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CHEMICAL DIFFUSION MASTER EQUATIONS: ANALYTICAL SOLUTIONS AND APPLICATIONS

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Contents

Abstract

This thesis is the compilation of 3 of mine and my supervisor's research, that are present in Chapters 4, 5 and 6 from the corresponding papers [Lanconelli et al., 2023, Lanconelli and Perçin, 2024a] and [Lanconelli and Perçin, 2024b] respectively. Our work is centered around the model, which is called the Chemical Diffusion Master Equation (CDME), which enables us to assign probabilities to different configurations of particles undergoing in a reaction of interest at time t. Due to this nature of the model, the model fits into the category of stochastic hybrid systems, where continuous dynamics and discrete events coexist in the same process, which makes the analysis more realistic and more complex compared to other well known models such as Chemical Master Equation (CME) (see [Erban and Chapman, 2020, del Razo et al., 2022]). Because the model is very complex most of the time the research including CDME is only focused at computer simulations.

However in Chapters 4 and 5 we report a general method to treat the system analytically for any reaction where the *reaction* and *diffusion* are considered to be independent. This is very important given the low abundance of such solutions. Moreover we believe seeing an explicit solution gives better insights on how the parameters of the model plays a role. Moreover as will be seen in Chapter 6, the CDME of a *reaction-diffusion* system where the reaction and diffusion *are not* independent will be reported and solved explicitly with an approach particular to the process considered.

Introduction and Organization of the Thesis

In order to describe biochemical dynamics, one has to investigate two main subjects: ***diffusion*** and ***reaction***. The reaction part is well known in general chemistry and diffusion is a well-known topic in stochastic analysis. In this thesis, these two topics will be combined to analyze a reaction-diffusion system, which is extremely useful to model complex biological and chemical phenomena. This analysis will be mainly done via a mathematical model called the Chemical Diffusion Master Equation (CDME) which is used to quantify the probability of observing a given configuration of chemical specimens' locations at a fixed time point in chemical reactions. The nature of the model enables us to utilize many tools from Stochastic Processes and Malliavin Calculus in order to tackle the reaction of interest.

To introduce and work on the idea, there should be other series of topics that should be introduced first. This is why in Chapter 1, we start introducing what are chemical reactions and what are the common ways of analyzing them as done in chemistry. Then towards the end of the chapter, we are going to argue that all these deterministic tools are not sufficient to fully describe the observed deviation from the theory.

Then in Chapter 2 we introduce the so called Chemical Master Equation (CME). This model is the well-known method to introduce the *randomness* to the reaction kinetics by writing a system of ordinary differential equations (ODEs) for the *probability densities* for obtaining a given number of particles at time t, while reflecting the dynamics of the original reaction simultaneously. This way the solution of the system becomes the probability to obtain a given number of particles at a fixed time and hence the randomness element was successfully added to the number of particles. This idea is introduced based on two simple example reactions in Sections 2.2 and 2.3. However it is worth to mention that, all the ideas that are introduced can easily be generalized to any reaction. In the later parts of the aforementioned sections we also provide an analytical approach for the model that is general enough to solve rather simple reactions. Then in Chapter 2.4, a numerical approach called the Gillespie algorithm is introduced and applied to the birth-death type of reaction.

In Chapter 3, finally the CDME model, as described in [del Razo et al., 2022], is introduced and its advantages over the CME are reported. As it will be seen in Chapter 2, the CME is a way of introducing a source of randomness to the number of particles at time t. However, the way that it does so is improved to be significantly more realistic in the CDME. Now in this new model, one can quantify the probability of obtaining any given configuration of particles at time "t". In simpler terms, using this new model, in addition to be able to quantify the number of particles at any given time, one can also assign probabilities to observe the particles in different locations and this is the main advantage of the CDME over the CME. The location dependency introduced in this new model can be used to model the reactions more realistically because the underlying dynamics of the chemical reactions actually depends on it. Mostly, chemical specimens must meet in order to carry out a change in their chemical structure, as one can see in reactions (2.3.1) and (1.1.2) later in this thesis. The fact that the location information already being incorporated in the CDME makes it very useful to realistically model chemical reactions.

Chapters 4, 5 and 6 are original contributions to the literature performed by me and my supervisor. The corresponding papers can be found in [Lanconelli et al., 2023, Lanconelli and Perçin, 2024a] and [Lanconelli and Perçin, 2024b] respectively. In chapters 4 and 5 the CDME is introduced for the birth-death type and mutual annihilation with creation type reactions, followed by the application of the solution methodology developed in [Lanconelli, 2023] (see Chapter 3.4). In Chapter 4, we were able to find an explicit solution for the birth-death type reaction (2.2.1), which is quite important given the low abundance of such results in literature. In Chapter 5 we were able to reach to a partial differential equation (PDE), which that single equation, fully governs the dynamics of a mutual annihilation with creation reaction (2.3.1). We were not able to solve it, nevertheless if it is solved, then using the methodology mentioned in Chapter 3.4 it is possible to explicitly represent the system. In other words, the problem of solving a coupled system of PDEs were transformed to solve a single PDE by us. We believe this can be done by other researchers who specialized in PDE theory in the future, unleashing the dynamics of this reaction. Although an alternative construction for the CDME is already present in [del Razo et al., 2022], it is worth mentioning in the Chapter 5 the new derivation of the CDME is carried out from a more mathematical perspective, very similar to the common derivation for the CME as done in Chapter 2. The novelty of this derivation is that, by only assuming the following set of assumptions below, one can directly reach to the CDME by only using the law of total probability, fully explicitly:

- A single reaction can take place in a sufficiently small time interval.
- The diffusion and reaction of particles are independent.

Where the first assumption is also necessary in the derivation of the CME (see Chapter 2) and the last assumption is expected due to the nature of chemical reactions. With this new derivation scheme, one can see the current construction for the CDME that is presented in [del Razo et al., 2022], is the only one that you reach by following this set of assumptions. Lastly in Chapter 6, a completely new challenge is pursued, where now the derivation and the solution of the CDME of a branching Brownian motion (BBM) process is reported. It is important because as explained in later sections, the key of writing the CDME is having the reaction and diffusion processes being completely independent of each other. However in the BBM the splitting reaction affects the location of the daughter particles, hence the construction in paper [del Razo et al., 2022] is not applicable in this case. Instead we follow a new pipeline to first find the expression that describes the dynamic of the BBM and then see which PDE that it satisfies, corresponding to be the CDME of the branching process. In order to do so, as it will be seen in great detail in Chapter 6, we utilize the common associated properties of the BBM such as the F-KPP equation, McKean representation with the not so common Wick Product to analyze the reaction diffusion systems. Therefore, the resulting PDE is completely novel to our knowledge and we believe this methodology with new tools will open more doors in this field.

Lastly, in the Appendix A, the techniques of Stochastic Calculus used in our research will be provided for the readers to consult when necessary. Due to completeness the techniques are introduced starting from the preliminaries.

Chapter 1

Chemical Kinetics and Reaction Rates

1.1 Deterministic Chemical Kinetics

The main aim of this section, is to systematically describe the chemical reactions as mathematical systems and if possible also solve them. In order to do so, we should mention the field of Chemical Kinetics. Chemical Kinetics is the branch of chemistry where the *"rates"* of reactions are investigated. This deterministic approach, called the chemical kinetics is used by chemists and life scientists to characterize the time evolutions of chemical reactions in large systems to answer questions like: "*How much of this drug will be left at time t*" or "*How much time do we need to see the affect of the reactions?*"

The mathematical system that is introduced should conserve the amount of substances while no reaction takes place. However the number of concentration of particles can alter upon reactions. This is why the logic is always:

$$\big(\text{Generation} - \text{Consumption}\big)_j = \sum_i \mathcal{R}_i v_{i,j} \tag{1.1.1}$$

where the difference of generation and consumption of j'th chemcial species is given as the sum on all possible reaction rates, $\mathcal{R}_i$ (explained in next section) and $v_{i,j} \in \mathbb{R}$, where it is the so called stoichiometric coefficient of the j'th species in i'th reaction. The stoichiometric coefficient explains about the nature of the specimen in the reaction ie. if it is a reactant (used in the reaction) or a product (produced using the reactants) of the reaction. As an example in the following chemical reaction:

$$\begin{matrix} \underline{\mathcal{R}_1} & \qquad\qquad & \underline{\mathcal{R}_2} \\ aA + bB \to cC, & \qquad\qquad & \emptyset \to A, \end{matrix} \tag{1.1.2}$$

where there are two reactions and the stoichiometric coefficients of this reaction are: $v_{1,A} = -a$, $v_{1,B} = -b$, $v_{1,C} = c$ and $v_{2,A} = 1$. It is worth to mention that because the specimens A and B are getting used in the reaction proportional to the constants multiplying them, their stoichiometric coefficients are negative and equal in magnitude to a and b. Using the ideas introduced in expression (1.1.1) on the reaction (1.1.2), one can write the following system of Ordinary Differential Equations (ODE)s:

$$\begin{aligned}\frac{dA}{dt} &= 1\mathcal{R}_2 - a\mathcal{R}_1,\\ \frac{dB}{dt} &= -b\mathcal{R}_1\\ \frac{dC}{dt} &= c\mathcal{R}_1\end{aligned} \tag{1.1.3}$$

with any set of initial conditions as, $A(0) = A_0$, $B(0) = B_0$ and $C(0) = C_0$ where $A_0, B_0, C_0 \geq 0$. When expressed in words, one can see according to the rate that reaction 1 happens (which is $\mathcal{R}_1$), a many A particles and b many B particles will be consumed to generate c many C particles in unit time. Similarly we expect to generate one A particle proportional to how frequent it is for reaction 2 to take place, so $\mathcal{R}_2$, in unit time.

1.1.1 The Rate Law

With the help of the previous section we're able to formalize the reaction (1.1.2) in mathematical form in (1.1.3). However we need to define appropriate reaction rates $\mathcal{R}_i$ if we want to make this approach useful. As shown in [Lecca et al., 2013], it is done using the so called Rate Law. According to it we know the term $\mathcal{R}$ should be a function of the reactants and the products. For the reaction (1.1.2), it is in the form:

$$\mathcal{R} := f(A, B, C). \tag{1.1.4}$$

This explicit formulation of the reaction rate is generally not known a priori. This means that for each type reactions, experimentally the reaction rate should be measured and fitted to a candidate function in the form of (1.1.4), namely with respect to the concentrations (or numbers if the volume of the environment is known) of chemical specimens present. Fortunately due to chemistry being well studied for centuries, for elementary types of reactions in the form

$$aA + bB + \cdots + zZ \to pP$$

the reaction rate is given as:

$$\mathcal{R} = k\, A^{|a|}\, B^{|b|}\, \ldots\, Z^{|z|}. \tag{1.1.5}$$

Where $k \in \mathbb{R}^+$ is the *rate constant* that should be determined empirically and the exponents are the absolute value of the stoichiometric coefficients of the specimens present in the reaction. The *elementary reactions* mentioned here stands for reactions:

1. That happens once the reactants contact with each other.
2. That doesn't have an intermediary step. Meaning when reactants contact, the reaction happens and produces the product.

However it is worth to mention that there are more complex reactions in nature such as enzymatic reactions, where there is a intermediate complex that eases the reaction process as shown in section 8.3 of [Berg et al., 2015]. Thus in such reactions the observed reaction rate is higher than the anticipated reaction rate given by formula (1.1.4), even though the same reactants and products are present. In such cases the formula (1.1.5) is modified to be:

$$\mathcal{R} = k\, A^{\alpha}\, B^{\beta}\, \ldots\, Z^{\zeta}.$$

Where each positive coefficient $\alpha, \beta, \ldots, \zeta$ is fitted experimentally from the data. However for the sake of this thesis we will only focus on elementary reactions because fitting the exponents of formula (1.1.4) is not of our concern. Our research can easily be applied to any reaction, once the exponents are fixed.

1.1.2 Analysis of the Isomerization Reaction

Consider a spontaneous isomerization of a molecule

$$A \underset{k_2}{\overset{k_1}{\rightleftharpoons}} B \tag{1.1.6}$$

where k_1 is the forward reaction rate constant quantifying the dependence of forward reaction rate based on the concentration of A and similarly k_2 is called the backward reaction rate constant and quantifying the dependence of backward reaction rate based on the concentration of B.

As seen in section 33.3 in [Berg et al., 2015] the reaction (1.1.6) is actually present in our ability to perceive the world already. Because a receptor in our eyes called rhodopsin is able to convert itself to an isomerized form in the presence of light and generate visual signals for our nervous system.

Assuming this reaction is an elementary one, we can directly write down the system of ODEs governing the isomerization reaction using the ideas introduced in the previous sections.

$$\begin{aligned} \frac{dA}{dt} &= k_2 B - k_1 A \\ \frac{dB}{dt} &= k_1 A - k_2 B, \end{aligned} \tag{1.1.7}$$

where $A(t)$ and $B(t)$ denote the concentration of the corresponding particles and we choose the initial conditions as $A(0) = A_0$ and $B(0) = 0$. This system can also be written as in matrix notation:

$$\frac{d\mathbf{c}(t)}{dt} = \mathbf{A}\mathbf{c}(t) \qquad \text{where } \mathbf{c}(0) = \mathbf{c}_0,$$

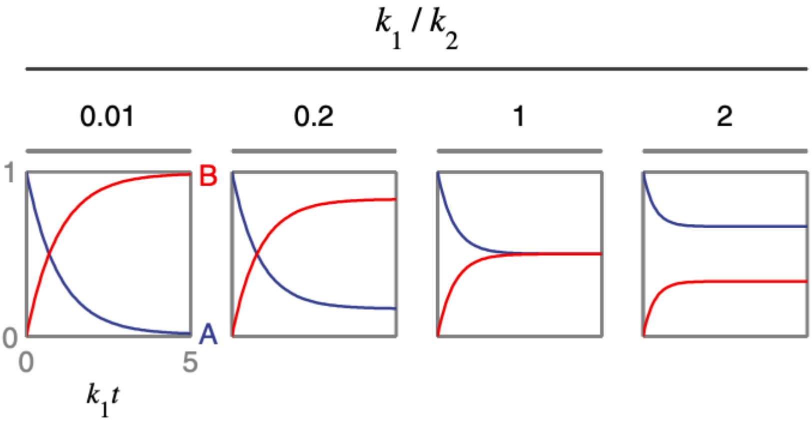


Figure 1.1: The dynamcis of the isomerization reaction (1.1.6), taken from the book [Lecca et al., 2013]. The y-axis is the ratios of $A(t)/A_0$ in blue and $B(t)/A_0$ in red.

where

$$\mathbf{c}(t) := \begin{pmatrix} A(t) \\ B(t) \end{pmatrix} \qquad \text{and} \qquad \mathbf{A} := \begin{pmatrix} -k_1 & k_2 \\ k_1 & -k_2 \end{pmatrix}.$$

Because the system is a linear constant coefficient system of ODEs, one can easily solve it by utilizing Laplace transform (see section 1.4.1 of [Lecca et al., 2013]). Define $\mathbf{C}(s) := \int_0^\infty e^{-st}\mathbf{c}(t)dt$ and it satisfies:

$$s\mathbf{C}(s) - \mathbf{c}_0 = \mathbf{A}\mathbf{C}(s).$$

By rearranging, one gets:

$$\mathbf{C}(s) = \left(s\mathbf{I} - \mathbf{A}\right)^{-1}\mathbf{c}_0.$$

where $\mathbf{I}$ is the identity matrix. Now we can go on and evaluate the inverse of the 2×2 matrix

$$\left(s\mathbf{I} - \mathbf{A}\right)^{-1} = \frac{\begin{pmatrix} s + k_2 & k_2 \\ k_1 & s + k_1 \end{pmatrix}}{s(s + k_1 + k_2)}.$$

Using this explicit relation we can find out the Laplace transformed concentrations:

$$\mathbf{C}(s) = \begin{pmatrix} (s + k_2)A_0 \\ k_1 A_0 \end{pmatrix} \frac{1}{s(s + k_1 + k_2)}.$$

This expression can be inversely Laplace transformed to yield the original solutions:

$$\begin{aligned} A(t) &= A_0 e^{-(k_1+k_2)t} + \frac{k_2}{k_1 + k_2} A_0 \left(1 - e^{-(k_1+k_2)t}\right) \\ B(t) &= \frac{k_1}{k_1 + k_2} A_0 \left(1 - e^{-(k_1+k_2)t}\right). \end{aligned} \tag{1.1.8}$$

The resulting dynamics can be seen in Figure 1.1 for various coefficients for the readers to better visualize the dynamics of the reaction.

