_0) \quad (1.184)$$

which is very similar to the diffusion equation:

$$\partial_t W(x, t) = D \partial_x^2 W(x, t) \quad W(x, t|x_0, 0) \Big|_{t=0} = \delta(x - x_0) \quad (1.185)$$

In fact, we can map (1.184) to (1.185) by defining a *quantum diffusion coefficient*  $D_{QM} = i\hbar/(2m)$ .

Does this mean that all properties of the diffusion equation - and its solution - can be mapped to the quantum case? Unfortunately, the answer is a bit complex.

Recall that the solution of (1.185) for a particle initially starting in  $x_0$  at  $t_0$  is:

$$W(x, t|x_0, t_0) = \frac{1}{\sqrt{4\pi D(t-t_0)}} \exp\left(-\frac{(x-x_0)^2}{4D(t-t_0)}\right) \quad (1.186)$$

By substituting  $D \leftrightarrow D_{QM}$  we can construct the analogous *quantum* solution:

$$\psi(x, t) = \sqrt{\frac{2m}{4\pi(t-t_0)i\hbar}} \exp\left(i \frac{m}{2\hbar} \frac{(x-x_0)^2}{t-t_0}\right) \quad (1.187)$$

Note that now the exponential argument is *complex*, making basic properties of (1.186) not-trivial. For example, if  $t \rightarrow t_0$ , the exponential in (1.186) tends to a  $\delta$ :

$$\lim_{t \rightarrow t_0} W(x, t | x_0, t_0) = \delta(x - x_0)$$

giving back the starting distribution, as expected.

The same, however, does not happen for (1.187), given the presence of the  $i$ . Nonetheless, it is true that in the limit  $t \rightarrow t_0$ , (1.187) is a *infinitely oscillating function*, meaning that it is 0 *almost* everywhere. This can be proven by using more sophisticated techniques, such as the *stationary phase approximation*.

What about path integrals? If we start with the usual definition and make the substitution  $D \leftrightarrow D_{QM}$  we get:

$$\begin{aligned} \psi(x, t) &= \langle \delta(x(t) - x) \rangle_W = \\ &= \int_{\mathbb{R}^T} \prod_{\tau=0^+}^t \frac{dx(\tau)}{\sqrt{4\pi D_{QM}}} \exp \left( -\frac{1}{4D_{QM}} \int_0^t \left( \frac{dx(\tau)}{d\tau} \right)^2 d\tau \right) \delta(x(t) - x) = \\ &= \int_{\mathbb{R}^T} \prod_{\tau=0^+}^t \frac{dx(\tau)}{\sqrt{4\pi D_{QM}}} \exp \left( \frac{i}{\hbar} \frac{1}{2} m \int_0^t \left[ \frac{dx(\tau)}{d\tau} \right]^2 d\tau \right) \delta(x(t) - x) \end{aligned}$$

Note that now *trajectories* are weighted by a *complex number*. This means that they *are not probabilities* - and in particular, we cannot use Kolmogorov extension theorem to prove the existence of such a measure as the *continuum limit* of a measure defined on *discretized paths*.

However, we note that in the limit  $\hbar \rightarrow 0$ , the integral can be approximated with the saddle-point method, which returns the *classical trajectory* - the one where the *phases oscillate slowly*.

In fact, it can be proven that  $QM$  cannot be derived by statistical mechanics alone: quantum “noise” is very much different from thermal “noise”!

Consider now the more general case of non-zero potential:

$$\frac{\partial}{\partial t} \psi(x, t) = i \frac{\hbar}{2m} \partial_x^2 \psi(x, t) - \frac{iV(x)}{\hbar} \psi(x, t)$$

which is just the quantum evaluated version of the Fokker-Planck equation:

$$\partial_t W(x, t) = D \partial_x^2 W(x, t) - V(x) W(x, t)$$

with the substitutions:

$$\begin{aligned} D &\rightarrow D_{QM} = \frac{i\hbar}{2m} \\ V &\rightarrow \frac{i}{\hbar} V \end{aligned} \tag{1.188}$$

The solution we obtained from discussing the diffusion process is:

$$\begin{aligned} W(x, t | x_0, t_0) &= \langle \exp \left( - \int_0^t V(x(\tau)) d\tau \right) \delta(x(t) - x) \rangle_W = \\ &= \int_{\mathbb{R}^T} \prod_{\tau=0^+}^t \frac{dx(\tau)}{\sqrt{4D\pi}} \exp \left( -\frac{1}{4D} \int_0^t \dot{x}^2(\tau) d\tau - \int_0^t V(x(\tau)) d\tau \right) \delta(x(t) - x) \end{aligned}$$

Applying (1.188) we arrive to the **Feynman path integral**:

$$\psi(x, t) = \int_{\mathbb{R}^T} \prod_{\tau=0^+}^t \frac{dx(\tau)}{\sqrt{4\pi D_{QM}} d\tau} \exp \left( \frac{i}{\hbar} \int_0^t d\tau \underbrace{\left[ \frac{\dot{x}^2(\tau)}{2} - V(x(\tau)) \right]}_{L(\dot{x}, x)} \right) \delta(x(t) - x)$$

To compute it we can resort to variational methods. We define the action functional  $S$  as:

$$S \equiv \int_0^t d\tau L(\dot{x}(\tau), x(\tau))$$

Note that the Feynman path integral *weights* every trajectory with the following quantity:

$$\exp \left( \frac{i}{\hbar} S \left( \{x(\tau)\}_{\tau \in [0, t]} \right) \right)$$

Then, according to the variational method, we can approximate  $\psi(x, t)$  by evaluating it only for the *most contributing trajectory*, i.e. the one that *stationarizes*  $S$ :  $\delta S = 0$ , implying:

$$x_c: \frac{\partial L}{\partial x} - \frac{d}{dt} \frac{\partial L}{\partial \dot{x}} \Big|_{x_c} = 0$$



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