1.1.3 Emergence of Randomness, Example of Radioactive Decay

Now we are going to investigate a special case of the previous isomerization example. Consider a radioactive decay reaction:

$$A \xrightarrow{k} \emptyset \tag{1.1.9}$$

where the substance A decays with time and with rate constant $k \in \mathbb{R}^+$. Plugging $B(t) = 1 \ \forall t \geq 0$, $k_1 = k$ and $k_2 = 0$ in isomerization reaction (1.1.6) yields the radioactive decay reaction (1.1.9) considered above. Likewise plugging the same values in equations (1.1.7) and (1.1.8) one gets the ODE that governs the dynamics of the radioactive decay.

$$\frac{dA(t)}{dt} = -kA(t), \qquad A(0) = A_0,$$

and the solution is:

$$A(t) = A_0 e^{-kt} \tag{1.1.10}$$

which the solution intuitively makes sense. Due to the radioactive decay we will have an exponential decay in the number of reactants we have with time. Also in this explicit formula we see how the reaction rate k plays a role, it determines how fast the reactant A will be consumed in the reaction. However what we obtain when we take measurements of an actual radioactive decay is not quite the same:

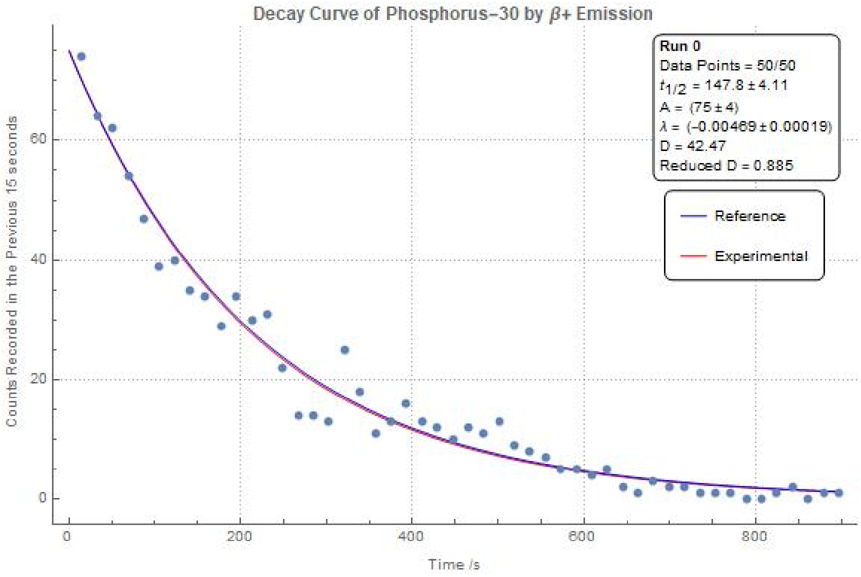


Figure 1.2: A real experimental result published online of Phosphorus-30 radioactive decay. The dots are measured the number of counted emissions blue solid line is the theoretical prediction and red solid line is the fit of expression (1.1.10).

As you can see from Figure 1.2 there will be deviation from the theory and not just due to measurement errors. Each phosphorus atom has a "fixed probability" to decay, so sometimes more will decay and sometimes less and follow the exponential decay *on average*. As stated in [Vlysidis and Kaznessis, 2018], the deterministic chemical kinetics equations are idealized behavior of these reactions in the thermodynamic limit (i.e. infinitely many well mixed specimens in an infinitely large volume). However as you deviate from this idealized case with either low number of specimens or with less mixed conditions, then you start to observe more randomized behavior in these reactions. This leads to the question to be addressed in this thesis: *How to introduce this randomness in the theory?*

Chapter 2

Chemical Master Equation (CME)

2.1 Introduction

The Chemical Master Equation (CME) is the most popular way of introducing randomness to Chemical Kinetics in the literature. The logic is to write down a deterministic system of ordinary differential equations (ODEs) according to the dynamics of the reaction of interest as it is explained in (1.1.1) and shown in examples (1.1.2) and (1.1.6). However this time, the solution of this system will be $\mathbb{P}(N_t = n)$ being the probability to have "n" particles at time "t". In other words, the randomness is introduced in this deterministic system due to solution being the probability density of the stochastic process N_t, the number of particles at time t.

In order to better explain the concept, we start introducing the model on a toy example that is the CME of a birth-death type of reaction. However it should be noted that the procedure can easily be generalized to any higher order reaction.

2.2 The Derivation of the CME of Birth-Death Reaction

Without loss of generality, consider the reaction

$$A \underset{\lambda_c}{\overset{\lambda_d}{\rightleftharpoons}} \varnothing, \tag{2.2.1}$$

where $\lambda_d, \lambda_c \in \mathbb{R}^+ \cup \{0\}$ and A stand for the concentration of the specimen. In this reaction the specimen A is being degraded with a rate constant λ_d and with a constant rate λ_c new A molecules are pumped in to our system. In this new setting our understanding of the reaction rate constants should be modified as *"The real number that quantifies the probability to have the reaction per unit time"*. In the light of this knowledge, the master equation for this reaction can be written with an assumption that is:

Assumption 2.2.1. *For a sufficiently small time interval $[t, t+h)$ it is assumed that only a single reaction can take place.*

With the assumption 2.2.1, the law of total probability and the nature of the reaction we can write the following about the birth-death type reaction (2.2.1):

$$\begin{aligned}\mathbb{P}(N^A_{t+h}=n) = &\underbrace{\mathbb{P}(N^A_{t+h}=n|N^A_t=n-1)}_{h\lambda_c}\mathbb{P}(N^A_t=n-1)\\ &+\underbrace{\mathbb{P}(N^A_{t+h}=n|N^A_t=n+1)}_{h(n+1)\lambda_d}\mathbb{P}(N^A_t=n+1)\\ &+\underbrace{\mathbb{P}(N^A_{t+h}=n|N^A_t=n)}_{\substack{(1-h\lambda_c)(1-hn\lambda_d)\\ =1-h\lambda_c-hn\lambda_d+\mathcal{O}(h^2)}}\mathbb{P}(N^A_t=n)\\ &+\underbrace{\mathbb{P}\{\text{multiple particle reactions}\}}_{\mathcal{O}(h^2)}\end{aligned} \tag{2.2.2}$$

where $n \in \mathbb{Z}^+ \cup \{0\}$. Now each term will be explained:

- $\mathbb{P}(N^A_{t+h}=n)$ is the probability to obtain n many particles of specimen A at time $t+h$.
- $\mathbb{P}(N^A_{t+h}=n|N^A_t=n-1)$ is the probability to obtain n many particles of specimen A at time $t+h$, given that there were $n-1$ particles at time t. This means a creation reaction should take place in time window $[t, t+h)$ and this is why this term is also equal to $\lambda_c h$.
- Similarly, $\mathbb{P}(N^A_{t+h}=n|N^A_t=n+1)$ is the probability to obtain n many particles of specimen A at time $t+h$, given that there were $n+1$ particles at time t. This means a degradation reaction should take place in time window $[t, t+h)$ among any of the $n+1$ particles and this is why this term is also equal to $(n+1)h\lambda_d$.
- $\mathbb{P}(N^A_{t+h}=n|N^A_t=n)$ is the probability to obtain n many particles of specimen A at time $t+h$, given that there were already n particles at time t. This means in no reaction should happen in time window $[t, t+h)$, which is product of the probabilities of $\{\text{No creation}\}\times\{\text{No degradation}\}$. This identity is given by

  $$(1-h\lambda_c)\times(1-nh\lambda_d) = 1-h\lambda_c-nh\lambda_d+\mathcal{O}(h^2).$$

- $\mathbb{P}\{\text{multiple particle reactions}\}$ is the term taking into account of all other possible reactions. Like $\mathbb{P}(N^A_{t+h}=n|N^A_t=n-2)\mathbb{P}(N^A_t=n-2)$, which will be possible only if 2 *net* creation reactions happens (i.e. 2 creations or 3 creations and 1 degradation, 4 creations and 2 degradation etc.). However because of assumption 2.2.1 all reactions will scale with h so having more than 1 reaction will scale with $\mathcal{O}(h^2)$ as shown in expression (2.2.2).

Bearing all these facts in mind and easing the notation by letting $\mathbb{P}(N_t = n) := \rho_n(t)$ equation (2.2.2) becomes:

$$\begin{aligned}\rho_n(t+h) &= h\lambda_c\rho_{n-1}(t) + h(n+1)\lambda_d\rho_{n+1}(t)\\ &\quad + (1 - h\lambda_c - hn\lambda_d)\rho_n(t) + O(h^2)\end{aligned}$$

Rearanging the terms and taking the limit $h \to 0$ yields:

$$\begin{aligned}\frac{d\rho_n(t)}{dt} &= \lambda_c\rho_{n-1}(t) + (n+1)\lambda_d\rho_{n+1}(t)\\ &\quad - (\lambda_c + n\lambda_d)\rho_n(t)\end{aligned} \tag{2.2.3}$$

for $n \in \{0, 1, 2, ...\}$ and with the initial condition of our choice:

$$\rho_0(0) = 1 \text{ and } \rho_n(0) = 0\,\forall n, \tag{2.2.4}$$

so this means initially there were no particles present. The infinite system of ODE's in expression (2.2.3) is called the Chemical Master Equation or CME for the reaction (2.2.1) and the solution $\rho_n(t)$ is the probability of observing n particles at time t. It is evident that the expression (2.2.3) resembles the deterministic dynamics since if we just set focus on the isomerization example in (1.1.6) and make the substitutions $k_1 = \lambda_d$, $k_2 = \lambda_c$, $B(t) = 1\ \forall t \geq 0$ and $A_0 = 0$ one gets the birth-death reaction introduced in (2.2.1) with the dynamics.

$$\frac{dA(t)}{dt} = \lambda_c - \lambda_d A(t),$$

where again the degradation term depends on the *number* of particles through the term $-\lambda_d A(t)$, resembling the term $-\lambda_d n$ in (2.2.3) and we see fixed number of particles being created via the constant λ_c, similar to the term $\lambda_c\rho_{n-1}(t)$. In the CME version, there are additional terms such as $-\lambda_c\rho_n(t)$ and $(n+1)\lambda_d\rho_{n+1}(t)$ due to the nature of the problem. As stated earlier, these terms arise due to the derivation of the model where instead of the exact number of particles, we are interested in probability densities and probability flows for each state n.

In other words, one can see from our example starting with the reaction (2.2.1), we were able to preserve the creation and degradation dynamics of the reaction inside the system (2.2.3) and still able to introduce randomness in the number of particles N_t. Lastly it is important to see how self-justified assumption 2.2.1 is. The assumption states that for a sufficiently short time frame only a single reaction can take place and then one can see that just before of equation (2.2.3), h is considered to approach 0.

2.2.1 Using Generating Function Method for Analytical Solution of the CME of Birth-Death Type Reactions

The complexity of solving the CME analytically is apparent from the expression (2.2.3). It is because the solution of all the states are entangled, that is you need the solution of states $\rho_{n-1}(t)$ and $\rho_{n+1}(t)$ too in order to solve $\rho_n(t)$ and this is true for all of the infinitely many n's. This means one has to solve the whole system all at once. The most common way to approach this problem is the so called probability generating function as explained in detail in [Erban and Chapman, 2020]. Basically one defines a function

$$G(z,t) := \sum_{n\geq 0} z^n \rho_n(t) \tag{2.2.5}$$

where $z \in [-1,1]$ to prevent the divergence of the series.

Remark 2.2.2. *Note that $G(1,t) = 1$ due to the law of total probability.*

It turns out when one multiplies the n'th state of the CME by z^n and sum all of the states, one can express the result as a single partial differential equation (PDE) in terms of $G(z,t)$. If that resulting PDE is solvable then the CME of interest is solvable as well. For illustration let's continue with our previous example, so we consider the reaction (2.2.1) and we have the CME (2.2.3), then for each state we multiply with corresponding z^n and get:

$$\begin{aligned}\frac{d(z^n\rho_n(t))}{dt} =& \lambda_c z^n \rho_{n-1}(t) + (n+1)\lambda_d z^n \rho_{n+1}(t) \\ &- z^n(\lambda_c + n\lambda_d)\rho_n(t)\end{aligned}$$

which can also be written as:

$$\begin{aligned}\frac{d(z^n\rho_n(t))}{dt} =& z\lambda_c z^{n-1} \rho_{n-1}(t) + \lambda_d \frac{dz^{n+1}}{dz} \rho_{n+1}(t) \\ &- z^n(\lambda_c + n\lambda_d)\rho_n(t)\end{aligned}$$

then when this equation is summed over all the possible values of n, one gets:

$$\frac{\partial G(z,t)}{\partial t} = (z-1)\lambda_c G(z,t) + \lambda_d(1-z)\frac{\partial G(z,t)}{\partial z} \tag{2.2.6}$$

Remark 2.2.3. *The partial derivative with respect to z is present due to the degradation reaction of the particle. So in single particle reactions,when the generating function methodology is used, the resulting PDE can be at most first order.*

As also done in [Lanconelli et al., 2023, McQuarrie, 1967a] considering the initial condition in (2.2.4) with the boundary condition in remark 2.2.2 the solution is:

$$G(z,t) = \exp\left\{\frac{\lambda_c}{\lambda_d}\left(1-e^{-\lambda_d t}\right)(z-1)\right\} \tag{2.2.7}$$

and it can be checked by direct verification. Because the $G(z,t)$ is already present we can use it to work our way back to $\rho_n(t)$ due to the relation stated in (2.2.5). As one can see, due to this relation:

$$\rho_n(t) = \frac{1}{n!}\left(\frac{\partial^n G(z,t)}{\partial z^n}\right)\bigg|_{z=0},$$

since now we have the explicit expression of $G(z,t)$ in (2.2.7) the solution of our interest is:

$$\rho_n(t) = \frac{\left(\frac{\lambda_c}{\lambda_d}(1-e^{-\lambda_d t})\right)^n}{n!} e^{-\frac{\lambda_c}{\lambda_d}(1-e^{-\lambda_d t})}$$

which we notice as a Poisson distribution with parameter $\frac{\lambda_c}{\lambda_d}(1-e^{-\lambda_d t})$. The whole pipeline followed for this example of reaction (2.2.1) can be summarized in Figure 2.1.

Moreover we notice that as $t \to \infty$ the density $\rho_n(t)$ converges to another function:

$$\phi(n) := \frac{(\lambda_c/\lambda_d)^n}{n!} e^{-\lambda_c/\lambda_d}, \tag{2.2.8}$$

which is called the *stationary distribution* of the birth-death type of reaction (2.2.1) because it won't change with time anymore. We also see that it is again a Poisson density with parameter λ_c/λ_d. Another example is provided in the next section.

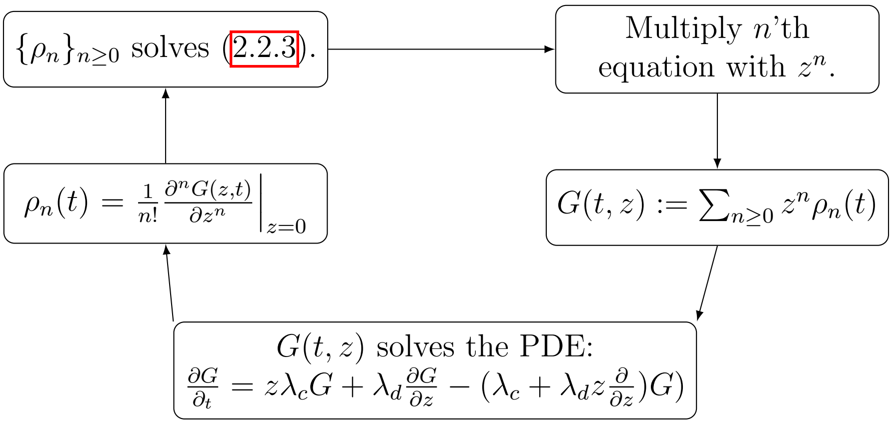


Figure 2.1: The figure summarizing the analytical pipeline followed to approach the system of ODEs in (2.2.3).

2.3 The Derivation of the CME of Mutual Annihilation Reaction

In this section we will reinforce the understanding of the CME and see how to apply it to another reaction. This time consider the reaction:

$$A + A \xrightarrow{\lambda_d} \varnothing, \tag{2.3.1}$$

where it means 2 A molecules collide on average with reaction rate constant λ_d and annihilate each other. This is an example of a *bimolecular* reaction that often tends to be harder to solve analytically. This is because similar to the explanation given in Remark 2.2.3, reactions involving 2 particles will yield a second order term in z in the resulting PDE of the generating function methodology, as will be demonstrated later. Similar to the previous case we can write the system of equations obeyed by the densities of the N_t according to our reaction of interest (2.3.1) as.

$$\begin{aligned}\mathbb{P}(N^A_{t+h} = n) = &\underbrace{\mathbb{P}(N^A_{t+h} = n | N^A_t = n+2)}_{h\frac{(n+2)(n+1)}{2}\lambda_d}\mathbb{P}(N^A_t = n+2)\\ &+ \underbrace{\mathbb{P}(N^A_{t+h} = n | N^A_t = n)}_{1-h\frac{n(n-1)}{2}\lambda_d}\mathbb{P}(N^A_t = n)\\ &+ \underbrace{\mathbb{P}\{\text{multiple particle reactions}\}}_{\mathcal{O}(h^2)},\end{aligned} \tag{2.3.2}$$

where the first thing to notice is that there is no creation term as before in (2.2.2) due to the nature of the reaction (2.3.1) being only composed of mutual annihilation. Then we can argue that, in the small time interval h, the probability to choose 2 particles among $n+2$ particles and annihilate them ($\mathbb{P}(N^A_{t+h} = n | N_t = n+2)$) is given by the expression $\frac{(n+2)(n+1)}{2}h\lambda_d$, this is due to the fact that the degradation reaction should happen in time frame $[t, t+h]$ by the term $h\lambda_d$ and we need to select 2 particles among the $n+2$ particles to degrade by the term $(n+2)(n+1)/2$. Similarly the probability of no reaction ($\mathbb{P}(N^A_{t+h} = n | N_t = n)$) is set as: $1 - \frac{n(n-1)}{2}h\lambda_d$ so that it is 1 minus the probability of selecting 2 particles among n many and annihilate them in small time interval h.

When the terms are rearranged and $h \to \infty$ limit is considered, the result is:

$$\frac{d\rho_n(t)}{dt} = \frac{(n+2)(n+1)}{2}\lambda_d\rho_{n+2}(t) - \frac{n(n-1)}{2}\lambda_d\rho_n(t) \tag{2.3.3}$$

2.3.1 Using Generating Function Method for Analytical Solution of the CME of Mutual Annihilation Type Reactions

When in a similar sense one defines the $G(t,z) := \sum_{n\geq 0} z^n\rho_n(t)$ for $z \in [-1,1]$ and multiplies the n'th equation with z^n and sum all the system, the equation that $G(t,z)$ satisfies is:

$$\frac{\partial G(t,z)}{\partial_t} = \frac{\lambda_d}{2}(1-z^2)\frac{\partial^2 G(t,z)}{\partial z^2} \tag{2.3.4}$$

Remark 2.3.1. *Due to the same reason explained in Remark 2.2.3, it can be seen that the terms:*

$$n(n-1)\rho_n(t)z^n = z^2\rho_n(t)\frac{d^2z^n}{dz^2} \quad \text{and} \quad (n+2)(n+1)\rho_{n+2}(t)z^n = \rho_{n+2}(t)\frac{dz^2z^{n+2}}{dz^2},$$

give rise to the second order derivative with respect to z, which makes it significantly harder to solve the equation (2.3.4) than (2.2.6).

Noting the reason of the presence of second order derivative it can be said that bimolecular reactions result in second order PDEs in generating function method. This is the main reason of finding analytic solutions to higher order reactions.

Nevertheless this reaction with only a mutual annihilation part can again be solved analytically by following the steps of [McQuarrie, 1967b] in Section III-b Bimolecular reactions. One can use the separation of variables methodology to guess a solution in the form $G(t, z) := T(t)C(z)$ and equate

$$\frac{dT(t)}{d_t}\frac{1}{T(t)}\frac{2}{\lambda_d} = (1-z^2)\frac{d^2C(z)}{dz^2}\frac{1}{C(z)} = constant.$$

Since otherwise two functions that depend on different parameters t and z can't be equal to each other. Since the equation is linear any solution's linear combination is also a solution. This is why if one chooses the constant as $-n(n-1)$ for $n \in \mathbb{N}$ then one can obtain all the non-exploding solutions $T(t)$ and $C(z)$. Following the results of the book [McQuarrie, 1967b], same chapter the solution of (2.3.4) is stated as:

$$G(t, z) = \sum_{n\geq 0} A_n C_n(z) T_n(t), \tag{2.3.5}$$

where

$$T_n(t) = e^{-\frac{\lambda_d}{2}n(n-1)t}$$

and $C_n(z)$ is the function so called *Gegenbauer polynomial* and it is the solution to the ODE:

$$(1-z^2)\frac{d^2C_n(z)}{dz^2} = -n(n-1)C_n(z).$$

Moreover the book also uses the initial condition that at time 0, there are n_0 many particles only so $G(0, z) = z^{n_0} \Rightarrow \frac{\partial G(t,z)}{\partial z} = n_0 z^{n_0-1}$ together with the properties of the Gegenbauer polynomials, finds the coefficients A_n too. One can see how demanding it is to just consider a mutual annihilation itself (without any creation reaction as it will be investigated in Chapter 5). Since $G(t, z)$ can be expressed using (2.3.5) where everything on the right hand side is known, similar to what have been explained in Figure 2.1, one can work their way back to $\rho_n(t)$ utilizing the analytical solution of $G(t, z)$.

However all this work was to solve a simple mutual annihilation reaction and it gives an idea on how fast the problem gets complicated with a little change. Imagine another more complex but still a lot simpler than real life reactions. Imagine

$$\begin{aligned} A + A &\xrightarrow{k_1} \emptyset, \qquad & A + B &\xrightarrow{k_2} \emptyset, \\ \emptyset &\xrightarrow{k_3} A, & \emptyset &\xrightarrow{k_4} B. \end{aligned} \tag{2.3.6}$$

Where this time similar to the approach in Figure 2.1, one can let $\rho_{n,m}(t)$ be the probability of having n many A particles and m many B particles at time t and write down the CME. Then similarly define a function:

$$G(w, z, t) := \sum_{n\geq 0, m\geq 0} w^m z^n \rho_{n,m}(t).$$

So the same idea prevails, if one can obtain an explicit representation for $G(w, z, t)$, then it can be used to reach back to $\rho_{n,m}(t)$. However the problem lies in the complexity of the PDE satisfied by $G(w, z, t)$. As explained in Remark 2.3.1, the result will be 2nd order in derivatives with respect to w and z. This means the system is very complex to treat analytically. As you can imagine for more realistic reactions most of the time the PDE of $G(z, t)$ is not analytically solvable and in literature mostly algorithms like Gillespie or other numerical simulation techniques are used. This situation makes the analytical solutions of any reaction be extremely valuable because they are not very abundant and these analytical solutions can be used to check the accuracy of the numerical methods as well.

2.4 The Gillespie Algorithm

The most popular algorithm to track down any Chemical Master Equation is the so called *Gillespie Stochastic Simulation Algorithm.* Now in this section it will be introduced for any reaction and the results simulations from the book [Erban and Chapman, 2020] will be given for the birth-death type of reactions mentioned above in Chapter 2.2. In general it works as the following, for any reaction of interest:

Sketch of Gillespie Algorithm

1. Given that there are fixed number of specimen(s) at time t. Simulate the time required for the next reaction to take place (τ).
2. Decide according to the reaction rates which reaction should happen.
3. Repeat the process for the time point $t + \tau$.

Let's define τ as the time required to have a reaction. Namely if at time t we have a fixed number of chemical specimens than at time $t+\tau$ due to one of the reactions we consider, this distribution will change. Surely τ is a random variable and we're interested in its density to simulate the dynamics. The following result ensures the pdf of *tau*.

Proposition 2.4.1. *The length of time without a reaction, in other words the τ is an exponential random variable with parameter λ being the sum of every rate of reaction we consider.*

Proof. Let $\mathbf{N}(t)$ be the vector of all the number of specimen(s) considered in reaction(s) of interest. For example $\mathbf{N}_t = N_t^A$ in (2.2.2) and (2.3.2) since there is only a single specimen, which is A. However if one considers a reaction such as $A + B \xrightarrow{\lambda} C$, then $\mathbf{N}_t$ becomes $(N_t^A, N_t^B, N_t^C)^T$. Define the density of τ as:

$$f(\mathbf{N}_t, s)ds = \begin{array}{c}\text{Probability that the number of}\\ \text{particles at time } t \text{ is } \mathbf{N}_t \text{ and next}\\ \text{reaction will take place in interval}\\ [t+s, t+s+ds).\end{array}$$

similarly define:

$$g(\mathbf{N}_t, s) = \begin{array}{c}\text{Probability that the number of} \\ \text{particles at time } t \text{ is } \mathbf{N}_t \text{ and no} \\ \text{reaction will happen in interval} \\ [t, t+s)\end{array} .$$

This means, one can also express $f(\mathbf{N}_t, s)ds$ as:

$$f(\mathbf{N}_t, s)ds = g(\mathbf{N}_t, s)\lambda(t)ds \tag{2.4.1}$$

where $\lambda(t)$ is the sum of all the rates of the reactions considered at time t. For example for the birth death reaction considered in (2.2.1) $\lambda(t) = \lambda_c + N_t^A\lambda_d$ and similarly for the mutual annihilation reaction (2.3.1) $\lambda(t) = N_t^A(N_t^A - 1)\lambda_d/2$. Moreover because we assume no reaction will take place in interval $[t, t+s)$, note that $\lambda(t) = \lambda(t+s)$.The expression (2.4.1) makes sense because the probability that one reaction will take place in the interval $[t+s, t+s+ds)$ means for the interval $[t, t+s)$ it shouldn't happen (the function $g(\mathbf{N}_t, s)$ takes care of that) times the probability to have one of the reactions in that infinitesimal time interval, $\lambda(t)ds$.

Now we will focus on expression what $g(\mathbf{N}_t, s)$ looks like explicitly. Note that the following relation is true:

$$g(\mathbf{N}_t, s+\Delta s) = g(\mathbf{N}_t, s)(1 - \lambda(t)\Delta s).$$

What is written above is nothing but simply the probability for no reaction to take place for the interval $[t, t+s+\Delta s)$ is prodcut of the probability to have no reaction in interval $[t, t+s)$ times $[t+s, t+s+\Delta s)$. When the terms are rearranged and lim δs goes to 0 is considered:

$$\lim_{\Delta s \to 0} \frac{g(\mathbf{N}_t, s+\Delta s) - g(\mathbf{N}_t, s)}{\Delta s} = \frac{dg(\mathbf{N}_t, s)}{ds} = -g(\mathbf{N}_t, s)\lambda(t),$$

and this ODE can be solved uniquely using the initial condition that $g(\mathbf{N}_t, 0) = 1$ so that

$$g(\mathbf{N}_t, s) = e^{-\lambda(t)s}. \tag{2.4.2}$$

Substituting equation (2.4.2) to (2.4.1) one gets:

$$f(\mathbf{N}_t, s)ds = \lambda(t)e^{-\lambda(t)s}ds \tag{2.4.3}$$

which for a fixed t, is the exponential distribution with parameter $\lambda(t)$. ☐

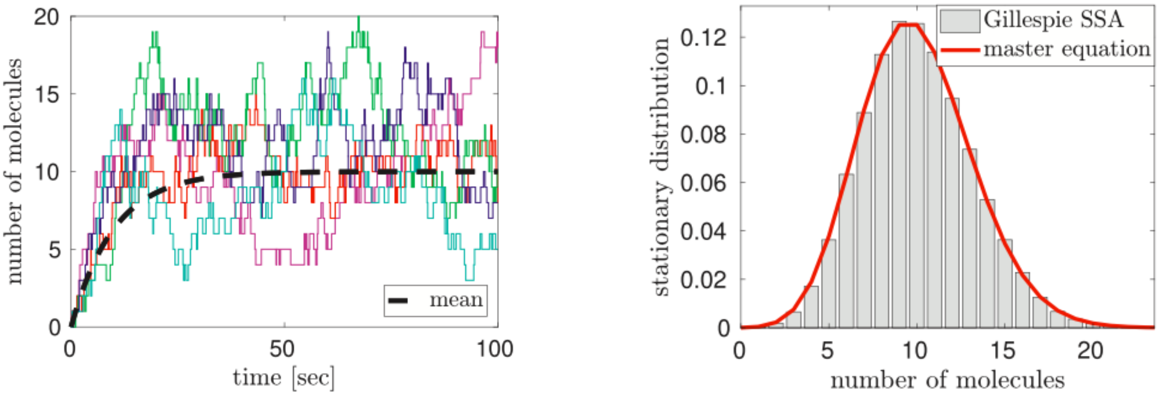
The Lemma 2.4.1 enables us to simulate τ on computer and perform the 1'st step of the Gillespie Algorithm. The only need is to generate a random number that is exponentially distributed.

2.4.1 Case Study for Birth-Death Type of Reactions

In the book [Erban and Chapman, 2020] the algorithm is applied on birth-death type reactions and the explicit algorithm and results are given below in Figure 2.2:

The Gillespie Algorithm for bdCME in (2.2.1)

1. For the state at time t. Generate 2 random numbers, r_1 and r_2, uniformly distributed in $[0, 1]$.
2. Compute when the next reaction will take place by
$$\tau = \frac{1}{\lambda(t)} \ln \left[\frac{1}{r_1} \right]$$
where $\lambda(t) = \lambda_c + N_t^A \lambda_d$. This way τ will be a random number generated according to an exponential distribution with parameter $\lambda(t)$.
3. Decide which reaction to take place, based on the relative magnitude of the reactions
$$N_{t+\tau}^A = \begin{cases} N_t^A + 1 & \text{if } r_2 < \lambda_c/\lambda(t) \\ N_t^A - 1 & \text{if } r_2 \geq \lambda_c/\lambda(t) \end{cases}$$
4. Apply the first step for the state at time $t + \tau$.



(a) (b)

Figure 2.2: The simulation results of the birth-death type of reactions by the Gillespie algorithm with parameters $N_0^A = 0$, $\lambda_d = 0.1$ and $\lambda_c = 1$. In Figure 2.2a we see many sample paths simulated via the algorithm and the mean of simulations reported in dashed black line. Figure 2.2b is the histogram generated by the numerical distribution of simulation results of Figure 2.2a for 10^5 reactions to take place and then normalized. The red line is the stationary distribution (2.2.8) for comparison.

It is worth showing how the CME, to some extend, preserves the dynamics of the deterministic chemical kinetics. The black dashed line in Figure 2.2a is the mean of the simulations where it clearly reflects the overall dynamics of the deterministic isomerization reaction shown in Figure 1.1 under the substitutions: $k_2 = \lambda_d$, $k_1 = \lambda_c$, $A(t) = 1$ $\forall t > 0$, yields the same birth-death type of reaction for particle B.

As one can see this algorithm is very handy since it can be applied to *any* reaction. In the book [Erban and Chapman, 2020] one can see that in section 1.5 it is applied to the reaction (2.3.6), which we emphasized on how demanding it is to approach analytically. In the same section of the book there are also the results of the simulation reported in Figure 1.5.

It is very impressive to have a method that can be applied to any reaction without restriction, still without an analytic solution at hand, one can't tell how good or bad the simulation results are which is why the red line in Figure 2.2b is reported.

Chapter 3

Chemical Diffusion Master Equation (CDME)

3.1 Introduction

As stated in [del Razo et al., 2022], in real life most of the biological and chemical phenomena one observes is a combination of reaction and diffusion of particles. Some examples are already provided in [Fisher, 1937, Kolmogorov et al., 1937, Fradin, 2017]. Because CME simply misses the location information of the specimens the model can be improved further by utilizing the same principles we already used but also including the location of the particles and therefore also incorporating the *diffusion* concept in our reaction equations. This way, the resulting model becomes the Chemical Diffusion Master Equation (CDME).

The CDME is first described in [del Razo et al., 2022] as a family of Fokker-Planck equations where each equation describes the diffusion processes for a given n-particle probability densities, also reflecting the dynamics of the reaction that it models, in a similar way to CME. In this chapter basically the approach of [del Razo et al., 2022] will be summarized, then on Chapter 4 the model will be applied to a birth-death type of reaction (as in (2.2.1)) and in Chapter 5, first the model will be derived and then applied on a mutual annihilation (reaction (2.3.1)) with a constant creation reaction and then analyzed. This is why instead of the actual derivation that is present in Chapter 5, in this chapter the intuitive description of the model will be present. Lastly in Chapter 6, we will see how to write down and solve CDME of a branching Brownian motion. A reaction where the reaction and diffusion processes are *not* independent, hence the remark 3.2.1 won't be true for that example, which is the main obstacle.

3.2 Description of the Chemical Diffusion Master Equation (CDME)

The main objective of this section is to propose a system of PDEs and explain their connection with the reaction diffusion systems such as chemical reactions. In the light of the paper [del Razo et al., 2022] we propose the system:

$$\begin{aligned}\partial_t \rho(t) &= \left(\mathcal{D} + \sum_{r=1}^{S} \mathcal{R}_r\right) \rho(t), \\ \partial_v \rho_n(t, \mathbf{x_n}) &= 0, \ \forall n \geq 1, \ \mathbf{x_n} \in \partial \mathbb{X}_\mathbf{n}\end{aligned} \tag{3.2.1}$$

where each element will be now explained in detail:

- $\rho(t)$ is the vector of probability densities for all number of particles:

  $$\rho(t) := (\rho_0(t), \rho_1(\cdot, t), \dots, \rho_n(\cdot, t), \dots)^T.$$

  In this setting $\rho_n(\mathbf{x_n}, t)$ is read as the probability to obtain a total of n particles reported in the vector $\mathbf{n} = (n, m, \dots)^T$ depending on how many specimens are considered, at time t around the location vector $\mathbf{x_n}$. One can see the length of the vector $\rho(t)$ can be infinite because the nature of the chemical reactions the number of particles are unbounded. As an example consider a case of pure creation by setting $\lambda_d = 0$ in reaction (2.2.1). One important thing to highlight is that, because the particles belonging to the same chemical specimen are indistinguishable, the densities $\rho_n(\mathbf{x_n}, t)$ are required to be symmetric in the location variables. If there is a single chemical specimen, then there is no need to vectorize the model and hence:

  $$\rho_n(x_1, x_2, \dots, x_n, t) = \rho_n(x_{\sigma_1}, x_{\sigma_2}, \dots, x_{\sigma_n}),$$

  where $\sigma_j, \ j \in \{1, 2, \dots, n\}$ are the permutations of the set $\{1, 2, \dots, n\}$.

- The vector $\mathcal{D}$ is a collection of operators $\mathcal{D}_n$ that are describing the movement of the particles, meaning the the operator making n particles move in the space without any reactions. If one separates $\rho_n(\mathbf{x_n}, t)$ as:

  $$\rho_n(\mathbf{x_n}, t) = p_n(\mathbf{x_n}, t | \mathbf{N}_t = \mathbf{n}) \mathbb{P}[\mathbf{N}_t = \mathbf{n}].$$

  Meaning the $p_\mathbf{n}(\mathbf{x_n}, t | \mathbf{N}_t = \mathbf{n})$ is the probability to obtain the n particles around location $\mathbf{x_n}$ at time t if it is given that there are specified number of particles ($\mathbf{n}$) for all chemical specimens. So in some sense, because the number of particles are given, the reaction nature of the dynamics can be ignored and only the particle movements can be described by $p_n(\mathbf{x_n}, t | \mathbf{N}_t = \mathbf{n})$.

  Then explicit form of the operator $\mathcal{D}_n$ is:

  $$\mathcal{D}_n p_n = -\sum_{i=1}^{n} \nabla_i \cdot (A_i p_n) + \sum_{i,j}^{n} \nabla_i \cdot (D_{ij} \nabla_i p_n),$$

where $A_i(\mathbf{x_n}, t)$ describes the drift of the particles and the D_{ij} is the element in the ith row and jth column of the 3×3 diffusion matrix if a 3D diffusion is considered.

As an example when the movement of the particles are sourced by a potential $U(\mathbf{x_n})$, then the operator A_i has the explicit form:

$$A_i = -\sum_{j=1}^{n} D_{ij}\nabla_j U.$$

However for the sake of this thesis we will always assume pure diffusion for the particles without any deterministic drift. This assumption simplifies the operator $\mathcal{D}_n$:

$$\mathcal{D}_n\rho_n = D\Delta\rho_n,$$

where D is the diffusion coefficient and Δ is the Laplacian operator. This assumption makes the particles diffuse as the regular Brownian motion.

- The space that only one particle freely diffuses is denoted as $\mathbb{X}$ and $\mathbb{X} \subseteq \mathbb{R}$ or $\mathbb{X} \subseteq \mathbb{R}^3$, depending on if the particles are considered to diffuse only in 1 dimension or in 3 dimensions respectively. Then one can express the space of n particles diffusing as the tensor space $\mathbb{X}_n := \mathbb{X}^{\otimes n}$, in words it is the tensor product of n many single particle spaces.
- ∂_v is denoting the unit normal vector along the surface of $\mathbb{X}_n$, which is also denoted as $\partial\mathbb{X}_n$. The boundary conditions in equation (3.2.1) is the reflective boundary conditions enabling there is no probability flux at the boundaries of the diffusive space. In other terms the probability is conserved inside the space $\mathbb{X}_n$ $\forall n > 0$.
- Lastly, $\mathcal{R}_r$ is the r'th reaction among the S ones considered. Which is parametrized by the r'th reaction rate λ_r. If one collects all reactions into

  $$\mathcal{R} = \sum_{r=1}^{S} \mathcal{R}_r$$

  then one can utilize the simplified matrix notation (3.2.2).

Now 2 remarks will be introduced about the model in general

Remark 3.2.1. *A* pure *movement process without any reaction would look like,*

$$\frac{\partial\rho(t)}{\partial t} = \mathcal{D}\rho(t).$$

Similarly if you consider a process with pure S *many reactions without any diffusion, one can express this dynamic by the following equation:*

$$\frac{\partial\rho(t)}{\partial t} = \sum_{r=1}^{S} \mathcal{R}_r\rho(t).$$

Which is analogous to the equation in (1.1.1). Note that the fact that we can combine both of these operators linearly on $\rho(t)$ in the expression (3.2.1), is the assumption of independence between the reaction and diffusion processes. This is the core of the assumption for writing the CDME of any reaction. If the reaction and diffusion are not assumed to be independent than the explicit form of expression is not straightforward (as it will be seen in Chapter 6).

Remark 3.2.2. *Due to how the boundary conditions of expression (3.2.1) are chosen, when the spatial parameters of the CDME (3.2.1) are integrated out one can obtain the pure reaction process. Which is nothing but the CME of the related reaction.*

Proof. Fix n, then integrate out the location parameters of the following equation:

$$\frac{\partial \rho_n(t,\mathbf{x_n})}{\partial t} = \mathcal{D}_n\rho_n(t,\mathbf{x_n}) + \mathcal{R}\rho_n(t,\mathbf{x_n}),$$
$$\frac{\partial \rho_n(t,\mathbf{x_n})}{\partial t} = D\Delta\rho_n(t,\mathbf{x_n}) + \mathcal{R}\rho_n(t,\mathbf{x_n}),$$

to obtain:

$$\int_{\mathbb{X}} \frac{\partial \rho_n(t,\mathbf{x_n})}{\partial t} d\mathbf{x_n} = \int_{\mathbb{X}} D\Delta\rho_n(t,\mathbf{x_n})\rho_n(t,\mathbf{x_n})d\mathbf{x_n} + \int_{\mathbb{X}} \mathcal{R}\rho_n(t,\mathbf{x_n})d\mathbf{x_n},$$
$$\frac{\partial \rho_n(t)}{\partial t} = \int_{\partial X} D\nabla\partial_v\rho_n(t,\mathbf{x_n})d\mathbf{s} + \mathcal{R}\rho_n(t),$$
$$\frac{\partial \rho_n(t)}{\partial t} = \mathcal{R}\rho_n(t).$$

where the divergence theorem is utilized in the second line. As one can see the result of this operation is a pure reaction process without any notion of diffusion or location inside the model. Which is also called the CME, where marginal density, $\rho_n(t)$ is the probability to obtain n many particles at time t. In other words, it can be said that, truly the CDME is the generalization of CME. □

Now in order to explain better the formulation of the CDME we express equation (3.2.1) in matrix notation.

$$\frac{\partial}{\partial t}\underbrace{\begin{pmatrix}\rho_0\\ \rho_1\\ \vdots\\ \rho_n\\ \vdots\end{pmatrix}}_{\rho} = \underbrace{\begin{pmatrix}\mathcal{D}_0\rho_0\\ \mathcal{D}_1\rho_1\\ \vdots\\ \mathcal{D}_n\rho_n\\ \vdots\end{pmatrix}}_{\mathcal{D}\rho} + \underbrace{\begin{pmatrix}\mathcal{Q}_{0,0} & \mathcal{Q}_{0,1} & \dots & \mathcal{Q}_{0,n} & \dots\\ \mathcal{Q}_{1,0} & \mathcal{Q}_{1,1} & \dots & \mathcal{Q}_{1,n} & \dots\\ \vdots & \vdots & \dots & \vdots & \dots\\ \mathcal{Q}_{n,0} & \mathcal{Q}_{n,1} & \dots & \mathcal{Q}_{n,n} & \dots\\ \vdots & \vdots & \dots & \vdots & \dots\end{pmatrix}}_{\mathcal{R}}\underbrace{\begin{pmatrix}\rho_0\\ \rho_1\\ \vdots\\ \rho_n\\ \vdots\end{pmatrix}}_{\rho}, \tag{3.2.2}$$

where $\mathcal{Q}_{n,m}$ is the transition operator from a state with m particles to a state with n particles. It will yield non-zero result when applied on ρ_m if one of the S many reactions we consider in $\mathcal{R}$ permits such a transition.

3.3 CDME of the Birth-Death Reaction-Diffusion Process (2.2.1)

For example as done in [del Razo et al., 2022], if we consider the birth-death reaction (2.2.1), the matrix $\mathcal{R}$ can be written with only tridiagonal elements such as:

$$\begin{pmatrix} \mathcal{Q}_{0,0} & \mathcal{Q}_{0,1} & 0 & \dots & & & \\ \mathcal{Q}_{1,0} & \mathcal{Q}_{1,1} & \mathcal{Q}_{1,2} & 0 & \dots & & \\ & & & \vdots & & & \\ 0 & \dots & \mathcal{Q}_{n-1n} & \mathcal{Q}_{n,n} & \mathcal{Q}_{nn+1} & 0 & \dots \\ & & & \vdots & & & \end{pmatrix},$$

because the reactions can only create or destroy one particle at a time and we ignore reactions that scale with $\mathcal{O}(h^2)$, as done in Chapter 2. As one can see the equation (3.2.2) is a model that has continuous diffusion in its location variables (due to the diffusion operator $\mathcal{D}$) but a regular discrete jump process in its number of parameters. This way the model fits into the category of stochastic hybrid systems, where continuous dynamics and discrete events coexist in the same process. However, a particular challenge for the mathematical formalization is the change of dimensionality that is induced by the discrete jumps. Then one can imagine the process as in Figure 3.1

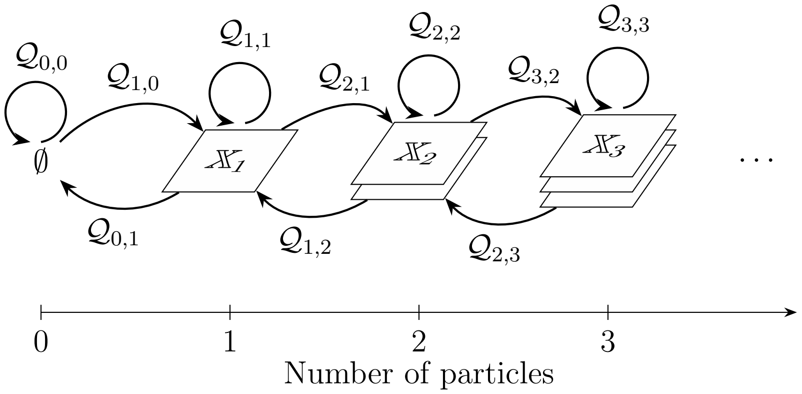


Figure 3.1: The illustration of the reaction-diffusion dynamics of the birth-death reaction (2.2.1). One can see the probability of *jumping* from nth state to m'th state as $\mathcal{Q}_{mn}$. Due to the nature of these jumpings can only cover 1 state at a time. The spaces $\mathbb{X}_n$ is the space where n particles are diffusing. One can also see while each creation of a particle necessarily creates another space where it can diffuse, each degradation removes the space of the corresponding particle.

Moreover because we have a reaction of interest in mind we can do more and express each $\mathcal{Q}_{n,m}$ in terms of the reaction rate *functions* $\lambda_d(x)$ and $\lambda_c(x)$.

Remark 3.3.1. *It is worth noting that because the location information is considered in CDME, the reaction rate* constants *in CME can be modified to be functions of location* *of particles. This feature of CDME adds additional realistic behaviour and complexity to the CDME compared to CME, as also mentioned in the beginning of this chapter. In the rest of the text the birth and death rates will be assumed to be functions of space variable* x.

Similar to the calculations done in equation (2.2.2) is we're assessing these $\mathcal{Q}_{n,m}$'s to be:

- The degradation of a particle happens via the operator $\mathcal{Q}_{n,n+1}$ acting on $\rho_{n+1}(t, \mathbf{x}_{n+1})$ to yield a system of n-particles. The explicit relation is:

  $$(\mathcal{Q}_{n,n+1}\rho_{n+1})(t, \mathbf{x}_n) = (n+1)\int_{\mathbb{X}} \lambda_d(y)\rho_{n+1}\left(t, y, \mathbf{x}_n\right) dy.$$

- A new particle is being created via the operator $\mathcal{Q}_{n,n-1}$ acting on $\rho_{n-1}(t, \mathbf{x}_{n-1})$ to yield a system of n-particles. The explicit relation is:

  $$(\mathcal{Q}_{n,n-1}\rho_{n-1})(t, \mathbf{x}_n) = \frac{1}{n}\sum_{i=1}^{n} \lambda_c\left(x_i\right)\rho_{n-1}(t, x_1, \ldots, x_{i-1}, x_{i+1}, \ldots, x_n).$$

  which also yields a symmetrized density ρ_n.

- The operator $\mathcal{Q}_{n,n}$, unlike of the previous two, when applied on $\rho_n(t, \mathbf{x}_n)$, ensures that no reaction will take place and the system will remain to have n particles. The explicit relation is:

  $$(\mathcal{Q}_{n,n}\rho_n)(t, \mathbf{x}_n) - \left[\sum_{i=1}^{n} \lambda_d(x_i) + \int_{\mathbb{X}} \lambda_c(x)dx\right]\rho_n(t, x_1, \ldots, x_n).$$

- For $n = 0$, the special cases that are presented above is:

  $$\begin{aligned}\mathcal{Q}_{0,1}\rho_1(t, x_1) &= \int_{\mathbb{X}} \lambda_d(x)\rho_1(t, x)dx,\\ \mathcal{Q}_{0,0}\rho_0(t) &= -\int_{\mathbb{X}} \lambda_c(x)\rho_0(t)dx.\end{aligned}$$

Using all these assigned operations above, if they are substituted to the expression (3.2.2), also assuming the diffusion is isotropic so without any deterministic drift, one gets:

$$
\begin{aligned}
\partial_t \rho_n(t, x_1, ..., x_n) = & \sum_{i=1}^{n} D\Delta_i \rho_n(t, x_1, ..., x_n) \\
& + (n+1) \int_{\mathbb{X}} \lambda_d(y) \rho_{n+1}(t, x_1, ..., x_n, y) dy \\
& - \sum_{i=1}^{n} \lambda_d(x_i) \rho_n(t, x_1, ..., x_n) \\
& + \frac{1}{n} \sum_{i=1}^{n} \lambda_c(x_i) \rho_{n-1}(t, x_1, ..., x_{i-1}, x_{i+1}, ..., x_n) \\
& - \int_{\mathbb{X}} \lambda_c(y) dy \cdot \rho_n(t, x_1, ..., x_n), \\
\text{for } n > 0, t > 0, (x_1, ..., x_n) \in \mathbb{X}_n & \quad \text{with the boundary condition:}
\end{aligned}
\tag{3.3.1}
$$

For the special case $n = 0$ of the system of equations shown in (3.3.1) can be simply written as below:

$$
\partial_t \rho_0(t) = \int_{\mathbb{X}} \lambda_d(x) \rho_1(t, x) dx - \int_{\mathbb{X}} \lambda_c(x) \rho_0(t) dx. \tag{3.3.2}
$$

So system of equations consisting of (3.3.1) together with (3.3.2) and with boundary conditions (3.2.1) with an initial condition that the researcher is free to choose, establishes the Chemical Diffusion Master Equation for the birth-death reaction. One important aspect is that similar to Remark 3.2.2, one can check when the reaction rates are assumed to be constants and the location parameters are integrated out one obtains the birth death CME (2.2.3) as shown in equation (1.6) of the paper [Lanconelli, 2023].

One can easily apply the same logic to other reactions by choosing the non-zero elements of the $\mathcal{R}$ matrix and expressing them in terms of the reaction rates of the considered reactions.

In system (3.3.1) and (3.3.2), we see that unlike of CME, the CDME is an infinite system of PDEs, with the solution $\rho_n(t, \mathbf{x_n})$ being the probability to obtain n many particles at time t around the location vector $\mathbf{x_n}$ of all the considered specimens. The derivation and analysis for various reactions will be the main focus in chapters 4, 5 and 6.

3.4 A Pipeline to Solve CDMEs: Infinite Dimensional Generating Function Method

In this section the methodology developed in [Lanconelli, 2023] will be summarized. The readers are encouraged to read the whole paper for any details. It turns out, for solving

CDME analytically, one can use an analogous approach similar to generating function methodology introduced in 2.2.1 and summarized in Figure 2.1.

The idea is to transform the system of CDME equations into an equivalent stochastic one by using iterated Itô integrals with respect to a one dimensional Brownian motion and the Wiener-Itô chaos expansion theorem. Then, exploiting the well known tools from stochastic calculus, we're able to reach to a single partial differential equation of Ornstein-Uhlenbeck type in infinitely many variables which will be connected to the solution of the CDME of interest via the so-called Stroock-Taylor formula. This approach provides an analytical representation for the solution of the original system.

Without loss of generality this approach can be applied on the CDME of birth-death type of reaction reported in (3.3.1) with initial and Neumann boundary conditions

$$\begin{aligned} \rho_0(0) &= 0; \\ \rho_1(0, x_1) &= \zeta(x_1), \quad x_1 \in [0,1]; \\ \rho_n(0, x_1, ..., x_n) &= 0, \quad n > 1, (x_1, ..., x_n) \in [0,1]^n; \\ \partial_\nu \rho_n(t, x_1, ..., x_n) &= 0, \quad n \geq 1, t \geq 0, (x_1, ..., x_n) \in \partial[0,1]^n. \end{aligned} \tag{3.4.1}$$

The initial condition above states that there are no molecules in the system at time zero while the Neumann boundary conditions prevents flux through the boundary of $\mathbb{X} := [0,1]$, thus forcing the diffusion of the molecules inside $[0,1]$. The symbol ∂_ν in (3.4.1) stands for the directional derivative along the outer normal vector at the boundary of $[0,1]^n$.

The main steps of the infinite dimensional generating function approach are summarized as follows:

1. Assume the existence of a classical solution $\{\rho_n\}_{n\geq 0}$ for (3.3.1)-(3.4.1); the continuity of $\rho_n(t,\cdot)$ together with its symmetry in the spatial variables imply the membership of $\rho_n(t,\cdot)$ to $L^2_s([0,1]^n)$, the space of symmetric square integrable functions. Then using first order contraction and symmetrized tensor product, which are explained in Appendix A.8, we express the equation (3.3.1) as:

$$\begin{aligned} \partial_t \rho_0(t) =& \lambda_d \otimes_1 \rho_1(t,\cdot) - \gamma \rho_0(t); \\ \partial_t \rho_n(t, x_1, ..., x_n) =& -\sum_{i=1}^{n} \mathcal{A}_i \rho_n(t, x_1, ..., x_n) + (n+1)(\lambda_d \otimes_1 \rho_{n+1}(t,\cdot))(x_1, ..., x_n) \\ &+ (\lambda_c \hat{\otimes} \rho(t,\cdot))(x_1, ..., x_n) - \gamma \rho_n(t, x_1, ..., x_n). \end{aligned} \tag{3.4.2}$$

   Where we define the operator $\mathcal{A} := -\partial_x^2 + \lambda_d(x)$ $\forall x \in [0,1]$ and $\gamma := \int_0^1 \lambda_c(y)dy$ and make the following assumption:

   Assumption 3.4.1. *There exists an orthonormal basis* $\{\xi_k\}_{k\geq 1}$ *of* $L^2([0,1])$ *that diagonalizes the operator*

$$\mathcal{A} := -\partial_x^2 + \lambda_d(x), \quad x \in [0,1], \tag{3.4.3}$$

with homogenous Neumann boundary conditions. This means that for all $j, k \geq 1$ *we have*

$$\int_0^1 \xi_k(y)\xi_j(y)dy = \delta_{kj}, \quad \xi_k'(0) = \xi_k'(1) = 0,$$

and there exists a sequence of non negative real numbers $\{\alpha_k\}_{k\geq 1}$ *such that*

$$\mathcal{A}\xi_k = \alpha_k \xi_k, \quad \textit{for all } k \geq 1.$$

2. Itô-integrate all the space variables of $\rho_n(t,\cdot)$ in (3.4.2) with respect to a one dimensional Brownian motion $\{B_x\}_{x\in[0,1]}$; this produces a sequence of multiple Itô integrals $\{I_n(\rho_n(t,\cdot))\}_{n\geq 0}$, as described in Appendix A.4. It will serve as a tag for the solution of each state n, analogous to multiplying each state with z^n as done in Chapter 2.2.1. This new system solves a new set of equations, namely:

$$\begin{aligned} \partial_t I_n(\rho_n(t,\cdot)) =& d\Gamma(-\mathcal{A})I_n(\rho_n(t,\cdot)) + D_{\lambda_d} I_{n+1}\left(\rho_{n+1}(t,\cdot)\right) \\ &+ D^{\star}_{\lambda_c} I_{n-1}\left(\rho_{n-1}(t,\cdot)\right) - \gamma I_n(\rho_n(t,\cdot)), \quad t>0, n\geq 0; \\ I_1(\rho_1(0,\cdot)) =& I_1(\zeta); \\ I_n(\rho_n(0,\cdot)) =& 0, \text{ for all } n \neq 1, \end{aligned} \tag{3.4.4}$$

with probability one. Here, we agree on setting $I_{-1}(\cdot) \equiv 0$. The system (3.4.4) is equivalent to (3.3.1) but expressed in terms of differential second quantization operators, Malliavin derivatives and their adjoints as introduced in Appendix A.8.

3. Define $\Phi(t) := \sum_{n\geq 0} I_n(\rho_n(t;\cdot))$; this is a generalized stochastic process, solution to a single infinite dimensional differential equation,

$$\begin{aligned} \partial_t \Phi(t) =& d\Gamma(-\mathcal{A})\Phi(t) + D_{\lambda_d}\Phi(t) + D^{\star}_{\lambda_c}\Phi(t) - \gamma\Phi(t), \quad t>0, \\ \Phi(0) =& I_1(\zeta). \end{aligned} \tag{3.4.5}$$

Whose kernels (from its Wiener-Itô chaos expansion) are by construction the elements of the sequence $\{\rho_n\}_{n\geq 1}$. The summation $\Phi(t) := \sum_{n\geq 0} I_n(\rho_n(t;\cdot))$ basically serves for the same purpose of the generating function $G(t,z)$ and similarly transforms the original coupled infinite system of equations to a single PDE.

4. For the sake of simplicity, we will skip some intermediary steps but for the full formal derivation we direct the readers to the paper itself [Lanconelli, 2023]. Because one can express an iterated Itô integral as:

$$I_n(\rho_n(t,\cdot)) = \varphi_n\left(t, I_1(\xi_1), I_1(\xi_2), ...\right),$$

where φ_n is a polynomial of degree n in the variables $\{I_1(\xi_1), I_1(\xi_2), \dots\}$, which are defined in the assumption 3.4.1, similarly one can apply the Malliavin operators on the $\Phi(t)$ too. It is due to the relation:

$$\Phi(t) := \sum_{n\geq 1} I_n(\rho_n(t,\cdot)) = \sum_{n\geq 1} \varphi_n\left(t, I_1(\xi_1), I_1(\xi_2), \dots\right)$$

$$= u(t, I_1(\xi_1), I_1(\xi_2), \dots)$$

Then one gets the PDE:

$$\begin{aligned}
\partial_t u(t,z) &= \sum_{k\geq 1} \alpha_k \partial^2_{z_k} u(t,z) + \sum_{k\geq 1} \left(d_k - c_k - \alpha_k z_k\right) \partial_{z_k} u(t,z) \\
&\quad + \left(\sum_{k\geq 1} c_k z_k - \gamma \right) u(t,z) \qquad (3.4.6) \\
u(0,z) &= \sum_{k\geq 1} \zeta_k z_k, \quad t \geq 0, z \in \mathbb{R}^N,
\end{aligned}$$

where, $d_k := \langle \lambda_d, \xi_k \rangle_{L^2([0,1])}$, $c_k := \langle \lambda_c, \xi_k \rangle_{L^2([0,1])}$ and $\zeta_k := \langle \zeta, \xi_k \rangle_{L^2([0,1])}$.

So what this pipeline ables you to do is, now one can map their problem of an infinite entangled system of PDEs to a single PDE (entangled being in the sense used in Chapter 2.2.1), as seen from the example of mapping from (3.3.1)-(3.4.1) to (3.4.6). It should be highlighted again that this methodology can be applied to any reaction and the birth-death type of reaction is focused in this section only for better explaining the technique. For example, in Chapter 5, it will be applied to mutual annihilation reaction with an additional creation term as well. This general method is the stochastic analogue of the Generating Function methodology explained in Chapter 2.2.1 and will be called *infinite dimensional generating function method* from now on.

It is worth to mention that the equation (3.4.6) will be fully solved in Chapter 4. In general, once the PDE is solved, by the generalized Stroock-Taylor formula described in Appendix A.9 in expression (A.9.1), an analytic representation for the corresponding $\{\rho_n(t, \mathbf{x})\}_{n\geq 0}$ where $\mathbf{x} \in [0,1]^n$ for each n, will be obtained. So that one will get a quantitative answer to what is the probability to obtain n particles around location vector $\mathbf{x}$ at time t.

The summary of the pipeline can be found in Figure 3.2.

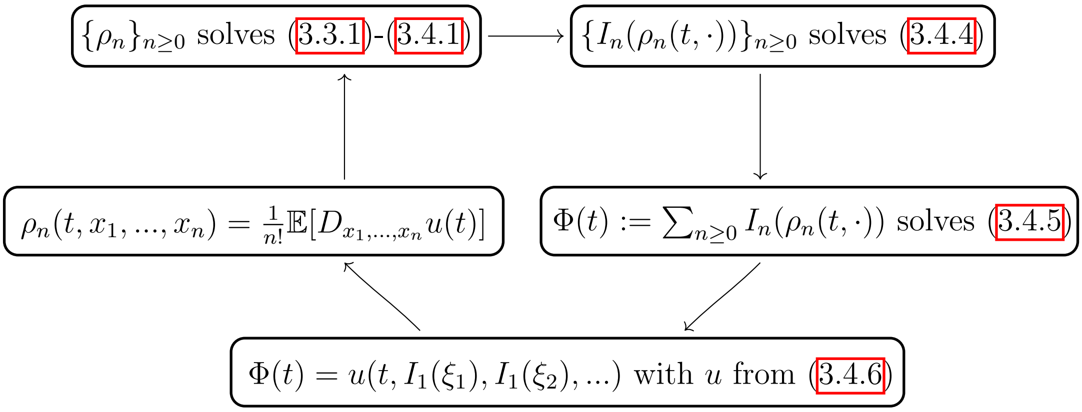


Figure 3.2: Solution pipeline of any CDME. Note the resemblence of the Figure 2.1.

Chapter 4

Solution Formula for the General Birth-Death CDME

Abstract

We propose a solution formula for chemical diffusion master equations of birth and death type. These equations, proposed and formalized in the recent paper [del Razo et al., 2022], aim at incorporating the spatial diffusion of molecules into the description provided by the classical chemical master equation. We start from the general approach developed in [Lanconelli, 2023] and perform a more detailed analysis of the representation found there. This leads to a solution formula for birth-death chemical diffusion master equations which is expressed in terms of the solution to the reaction-diffusion partial differential equation associated with the system under investigation. Such representation also reveals a striking analogy with the solution to the classical birth-death chemical master equations. The solutions of our findings are also illustrated for several examples.

4.1 Introduction and Statement of the Main Result

The CDME is the theoretical backbone of reaction-diffusion processes, and thus, it is fundamental to model and understand biochemical processes in living cells, as well as to develop multiscale numerical methods [del Razo et al., 2018, Flegg et al., 2012, Kostré et al., 2021, Smith and Yates, 2018] and hybrid algorithms [Chen et al., 2014, Dibak et al., 2018, del Razo et al., 2021]. The stochastic trajectories of the CDME can be often integrated using particle–based reaction–diffusion simulations [Andrews, 2017, Hoffmann et al., 2019]. However, analytic and approximate solutions have not yet been explored in detail. In this work, we work out a method to obtain an analytic solution of the CDME for a simple birth-death reaction system, with the aim to bring insight of the CDME solution of more complex systems.

We consider a system of indistinguishable molecules of a chemical species S which undergo

- *diffusion* in the bounded open region $\mathbb{X}$ of $\mathbb{R}^3$;
- *degradation* and *creation* chemical reactions

  $$\text{(I)} \quad S \xrightarrow{\lambda_d(x)} \varnothing \qquad\qquad \text{(II)} \quad \varnothing \xrightarrow{\lambda_c(x)} S,$$

  where $\lambda_d(x)$ denotes the propensity for reaction (I) to occur for a particle located at position $x \in \mathbb{X}$ (i.e., the probability per unit of time for this particle to disappear) while $\lambda_c(x)$ is the propensity for a new particle to be created at position $x \in \mathbb{X}$ by reaction (II).

To describe the evolution in time of such system the authors in [del Razo et al., 2022, del Razo et al., 2023] proposed a set of equations for the number and position of the molecules. Namely, for $t \geq 0$, $n \geq 1$ and $A \in \mathcal{B}(\mathbb{X}^n)$ they set

$$\begin{aligned} \mathcal{N}(t) &:= \text{ number of molecules at time } t, \\ \rho_0(t) &:= \mathbb{P}(\mathcal{N}(t) = 0) \\ \int_A \rho_n(t, x_1, ..., x_n) dx_1 \cdots dx_n &:= \mathbb{P}\left(\{\mathcal{N}(t) = n\} \cap \{(X_1(t), ..., X_n(t)) \in A\}\right); \end{aligned}$$

here, dx_i stands for the three dimensional integration volume $dx_i^{(1)} dx_i^{(2)} dx_i^{(3)}$. Then, according to [del Razo et al., 2022, del Razo et al., 2023], the time evolution of the reaction-diffusion process described above is governed by the following infinite system of equations we have in the expression (3.3.1) from the previous chapter with $D = 1$ for simplicity:

$$\left\{ \begin{aligned} \partial_t \rho_n(t, x_1, ..., x_n) = &\sum_{i=1}^n \Delta_i \rho_n(t, x_1, ..., x_n) \\ &+ (n+1) \int_{\mathbb{X}} \lambda_d(y) \rho_{n+1}(t, x_1, ..., x_n, y) dy \\ &- \sum_{i=1}^n \lambda_d(x_i) \rho_n(t, x_1, ..., x_n) \\ &+ \frac{1}{n} \sum_{i=1}^n \lambda_c(x_i) \rho_{n-1}(t, x_1, ..., x_{i-1}, x_{i+1}, ..., x_n) \\ &- \int_{\mathbb{X}} \lambda_c(y) dy \cdot \rho_n(t, x_1, ..., x_n), \quad n \geq 0, t > 0, (x_1, ..., x_n) \in \mathbb{X}^n; \end{aligned} \right. \tag{4.1.1}$$

where we agree on assigning value zero to the three sums above when $n = 0$. The term

$$\sum_{i=1}^n \Delta_i \rho_n(t, x_1, ..., x_n)$$

in (4.1.1) refers to spatial diffusion of the particles: here,

$$\Delta_i := \partial^2_{x_i^{(1)}} + \partial^2_{x_i^{(2)}} + \partial^2_{x_i^{(3)}}$$

stands for the three dimensional Laplace operator. We remark that to ease the notation we choose a driftless isotropic diffusion but the extension to the divergence-form second order partial differential operator

$$\mathtt{L}_{x_i} v := \sum_{l,m=1}^{3} \partial_{x_i^{(l)}} \left(a_{lm}(x_i) \partial_{x_i^{(m)}} v \right) - \sum_{l=1}^{3} \partial_{x_i^{(l)}} \left(b_l(x_i) v \right),$$

which models a general anisotropic diffusion with drift on $\mathbb{R}^3$, is readily obtained. The terms

$$(n+1) \int_{\mathbb{X}} \lambda_d(y) \rho_{n+1}(t, x_1, ..., x_n, y) dy - \sum_{i=1}^{n} \lambda_d(x_i) \rho_n(t, x_1, ..., x_n)$$

formalize gain and loss, respectively, due to reaction (I), while

$$\frac{1}{n} \sum_{i=1}^{n} \lambda_c(x_i) \rho_{n-1}(t, x_1, ..., x_{i-1}, x_{i+1}, ..., x_n) - \int_{\mathbb{X}} \lambda_c(y) dy \cdot \rho_n(t, x_1, ..., x_n)$$

relate to reaction (II). System (4.1.1) is combined with initial and Neumann boundary conditions

$$\begin{cases} \rho_0(0) = 1; & \\ \rho_n(0, x_1, ..., x_n) = 0, & n \geq 1, (x_1, ..., x_n) \in \mathbb{X}^n; \\ \partial_\nu \rho_n(t, x_1, ..., x_n) = 0, & n \geq 1, t \geq 0, (x_1, ..., x_n) \in \partial\mathbb{X}^n. \end{cases} \tag{4.1.2}$$

The initial condition above states that there are no molecules in the system at time zero while the Neumann condition prevents flux through the boundary of $\mathbb{X}$, thus forcing the diffusion of the molecules inside $\mathbb{X}$. The symbol ∂_ν in (4.1.2) stands for the directional derivative along the outer normal vector at the boundary of $\mathbb{X}^n$.

Aim of this note is to present the following solution formula for (4.1.1)-(4.1.2).

Theorem 4.1.1. *Let v be a classical solution of the problem*

$$\begin{cases} \partial_t v(t,x) = \Delta v(t,x) - \lambda_d(x) v(t,x) + \lambda_c(x), & t > 0, x \in \mathbb{X}; \\ v(0,x) = 0, & x \in \bar{\mathbb{X}}; \\ \partial_\nu v(t,x) = 0, & t \geq 0, x \in \partial\mathbb{X}. \end{cases} \tag{4.1.3}$$

Then, the chemical diffusion master equation (4.1.1) with initial and boundary conditions (4.1.2) has a classical solution given by

$$\rho_0(t) = \mathbb{P}(\mathcal{N}(t) = 0) = \exp\left\{ - \int_{\mathbb{X}} v(t,x) dx \right\}, \quad t \geq 0, \tag{4.1.4}$$

and for $n \geq 1$

$$\rho_n(t, x_1, ..., x_n) = \exp\left\{-\int_{\mathbb{X}} v(t,x)dx\right\}\frac{1}{n!}v(t,x_1)\cdots v(t,x_n), \quad t \geq 0, (x_1, ..., x_n) \in \mathbb{X}^n. \tag{4.1.5}$$

To prove the validity of the representations (4.1.4)-(4.1.5) one can trivially differentiate the right hand sides with respect to t and verify using (4.1.3) that they indeed solve (4.1.1)-(4.1.2). We will however provide in the next section a constructive derivation of the expressions (4.1.4)-(4.1.5) which is based on the general approach proposed in [Lanconelli, 2023]; here, an infinite dimensional version of the moment generating function method, which is commonly utilized to solve analytically some chemical master equations (see for details [McQuarrie, 1967b]), is developed. These techniques are also employed in an ongoing work which consider chemical diffusion master equations with higher order reactions.

Remark 4.1.2. *It is important to highlight the striking similarities between the representation formulas* (4.1.4)-(4.1.5) *for the solution of the CDME* (4.1.1)-(4.1.2) *and the solution*

$$\varphi_n(t) = \frac{\left(\frac{\mathtt{c}}{\mathtt{d}}(1-e^{-\mathtt{d}t})\right)^n}{n!}e^{-\frac{\mathtt{c}}{\mathtt{d}}(1-e^{-\mathtt{d}t})}, \quad t \geq 0, n \geq 0, \tag{4.1.6}$$

of the corresponding (diffusion-free) birth-death chemical master equation

$$\dot{\varphi}_n(t) = \mathtt{d}(n+1)\varphi_{n+1}(t) + \mathtt{c}\varphi_{n-1}(t) - \mathtt{d}n\varphi_n(t) - \mathtt{c}\varphi_n(t), \tag{4.1.7}$$

with initial condition

$$\varphi_n(0) = \delta_{0n}, \quad \textit{for all } n \geq 0. \tag{4.1.8}$$

Equation (4.1.7)-(4.1.8) *describes the evolution in time of the probability*

$$\varphi_n(t) := \mathbb{P}(\text{number of molecules at time } t = n)$$

for the reactions

$$\text{(I)} \quad S \xrightarrow{\mathtt{d}} \varnothing \qquad \text{(II)} \quad \varnothing \xrightarrow{\mathtt{c}} S,$$

with no molecules at time zero. Here, $\mathtt{d}$ *and* $\mathtt{c}$ *are the* stochastic rate constants *for degradation and creation reactions, respectively. (To see how* (4.1.6) *is derived from* (4.1.7)-(4.1.8) *one can for instance use the moment generating function method: see [McQuarrie, 1967b] for details). We note that the function*

$$t \mapsto \frac{\mathtt{c}}{\mathtt{d}}(1-e^{-\mathtt{d}t}),$$

appearing in (4.1.6) solves the deterministic rate equation

$$\begin{cases} \frac{d}{dt}v(t) = -\mathtt{d}v(t) + \mathtt{c}, & t > 0 \\ v(0) = 0 & . \end{cases} \tag{4.1.9}$$

This establishes a perfect agreement between (4.1.3),(4.1.4),(4.1.5), i.e. representation of the solution for (4.1.1)-(4.1.2) and reaction-diffusion PDE, on one side and (4.1.6),(4.1.9), i.e. representation of the solution for (4.1.7)-(4.1.8) and rate equation, on the other side.

Corollary 4.1.3. *In the reaction-diffusion model described by the CDME (4.1.1)-(4.1.2), conditioned on the event $\{\mathcal{N}(t) = n\}$ the positions of the molecules at time t are independent and identically distributed with probability density function*

$$p(t,x) := \frac{v(t,x)}{\int_{\mathbb{X}} v(t,x)dx}, \qquad x \in \mathbb{X}.$$

Moreover,

$$\mathbb{P}(\mathcal{N}(t) = n) = \frac{\left(\int_{\mathbb{X}} v(t,x)dx\right)^n}{n!} \exp\left\{-\int_{\mathbb{X}} v(t,x)dx\right\}.$$

Proof. Let $A \in \mathcal{B}(\mathbb{X}^n)$; then,

$$\begin{aligned} &\mathbb{P}((X_1(t),...,X_n(t)) \in A | \mathcal{N}(t) = n) \\ =&\frac{\mathbb{P}(\{(X_1(t),...,X_n(t)) \in A\} \cap \{\mathcal{N}(t) = n\})}{\mathbb{P}(\mathcal{N}(t) = n)} \\ =&\frac{\int_A \rho_n(t,x_1,...,x_n)dx_1 \cdots dx_n}{\int_{\mathbb{X}^n} \rho_n(t,x_1,...,x_n)dx_1 \cdots dx_n} \\ =&\frac{\int_A \exp\left\{-\int_{\mathbb{X}} v(t,x)dx\right\} \frac{1}{n!} v(t,x_1) \cdots v(t,x_n)dx_1 \cdots dx_n}{\int_{\mathbb{X}^n} \exp\left\{-\int_{\mathbb{X}} v(t,x)dx\right\} \frac{1}{n!} v(t,x_1) \cdots v(t,x_n)dx_1 \cdots dx_n} \\ =&\int_A \frac{v(t,x_1)}{\int_{\mathbb{X}} v(t,x)dx} \cdots \frac{v(t,x_n)}{\int_{\mathbb{X}} v(t,x)dx} dx_1 \cdots dx_n. \end{aligned}$$

The second part of the statement is proved as follows:

$$\begin{aligned} \mathbb{P}(\mathcal{N}(t) = n) &= \int_{\mathbb{X}^n} \rho_n(t,x_1,...,x_n)dx_1 \cdots dx_n \\ &= \int_{\mathbb{X}^n} \exp\left\{-\int_{\mathbb{X}} v(t,x)dx\right\} \frac{1}{n!} v(t,x_1) \cdots v(t,x_n)dx_1 \cdots dx_n \\ &= \frac{\left(\int_{\mathbb{X}} v(t,x)dx\right)^n}{n!} \exp\left\{-\int_{\mathbb{X}} v(t,x)dx\right\}. \end{aligned}$$

□

The paper is organized as follows: in Chapter 4.2 we propose a constructive proof of Theorem 4.1.1 which is based on the approach described in [Lanconelli, 2023] while in Chapter 4.3 we show graphical illustrations of our findings for some particular cases of physical interest that allow for explicit computations in the reaction diffusion PDE (4.1.3).

4.2 Constructive Proof of Theorem 4.1.1

In this section we propose a constructive method to derive the representation formulas (4.1.4)-(4.1.5) of Theorem 4.1.1. The method we propose steams from a further development of the ideas and results presented in Section 3.4, which is adapted from [Lanconelli, 2023].

For notational purposes we assume $\mathbb{X} =]0,1[$. Consider the birth-death CDME

$$\begin{cases} \partial_t \rho_n(t,x_1,...,x_n) = \displaystyle\sum_{i=1}^{n} \partial_{x_i}^2 \rho_n(t,x_1,...,x_n) \\ \qquad + (n+1)\displaystyle\int_0^1 \lambda_d(y)\rho_{n+1}(t,x_1,...,x_n,y)dy \\ \qquad - \displaystyle\sum_{i=1}^{n} \lambda_d(x_i)\rho_n(t,x_1,...,x_n) \\ \qquad + \dfrac{1}{n}\displaystyle\sum_{i=1}^{n} \lambda_c(x_i)\rho_{n-1}(t,x_1,...,x_{i-1},x_{i+1},...,x_n) \\ \qquad - \displaystyle\int_0^1 \lambda_c(y)dy \cdot \rho_n(t,x_1,...,x_n), \quad n \geq 0, t > 0, (x_1,...,x_n) \in]0,1[^n, \end{cases} \tag{4.2.1}$$

with the usual agreement of assigning value zero to the three sums above when $n = 0$, together with initial and Neumann boundary conditions

$$\begin{cases} \rho_0(0) = 1; \\ \rho_n(0,x_1,...,x_n) = 0, \quad n \geq 1, (x_1,...,x_n) \in [0,1]^n; \\ \partial_\nu \rho_n(t,x_1,...,x_n) = 0, \quad n \geq 1, t \geq 0, (x_1,...,x_n) \in \partial[0,1]^n. \end{cases} \tag{4.2.2}$$

We set

$$\mathcal{A} := -\partial_x^2 + \lambda_d(x), \quad x \in [0,1], \tag{4.2.3}$$

with homogenous Neumann boundary conditions and write $\{\xi_k\}_{k\geq 1}$ for the orthonormal basis of $L^2([0,1])$ that diagonalizes the operator $\mathcal{A}$; this means that for all $j,k \geq 1$ we have

$$\int_0^1 \xi_k(y)\xi_j(y)dy = \delta_{kj}, \quad \xi_k'(0) = \xi_k'(1) = 0,$$

and there exists a sequence of non negative real numbers $\{\alpha_k\}_{k\geq 1}$ such that

$$\mathcal{A}\xi_k = \alpha_k \xi_k, \qquad \text{for all } k \geq 1.$$

We observe that $\mathcal{A}$ is an unbounded, non negative self-adjoint operator.

Assumption 4.2.1. *The sequence of eigenvalues $\{\alpha_k\}_{k\geq 1}$ is strictly positive.*

We now denote by $\Pi_N : L^2([0,1]) \to L^2([0,1])$ the orthogonal projection onto the finite dimensional space spanned by $\{\xi_1, ..., \xi_N\}$, i.e.

$$\Pi_N f(x) := \sum_{k=1}^{N} \langle f, \xi_k \rangle_{L^2([0,1])} \xi_k(x), \quad x \in [0,1];$$

we also set

$$d_k := \langle \lambda_d, \xi_k \rangle_{L^2([0,1])}, \quad c_k := \langle \lambda_c, \xi_k \rangle_{L^2([0,1])}, \quad \gamma := \int_0^1 \lambda_c(y)dy. \tag{4.2.4}$$

Assumption 4.2.2. *There exists $N_0 \geq 1$ such that $\Pi_{N_0}\lambda_d = \lambda_d$; this is equivalent to say $\Pi_N \lambda_d = \lambda_d$ for all $N \geq N_0$.*

In the sequel we set $\Pi_N^{\otimes n}$ to be the orthogonal projection from $L^2([0,1]^n)$ to the linear space generated by the functions $\{\xi_{i_1} \otimes \cdots \otimes \xi_{i_n}, 1 \leq i_1, ..., i_n \leq N\}$. The next theorem was proved in [Lanconelli, 2023].

Theorem 4.2.3. *Let Assumptions 4.2.1-4.2.2 be in force and denote by $\{\rho_n\}_{n\geq 0}$ a classical solution of equation (4.1.1)-(4.1.2). Then, for any $N \geq N_0$ and $t \geq 0$ we have the representation*

$$\rho_0^{(N)}(t) = \mathbb{E}[u_N(t, Z)], \tag{4.2.5}$$

and for any $n \geq 1$ and $(x_1, ..., x_n) \in [0,1]^n$,

$$\Pi_N^{\otimes n} \rho_n(t, x_1, ..., x_n) = \frac{1}{n!} \sum_{j_1, \ldots j_n = 1}^{N} \mathbb{E}\left[\left(\partial_{z_{j_1}} \cdots \partial_{z_{j_n}} u_N\right)(t, Z)\right] \xi_{j_1}(x_1) \cdots \xi_{j_n}(x_n). \tag{4.2.6}$$

Here,

$$\mathbb{E}\left[\left(\partial_{z_{j_1}} \cdots \partial_{z_{j_n}} u_N\right)(t, Z)\right] = \int_{\mathbb{R}^N} \left(\partial_{z_{j_1}} \cdots \partial_{z_{j_n}} u_N\right)(t, z)(2\pi)^{-N/2} e^{-\frac{|z|^2}{2}} dz, \tag{4.2.7}$$

while $u_N : [0, +\infty[\times \mathbb{R}^N \to \mathbb{R}$ is a classical solution of the partial differential equation

$$\begin{aligned} \partial_t u_N(t,z) =& \sum_{k=1}^{N} \alpha_k \partial_{z_k}^2 u_N(t,z) + \sum_{k=1}^{N} (d_k - c_k - \alpha_k z_k)\, \partial_{z_k} u_N(t,z) \\ &+ \left(\sum_{k=1}^{N} c_k z_k - \gamma\right) u_N(t,z) \\ u_N(0,z) =& 1, \quad t \geq 0, z \in \mathbb{R}^N. \end{aligned} \tag{4.2.8}$$

We now start working out the details of formulas (4.2.5)-(4.2.6).

Lemma 4.2.4. *The solution to the Cauchy problem* (4.2.8) *can be represented as*

$$u_N(t,z) = \exp\Bigg\{ -\gamma t + \sum_{k=1}^{N} \Bigg(c_k z_k g_k(t) + c_k(d_k - c_k) \int_0^t g_k(s) ds \\ + c_k^2 \alpha_k \int_0^t g_k(s)^2 ds \Bigg) \Bigg\}, \tag{4.2.9}$$

where

$$g_k(t) := \frac{1 - e^{-\alpha_k t}}{\alpha_k}, \quad t \geq 0, k = 1, ..., N. \tag{4.2.10}$$

Proof. The solution to the Cauchy problem (4.2.8) admits the following Feynman-Kac representation (see for instance [Karatzas and Shreve, 1991])

$$u_N(t,z) = \mathbb{E}\left[\exp\left\{ \int_0^t \left(\sum_{k=1}^{N} c_k \mathcal{Z}_k^{z_k}(s) - \gamma \right) ds \right\} \right], \quad t \geq 0, z = (z_1, ..., z_N) \in \mathbb{R}^N. \tag{4.2.11}$$

Here, for $k \in \{1, ..., N\}$, the stochastic process $\{\mathcal{Z}_k^{z_k}(t)\}_{t\geq 0}$ is the unique strong solution of the mean-reverting Ornstein-Uhlenbeck stochastic differential equation

$$d\mathcal{Z}_k^{z_k}(t) = (d_k - c_k - \alpha_k \mathcal{Z}_k^{z_k}(t))\, dt + \sqrt{2\alpha_k} dW_k(t), \quad \mathcal{Z}_k^{z_k}(0) = z_k, \tag{4.2.12}$$

with $\{W_1(t)\}_{t\geq 0}$,...,$\{W_N(t)\}_{t\geq 0}$ being independent one dimensional Brownian motions. Using the independence of the processes $\mathcal{Z}_1^{z_1}$,...., $\mathcal{Z}_N^{z_N}$ we can rewrite (4.2.11) as

$$\begin{aligned} u_N(t,z) &= e^{-\gamma t}\mathbb{E}\left[\exp\left\{ \sum_{k=1}^{N} c_k \int_0^t \mathcal{Z}_k^{z_k}(s) ds \right\} \right] = e^{-\gamma t}\mathbb{E}\left[\prod_{k=1}^{N} \exp\left\{ c_k \int_0^t \mathcal{Z}_k^{z_k}(s) ds \right\} \right] \\ &= e^{-\gamma t} \prod_{k=1}^{N} \mathbb{E}\left[\exp\left\{ c_k \int_0^t \mathcal{Z}_k^{z_k}(s) ds \right\} \right]. \end{aligned} \tag{4.2.13}$$

We now want to compute the last expectation explicitly: first of all, we observe that equation (4.2.12) admits the unique strong solution

$$\mathcal{Z}_k^{z_k}(t) = z_k e^{-\alpha_k t} + \frac{d_k - c_k}{\alpha_k}\left(1 - e^{-\alpha_k t}\right) + \int_0^t e^{-\alpha_k(t-s)} \sqrt{2\alpha_k} dW_k(s),$$

(recall Assumption 4.2.1). Therefore,

$$\int_0^t \mathcal{Z}_k^{z_k}(s) ds$$

$$
\begin{aligned}
&= z_k\frac{1-e^{-\alpha_k t}}{\alpha_k} + (d_k - c_k)\int_0^t \frac{1-e^{-\alpha_k s}}{\alpha_k} ds + \int_0^t\int_0^s e^{-\alpha_k(s-u)}\sqrt{2\alpha_k}dW_k(u)ds\\
&= z_k\frac{1-e^{-\alpha_k t}}{\alpha_k} + (d_k - c_k)\int_0^t \frac{1-e^{-\alpha_k s}}{\alpha_k} ds + \sqrt{2\alpha_k}\int_0^t \frac{1-e^{-\alpha_k(t-s)}}{\alpha_k} dW_k(s);
\end{aligned}
$$

in the last equality we employed Fubini theorem for Lebesgue-Wiener integrals. The identity above yields

$$
\begin{aligned}
\mathbb{E}\left[\exp\left\{c_k\int_0^t \mathcal{Z}_k^{z_k}(s)ds\right\}\right] =& \exp\left\{c_k\left(z_k\frac{1-e^{-\alpha_k t}}{\alpha_k} + (d_k - c_k)\int_0^t \frac{1-e^{-\alpha_k s}}{\alpha_k} ds\right)\right\}\\
&\times \mathbb{E}\left[\exp\left\{c_k\sqrt{2\alpha_k}\int_0^t \frac{1-e^{-\alpha_k(t-s)}}{\alpha_k} dW_k(s)\right\}\right]\\
=& \exp\left\{c_k\left(z_k\frac{1-e^{-\alpha_k t}}{\alpha_k} + (d_k - c_k)\int_0^t \frac{1-e^{-\alpha_k s}}{\alpha_k} ds\right)\right\}\\
&\times \exp\left\{c_k^2\alpha_k\int_0^t\left(\frac{1-e^{-\alpha_k(t-s)}}{\alpha_k}\right)^2 ds\right\},
\end{aligned}
$$

where in last equality we used the fact that $\int_0^t \frac{1-e^{-\alpha_k(t-s)}}{\alpha_k} dW_k(s)$ is a Gaussian random variable with mean zero and variance $\int_0^t\left(\frac{1-e^{-\alpha_k(t-s)}}{\alpha_k}\right)^2 ds$. This, together with (4.2.13), gives

$$
\begin{aligned}
u_N(t,z) =& e^{-\gamma t}\prod_{k=1}^N \exp\left\{c_k\left(z_k\frac{1-e^{-\alpha_k t}}{\alpha_k} + (d_k - c_k)\int_0^t \frac{1-e^{-\alpha_k s}}{\alpha_k} ds\right)\right\}\\
&\times \prod_{k=1}^N \exp\left\{c_k^2\alpha_k\int_0^t\left(\frac{1-e^{-\alpha_k(t-s)}}{\alpha_k}\right)^2 ds\right\}\\
=& \exp\left\{-\gamma t + \sum_{k=1}^N\left(c_k z_k g_k(t) + c_k(d_k - c_k)\int_0^t g_k(s)ds + c_k^2\alpha_k\int_0^t g_k(s)^2 ds\right)\right\},
\end{aligned}
$$

(recall definition (4.2.10)). The proof is complete. □

Lemma 4.2.5. *Expectation (4.2.5) can be written as*

$$
\rho_0^{(N)}(t) = \exp\left\{t\left(\sum_{k=1}^N \frac{c_k d_k}{\alpha_k} - \gamma\right) + \sum_{k=1}^N c_k d_k\frac{e^{-\alpha_k t}-1}{\alpha_k^2}\right\}.
$$

In particular,

$$
\rho_0(t) = \lim_{N\to+\infty}\rho_0^{(N)}(t) = \exp\left\{\sum_{k\geq 1} c_k d_k\frac{e^{-\alpha_k t}-1}{\alpha_k^2}\right\}. \tag{4.2.14}
$$

Proof. Let $Z = (Z_1, ..., Z_N)$ be an N-dimensional vector of i.i.d. standard Gaussian random variables; then,

$$\begin{aligned}
\rho_0^{(N)}(t) =& \mathbb{E}[u_N(t, Z)] \\
=& \mathbb{E}\left[\exp\left\{-\gamma t + \sum_{k=1}^{N}\left(c_k Z_i g_k(t) + c_k(d_k - c_k)\int_0^t g_k(s)ds + c_k^2\alpha_k\int_0^t g_k(s)^2 ds\right)\right\}\right] \\
=& \exp\left\{-\gamma t + \sum_{k=1}^{N}\left(c_k(d_k - c_k)\int_0^t g_k(s)ds + c_k^2\alpha_k\int_0^t g_k(s)^2 ds\right)\right\} \\
& \cdot \mathbb{E}\left[\exp\left\{\sum_{k=1}^{N} c_k Z_i g_k(t)\right\}\right] \\
=& \exp\left\{-\gamma t + \sum_{k=1}^{N}\left(\frac{c_k^2 g_k(t)^2}{2} + c_k(d_k - c_k)\int_0^t g_k(s)ds + c_k^2\alpha_k\int_0^t g_k(s)^2 ds\right)\right\} \\
=& \exp\Bigg\{ -\gamma t + \sum_{k=1}^{N}\Bigg[c_k^2\left(\frac{g_k(t)^2}{2} - \int_0^t g_k(s)ds + \alpha_k\int_0^t g_k(s)^2 ds\right) \\
& + c_k d_k\int_0^t g_k(s)ds\Bigg]\Bigg\} \\
=& \exp\left\{-\gamma t + \sum_{k=1}^{N} c_k d_k\int_0^t g_k(s)ds\right\}.
\end{aligned}$$

The fourth equality follows from the expression of the exponential generating function of a Gaussian vector while the last equality is due to identity

$$\frac{g_k(t)^2}{2} - \int_0^t g_k(s)ds + \alpha_k\int_0^t g_k(s)^2 ds = 0, \quad t \geq 0$$

which follows from a direct verification (recall definition (4.2.10)). On the other hand, we have

$$\int_0^t g_k(s)ds = \frac{t}{\alpha_k} + \frac{e^{-\alpha_k t} - 1}{\alpha_k^2},$$

and hence

$$\rho_0^{(N)}(t) = \exp\left\{t\left(\sum_{k=1}^{N}\frac{c_k d_k}{\alpha_k} - \gamma\right) + \sum_{k=1}^{N} c_k d_k\frac{e^{-\alpha_k t} - 1}{\alpha_k^2}\right\}.$$

Moreover, letting N to infinity we get

$$\rho_0(t) = \lim_{N\to+\infty}\rho_0^{(N)}(t)$$

$$
\begin{aligned}
&= \lim_{N\to+\infty} \exp\left\{ t\left(\sum_{k=1}^{N} \frac{c_k d_k}{\alpha_k} - \gamma \right) + \sum_{k=1}^{N} c_k d_k \frac{e^{-\alpha_k t} - 1}{\alpha_k^2} \right\} \\
&= \exp\left\{ t\left(\sum_{k\geq 1} \frac{c_k d_k}{\alpha_k} - \gamma \right) + \sum_{k\geq 1} c_k d_k \frac{e^{-\alpha_k t} - 1}{\alpha_k^2} \right\} \\
&= \exp\left\{ \sum_{k\geq 1} c_k d_k \frac{e^{-\alpha_k t} - 1}{\alpha_k^2} \right\}.
\end{aligned}
$$

Here, we employed the identity

$$
\sum_{k\geq 1} \frac{c_k d_k}{\alpha_k} = \gamma,
$$

which follows from

$$
\begin{aligned}
\sum_{k\geq 1} \frac{c_k d_k}{\alpha_k} &= \langle \mathcal{A}^{-1}\lambda_c, \lambda_d \rangle_{L^2([0,1])} = \langle \mathcal{A}^{-1}\lambda_c, \mathcal{A}\mathtt{1} \rangle_{L^2([0,1])} = \langle \lambda_c, \mathcal{A}^{-1}\mathcal{A}\mathtt{1} \rangle_{L^2([0,1])} \\
&= \langle \lambda_c, \mathtt{1} \rangle_{L^2([0,1])} = \int_0^1 \lambda_c(x)\mathtt{1}(x)dx = \gamma.
\end{aligned}
$$

We also denoted $\mathtt{1}(x) = 1$, $x \in [0,1]$ and exploited the identity $\mathcal{A}\mathtt{1} = \lambda_d$. □

Lemma 4.2.6. *Expectation* (4.2.6) *can be written as*

$$
\Pi_N^{\otimes n} \rho_n(t, x_1, ..., x_n) = \rho_0^{(N)}(t) \frac{1}{n!} \left(\sum_{j=1}^{N} c_j g_j(t) \xi_j(x_1) \right) \cdots \left(\sum_{j=1}^{N} c_j g_j(t) \xi_j(x_n) \right).
$$

In particular,

$$
\begin{aligned}
\rho_n(t, x_1, ..., x_n) &= \lim_{N\to+\infty} \Pi_N^{\otimes n} \rho_n(t, x_1, ..., x_n) \\
&= \exp\left\{ -\sum_{k\geq 1} c_k d_k \frac{1 - e^{-\alpha_k t}}{\alpha_k^2} \right\} \frac{1}{n!} \left(\sum_{j\geq 1} c_j \frac{1 - e^{-\alpha_j t}}{\alpha_j} \xi_j \right)^{\otimes n} (x_1, ..., x_n).
\end{aligned}
\tag{4.2.15}
$$

Proof. We note that according to (4.2.9) we have

$$
\left(\partial_{z_{j_1}} \cdots \partial_{z_{j_n}} u_N \right)(t, z) = u_N(t, z) c_{j_1} g_{j_1}(t) \cdots c_{j_n} g_{j_n}(t),
$$

and hence

$$
\mathbb{E}\left[\left(\partial_{z_{j_1}} \cdots \partial_{z_{j_n}} u_N \right)(t, Z) \right] = \rho_0^{(N)}(t) c_{j_1} g_{j_1}(t) \cdots c_{j_n} g_{j_n}(t).
$$

Therefore,

$$\begin{aligned}\Pi_N^{\otimes n}\rho_n(t,x_1,...,x_n) &= \frac{1}{n!}\sum_{j_1,...j_n=1}^{N}\mathbb{E}\left[\left(\partial_{z_{j_1}}\cdots\partial_{z_{j_n}}u_N\right)(t,Z)\right]\xi_{j_1}(x_1)\cdots\xi_{j_n}(x_n)\\ &= \frac{1}{n!}\sum_{j_1,...j_n=1}^{N}\rho_0^{(N)}(t)c_{j_1}g_{j_1}(t)\cdots c_{j_n}g_{j_n}(t)\xi_{j_1}(x_1)\cdots\xi_{j_n}(x_n)\\ &= \rho_0^{(N)}(t)\frac{1}{n!}\left(\sum_{j=1}^{N}c_jg_j(t)\xi_j(x_1)\right)\cdots\left(\sum_{j=1}^{N}c_jg_j(t)\xi_j(x_n)\right).\end{aligned}$$

Moreover, letting N to infinity we obtain

$$\begin{aligned}\rho_n(t,x_1,...,x_n) =&\exp\left\{-\sum_{k\geq 1}c_kd_k\frac{1-e^{-\alpha_kt}}{\alpha_k^2}\right\}\frac{1}{n!}\left(\sum_{j\geq 1}c_jg_j(t)\xi_j(x_1)\right)\\ &\cdots\left(\sum_{j\geq 1}c_jg_j(t)\xi_j(x_n)\right)\\ =&\exp\left\{-\sum_{k\geq 1}c_kd_k\frac{1-e^{-\alpha_kt}}{\alpha_k^2}\right\}\frac{1}{n!}\left(\sum_{j\geq 1}c_j\frac{1-e^{-\alpha_jt}}{\alpha_j}\xi_j\right)^{\otimes n}(x_1,...,x_n).\end{aligned}$$

□

We are now in a position to show the equivalence between (4.2.14)-(4.2.15) and (4.1.4)-(4.1.5).
We start observing that

$$d_k:=\langle\lambda_d,\xi_k\rangle=\langle\mathcal{A}1,\xi_k\rangle=\langle 1,\mathcal{A}\xi_k\rangle=\alpha_k\langle 1,\xi_k\rangle=\alpha_k\int_0^1\xi_k(x)dx.$$

Therefore, from formula (4.2.14) we can write

$$\begin{aligned}\rho_0(t)=\mathbb{P}(\mathcal{N}(t)=0) &= \exp\left\{-\sum_{k\geq 1}c_kd_k\frac{1-e^{-\alpha_kt}}{\alpha_k^2}\right\}\\ &= \exp\left\{-\sum_{k\geq 1}c_k\int_0^1\xi_k(x)dx\frac{1-e^{-\alpha_kt}}{\alpha_k}\right\}\\ &= \exp\left\{-\int_0^1\left(\sum_{k\geq 1}c_k\frac{1-e^{-\alpha_kt}}{\alpha_k}\xi_k(x)\right)dx\right\}\\ &= \exp\left\{-\int_0^1 v(t,x)dx\right\},\end{aligned}$$

where we set

$$v(t,x) := \sum_{k\geq 1} c_k \frac{1-e^{-\alpha_k t}}{\alpha_k}\xi_k(x). \tag{4.2.16}$$

Note that with this notation we can also write according to (4.2.15) that

$$\rho_n(t,x_1,...,x_n) = \exp\left\{-\int_{\mathbb{X}} v(t,x)dx\right\}\frac{1}{n!}v(t,x_1)\cdots v(t,x_n), \quad t\geq 0, (x_1,...,x_n)\in\mathbb{X}^n.$$

If we now prove that the function v defined in (4.2.16) solves (4.1.3), then the equivalence between (4.2.14)-(4.2.15) and (4.1.4)-(4.1.5) will be established. Since

$$\partial_t v(t,x) = \partial_t\left(\sum_{k\geq 1} c_k\frac{1-e^{-\alpha_k t}}{\alpha_k}\xi_k(x)\right) = \sum_{k\geq 1} c_k e^{-\alpha_k t}\xi_k(x),$$

we can conclude that

$$\begin{aligned}\partial_x^2 v(t,x) - \lambda_d(x)v(t,x) &= -\mathcal{A}v(t,x) = -\mathcal{A}\left(\sum_{k\geq 1} c_k\frac{1-e^{-\alpha_k t}}{\alpha_k}\xi_k(x)\right)\\ &= \sum_{k\geq 1} c_k(e^{-\alpha_k t}-1)\xi_k(x) = \sum_{k\geq 1} c_k e^{-\alpha_k t}\xi_k(x) - \lambda_c(x)\\ &= \partial_t v(t,x) - \lambda_c(x),\end{aligned}$$

proving the desired property (the initial and boundary conditions in (4.1.3) are readily satisfied).

4.3 Case Study: One Dimensional Motion with Constant Degradation Function

In this section we illustrate through several plots our theoretical findings for some concrete models. According to formulas (4.1.4)-(4.1.5) the solution to the chemical diffusion master equation (4.1.1)-(4.1.2) is completely determined by the solution of equation (4.1.3). To solve this problem explicitly we decided to focus on the one dimensional case $\mathbb{X} =]0,1[$ with driftless isotropic diffusion (i.e. the framework of Chapter 4.2) and constant degradation function λ_d. This last restriction yields the advantage of knowing the explicit form of the eigenfunctions and eigenvalues of the operator $\mathcal{A}$ in (4.2.3) and hence the possibility of working with (4.2.14)-(4.2.15), which we recall to be equivalent to (4.1.4)-(4.1.5).
When $\lambda_d(x) = \lambda_d$, $x\in[0,1]$ for some positive constant λ_d, we get

$$\mathcal{A}f(x) = -f''(x) + \lambda_d f(x), \qquad \xi_k(x) = \cos((k-1)\pi x), \quad k\geq 1,$$

and

$$\alpha_k = (k-1)^2\pi^2 + \lambda_d, \quad k \geq 1. \tag{4.3.1}$$

Therefore, the degradation function $\lambda_d(x) = \lambda_d$ is proportional to the first eigenfunction $\xi_1(x) = \mathtt{1}(x)$ and hence orthogonal to all the other eigenfunctions $\xi_k(x)$ for $k \geq 2$; this gives

$$d_1 = \langle \lambda_d, \xi_1 \rangle = \lambda_d \quad \text{and} \quad d_k = \langle \lambda_d, \xi_k \rangle = 0 \text{ for all } k \geq 2;$$

note also that (4.3.1) implies $\alpha_1 = \lambda_d$. Combining these facts in (4.2.14) and (4.2.15) we obtain

$$\rho_0(t) = \mathbb{P}(\mathcal{N}(t) = 0) = \exp\left\{-c_1 \frac{1-e^{-\lambda_d t}}{\lambda_d}\right\}, \quad t \geq 0, \tag{4.3.2}$$

and, for $n \geq 1$, $t \geq 0$ and $(x_1, ..., x_n) \in [0,1]^n$,

$$\rho_n(t, x_1, ..., x_n) = \exp\left\{-c_1 \frac{1-e^{-\lambda_d t}}{\lambda_d}\right\} \frac{1}{n!} \left(\sum_{j\geq 1} c_j \frac{1-e^{-\alpha_j t}}{\alpha_j} \xi_j\right)^{\otimes n} (x_1, ..., x_n). \tag{4.3.3}$$

We now specify some interesting choices of the creation function λ_c.

4.3.1 Constant creation function

In the case $\lambda_c(x) = \lambda_c$, $x \in [0,1]$ for some positive constant λ_c, in other words the creation is uniform in the whole interval just like the degradation, we get from (4.3.2) and (4.3.3)

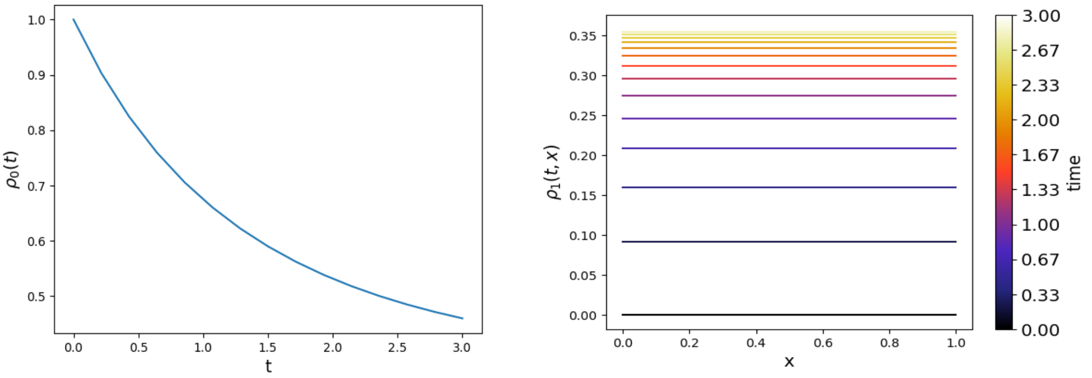
$$\rho_0(t) = \mathbb{P}(\mathcal{N}(t) = 0) = \exp\left\{-\lambda_c \frac{1-e^{-\lambda_d t}}{\lambda_d}\right\}, \quad t \geq 0,$$

and for $n \geq 1$

$$\begin{aligned}\rho_n(t, x_1, ..., x_n) &= \exp\left\{-\lambda_c \frac{1-e^{-\lambda_d t}}{\lambda_d}\right\} \frac{1}{n!} \left(\lambda_c \frac{1-e^{-\lambda_d t}}{\lambda_d} \xi_1\right)^{\otimes n} (x_1, ..., x_n) \\ &= \exp\left\{-\lambda_c \frac{1-e^{-\lambda_d t}}{\lambda_d}\right\} \frac{1}{n!} \left(\lambda_c \frac{1-e^{-\lambda_d t}}{\lambda_d}\right)^{n} 1(x_1) \cdots 1(x_n).\end{aligned}$$

This shows that for any $n \geq 1$ the function ρ_n is constant in $x_1, ..., x_n$ with height given by the n-th component of the solution to the birth-death chemical master equation with stochastic rate constants λ_d and λ_c (compare with (4.1.6)).

Figure 4.1 shows the solutions for ρ_0 and ρ_1 as a function of time. Figure 4.1a shows the the exponential decay of the probability of having 0 particles due to the constant creation of particles, and 4.1b shows the probability distribution of having 1 particle is uniform in space for all times, as well as its convergence to the stationary distribution.



(a) (b)

Figure 4.1: Solutions plots of the bdCDME generated with constant creation and degradation rates with $\lambda_c = \lambda_d = 0.5$. a. The solution of $\rho_0(t)$ as a function of time. b. The solution of $\rho_1(t, x_1)$ as a function of position and time.

4.3.2 Dirac delta creation function at $x = 0$

In this case we take $\lambda_c(x) = \lambda_c\delta_0(x)$, $x \in [0, 1]$ for some positive constant λ_c, so the creation takes place only in the leftmost point of the interval while degradation happens uniformly. This way one yields

$$c_j = \int_0^1 \lambda_c(x)\xi_j(x)dx = \int_0^1 \lambda_c\delta_0(x)\xi_j(x)dx = \lambda_c\xi_j(0) = \lambda_c, \qquad \text{for all } j \geq 1.$$

and formulas (4.3.2) and (4.3.3) now read

$$\rho_0(t) = \mathbb{P}(\mathcal{N}(t) = 0) = \exp\left\{-\lambda_c \frac{1 - e^{-\lambda_d t}}{\lambda_d}\right\}, \quad t \geq 0,$$

and for $n \geq 1$

$$\begin{aligned}\rho_n(t, x_1, ..., x_n) &= \exp\left\{-\lambda_c \frac{1 - e^{-\lambda_d t}}{\lambda_d}\right\} \frac{1}{n!} \left(\sum_{j\geq 1} \lambda_c \frac{1 - e^{-\alpha_j t}}{\alpha_j}\xi_j\right)^{\otimes n} (x_1, ..., x_n) \\ &= \exp\left\{-\lambda_c \frac{1 - e^{-\lambda_d t}}{\lambda_d}\right\} \frac{\lambda_c^n}{n!} \left(\sum_{j\geq 1} \frac{1 - e^{-\alpha_j t}}{\alpha_j}\xi_j\right)^{\otimes n} (x_1, ..., x_n).\end{aligned}$$

We note that even though $\lambda_c(x)$ is a generalized function the series

$$\sum_{j\geq 1} c_j \frac{1 - e^{-\alpha_j t}}{\alpha_j}\xi_j = \lambda_c \sum_{j\geq 1} \frac{1 - e^{-\alpha_j t}}{\alpha_j}\xi_j \tag{4.3.4}$$

appearing above converges in $L^2([0, 1])$.

In Figure 4.2 we plot solution of the bdCDME for this example. Figure 4.2a shows the exponential decay of the probability of having 0 particles due to the constant creation of particles. In contrast with Figure 4.1, in Figures 4.2b and 4.2c, one can see the effect of the creation happening only at $x = 0$ due to the peaks at the origin, while the highest peak is when $x_2 = x_1 = 0$. With increasing time the peaks at the origin smooth out due to diffusion and probability being distributed through the different particle number densities. Similar to before, the curves converge to their stationary distribution as time increases. Lastly, Figure 4.2d shows the solution of the bdCDME for 2 particles as a surface on x_1, x_2 axes, when time is fixed at $t = 0.25$.

4.3.3 Dirac delta creation function at $x = 1/2$

We now choose $\lambda_c(x) = \lambda_c \delta_{1/2}(x)$, $x \in [0,1]$ for some positive constant λ_c, so the creation takes place only on the middle of the interval and degradation happens uniformly. This way one obtains

$$c_j = \int_0^1 \lambda_c(x)\xi_j(x)dx = \int_0^1 \lambda_c\delta_{1/2}(x)\xi_j(x)dx = \lambda_c\xi_j(1/2) = \lambda_c \cos((j-1)\pi/2), \quad \text{for all } j \geq 1.$$

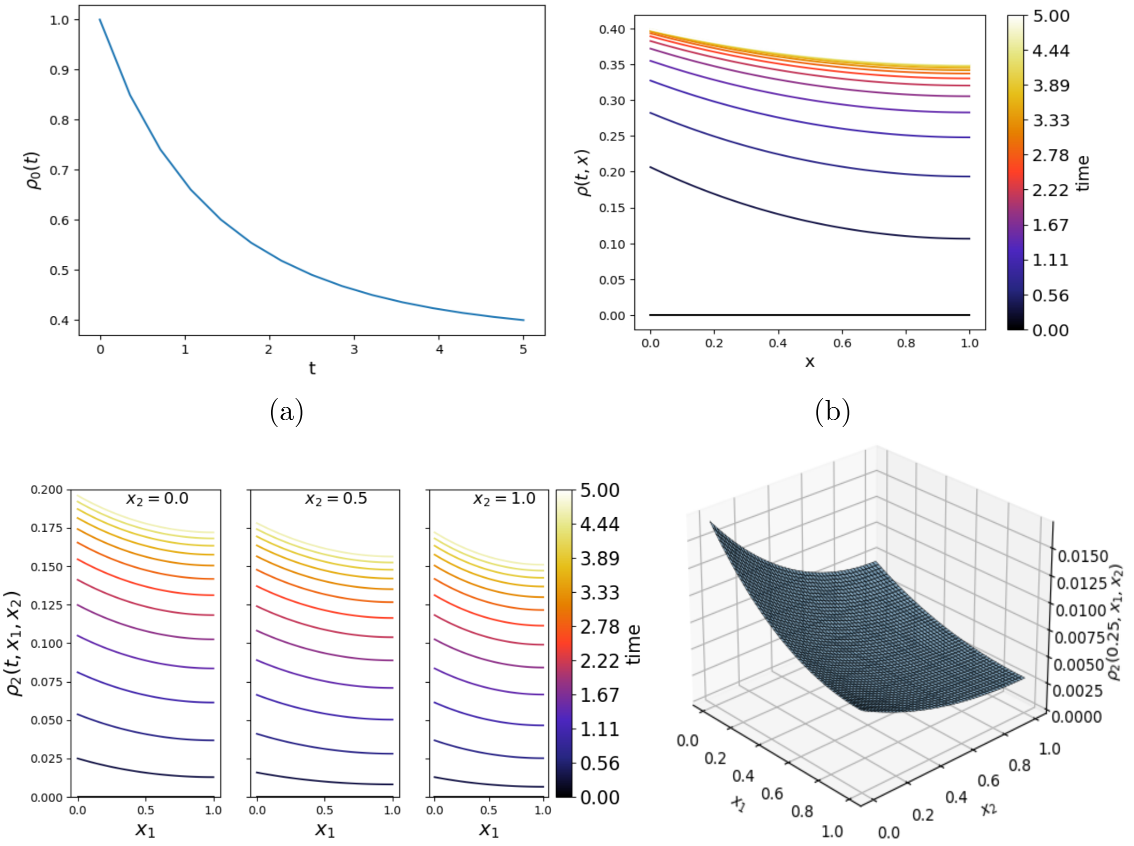
Therefore, equations (4.3.2) and (4.3.3) take now the form

$$\rho_0(t) = \mathbb{P}(\mathcal{N}(t) = 0) = \exp\left\{-\lambda_c \frac{1-e^{-\lambda_d t}}{\lambda_d}\right\}, \quad t \geq 0,$$

and for $n \geq 1$

$$\begin{aligned}\rho_n(t, x_1, ..., x_n) &= \exp\left\{-\lambda_c \frac{1-e^{-\lambda_d t}}{\lambda_d}\right\} \frac{1}{n!} \left(\sum_{j\geq 1} \lambda_c \cos((j-1)\pi/2) \frac{1-e^{-\alpha_j t}}{\alpha_j} \xi_j\right)^{\otimes n} \\ &\quad \cdot (x_1, ..., x_n) \\ &= \exp\left\{-\lambda_c \frac{1-e^{-\lambda_d t}}{\lambda_d}\right\} \frac{\lambda_c^n}{n!} \left(\sum_{k\geq 1} (-1)^{k-1} \frac{1-e^{-\alpha_{2k-1} t}}{\alpha_{2k-1}} \xi_{2k-1}\right)^{\otimes n} \cdot (x_1, ..., x_n)\end{aligned}$$

Figure 4.3 shows plots of the solution of the bdCDME for this example. Figure 4.3a shows the exponential decay of the probability of having 0 particles due to the constant creation of particles. However, in conrast with figures 4.1 and 4.2, in this case, the effect of creation in the middle of the interval can be seen in the peaks in the Figures 4.3b and 4.3c, while the highest peak is at $x_1 = x_2 = 0.5$, as expected. Similar to the previous example the effect of the location of the creation of particles on the distribution becomes less important with increasing time due to diffusion. Once again, the curves converge to their stationary distribution. Lastly, Figure 4.3d plots the solution of bdCDME as a surface for 2 particle case at fixed time $t = 0.25$, as a function of x_1 and x_2.



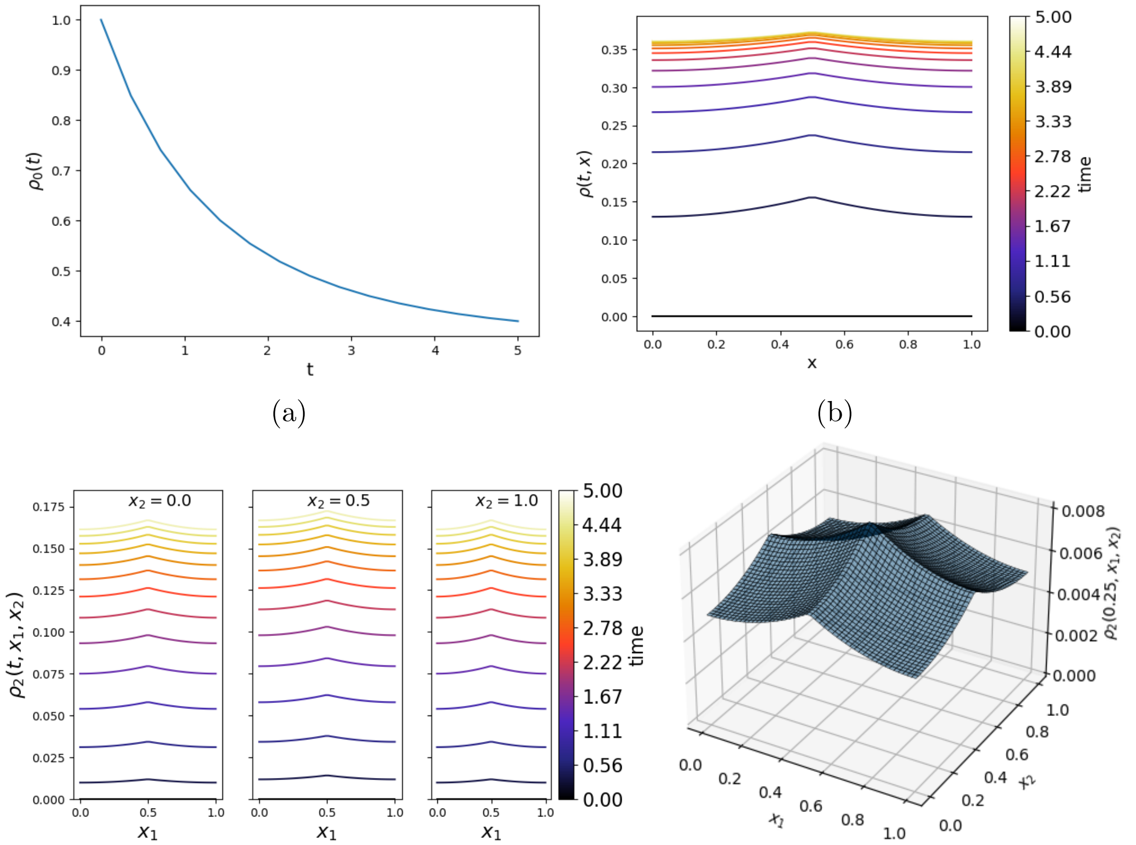
(a)

(b)

(c)

(d)

Figure 4.2: Solutions plots of the bdCDME generated with creation of particles at $x = 0$ and constant degradation in the whole domain, namely with $\lambda_c(x) = 0.5\delta_0(x)$ and $\lambda_d(x) = 0.5$. The first 1000 terms of the sum in eq. (4.3.4) are considered. a. The solution of the 0 particle density ($\rho_0(t)$) as a function of time. b. The solution of the 1 particle density ($\rho_1(t, x_1)$) for given position and time. c. The solution of the 2 particle density ($\rho_2(t, x_1, x_2)$) with respect to x_1 and t for three values of x_2. Time points as indicated in the color bar. d. The solution of the two particle density for fixed time, $\rho_2(t = 0.25, x_1, x_2)$, as a function of x_1 and x_2.



(a) (b)

(c) (d)

Figure 4.3: Solutions plots of the bdCDME generated with creation of particles at $x = 0.5$ and constant degradation in the whole domain, namely $\lambda_c = 0.5\delta_{1/2}(x)$ and $\lambda_d = 0.5$. The first 1000 terms of the sum in eq. (4.3.4) are considered. a. The solution of the 0 particle density ($\rho_0(t)$) as a function of time. b. The solution of the 1 particle density ($\rho_1(t,x_1)$) for given position and time. c. The solution of the 2 particle density ($\rho_2(t,x_1,x_2)$) with respect to x_1 and t for three values of x_2. Time points as indicated in the color bar. d. The solution of the two particle density for fixed time, $\rho_2(t = 0.25, x_1, x_2)$, as a function of x_1 and x_2.

Chapter 5

Solving the CDME With Mutual Annihilation and Creation

Abstract

We propose an infinite dimensional generating function method for finding the analytical solution of the so-called chemical diffusion master equation (CDME) for creation and mutual annihilation chemical reactions. CDMEs model by means of an infinite system of coupled Fokker-Planck equations the probabilistic evolution of chemical reaction kinetics associated with spatial diffusion of individual particles; here, we focus an creation and mutual annihilation chemical reactions combined with Brownian diffusion of the single particles. Using our method we are able to link certain finite dimensional projections of the solution of the CDME to the solution of a single linear fourth order partial differential equation containing as many variables as the dimension of the aforementioned projection space. Our technique extends the one presented in [Lanconelli, 2023] and [Lanconelli et al., 2023] which allowed for an explicit representation for the solution of birth-death type CDMEs.

5.1 Introduction

We consider a system of indistinguishable molecules of a chemical species S which undergo

- drift-less isotropic *diffusion* in the interval $[0,1]$;
- *creation* and *mutual annihilation* chemical reactions

$$\text{(I)} \quad \varnothing \xrightarrow{\lambda_c(x)} S \qquad\qquad \text{(II)} \quad S+S \xrightarrow{\lambda_d(x,y)} \varnothing,$$

where we consider an additional creation reaction unlike of the reaction (2.3.1) presented earlier, making the model model complex. Here, the function $[0,1] \ni x \mapsto \lambda_c(x)$ represents the stochastic rate function for reaction (I); it can be thought of being of the form $\lambda_c(x) = \gamma\pi_c(x)$ with γ being a positive constant representing the probability per unit of time for a new particle to be created while π_c is a probability density on $[0,1]$ which describes the random location for the birth of the new particle. Similarly, the function $[0,1]^2 \ni (x,y) \mapsto \lambda_d(x,y)$ is the stochastic rate function for reaction (II) to occur between two particles located at (x,y); for instance, when λ_d is constant then the location of the two particles is not relevant for reaction (II) to take place; on the contrary, if $\lambda_d(x,y) = \delta(x-y)$ (here δ stands for the Dirac delta function with mass at zero) then reaction (II) occurs (with rate one) only for particles having the same location.

To analyze the probabilistic evolution of such system the authors in [del Razo et al., 2022] (see also [del Razo et al., 2023] for a further discussion of the model) proposed a set of equations which describe how the number of molecules and their positions change with time. Namely, for $t \geq 0$, $n \geq 1$ and $A \in \mathcal{B}([0,1]^n)$ they set

$$\begin{aligned} \mathcal{N}(t) &:= \text{ number of molecules at time } t, \\ \rho_0(t) &:= \mathbb{P}(\mathcal{N}(t) = 0), \\ \int_A \rho_n(t, x_1, ..., x_n)dx_1 \cdots dx_n &:= \mathbb{P}\left(\{\mathcal{N}(t) = n\} \cap \{(X_1(t), ..., X_n(t)) \in A\}\right); \end{aligned}$$

here $(X_1(t), ..., X_n(t))$ is the vector collecting the positions at time t of the n particles constituting the system (we are also assuming that the stochastic processes under investigation are defined on a common probability space with reference measure $\mathbb{P}$). Then, following the steps in Chapter 3, they write the following infinite system of equations:

$$\begin{aligned} \partial_t\rho_n(t, x_1, ..., x_n) =& \sum_{i=1}^n \partial^2_{x_i}\rho_n(t, x_1, ..., x_n) \\ &+ \frac{(n+2)(n+1)}{2}\int_{[0,1]^2} \lambda_d(x,y)\rho_{n+2}(t, x_1, ..., x_n, x, y)dxdy \\ &- \sum_{i<j} \lambda_d(x_i, x_j) \cdot \rho_n(t, x_1, ..., x_n) \\ &+ \frac{1}{n}\sum_{i=1}^n \lambda_c(x_i)\rho_{n-1}(t, x_1, ..., x_{i-1}, x_{i+1}, ..., x_n) \\ &- \int_{[0,1]} \lambda_c(y)dy \cdot \rho_n(t, x_1, ..., x_n), \\ & \text{for all } n \geq 0, t > 0, (x_1, ..., x_n) \in [0,1]^n, \end{aligned} \tag{5.1.1}$$

where we agree on assigning value zero to the three sums above when $n = 0$. The term

$$\sum_{i=1}^n \partial^2_{x_i}\rho_n(t, x_1, ..., x_n)$$

in (5.1.1) refers to spatial diffusion of the particles; the terms

$$\frac{(n+2)(n+1)}{2}\int_{[0,1]^2}\lambda_d(x,y)\rho_{n+2}(t,x_1,...,x_n,x,y)dxdy$$

and

$$\sum_{i<j}\lambda_d(x_i,x_j)\cdot\rho_n(t,x_1,...,x_n)$$

formalize gain and loss, respectively, due to reaction (II), while

$$\frac{1}{n}\sum_{i=1}^{n}\lambda_c(x_i)\rho_{n-1}(t,x_1,...,x_{i-1},x_{i+1},...,x_n)$$

and

$$-\int_{[0,1]}\lambda_c(y)dy\cdot\rho_n(t,x_1,...,x_n)$$

represent gain and loss, respectively, associated to reaction (I). System (5.1.1) is combined with initial and Neumann boundary conditions

$$\begin{cases} \rho_0(0)=1; & \\ \rho_n(0,x_1,...,x_n)=0, & n\geq 1,(x_1,...,x_n)\in[0,1]^n; \\ \partial_\nu\rho_n(t,x_1,...,x_n)=0, & n\geq 1,t\geq 0,(x_1,...,x_n)\in\partial[0,1]^n. \end{cases} \tag{5.1.2}$$

The initial condition (first two equations in (5.1.2)) states that there are no molecules in the system at time zero while the Neumann condition prevents flux through the boundary of $[0,1]$, thus forcing the diffusion of the molecules inside $[0,1]$. The symbol ∂_ν in (5.1.2) stands for the directional derivative along the outer normal vector at the boundary of $[0,1]^n$.

5.2 Statement of the Main Result and Structure of the Section

Our main result links certain finite dimensional projections of the solution of (5.1.1) to a single linear partial differential equation thus providing a tool for finding analytical solutions to (5.1.1). Our techniques applies to the case where the function $\lambda_d:[0,1]^2\to$

$[0, +\infty[$ is constant. This means that the CDME in (5.1.1) simplifies to

$$\begin{cases} \partial_t \rho_n(t, x_1, ..., x_n) = & \sum_{i=1}^{n} \partial^2_{x_i} \rho_n(t, x_1, ..., x_n) \\ & + \lambda_d \frac{(n+2)(n+1)}{2} \int_{[0,1]^2} \rho_{n+2}(t, x_1, ..., x_n, x, y) dx dy \\ & - \lambda_d \frac{n(n-1)}{2} \rho_n(t, x_1, ..., x_n) \\ & + \frac{1}{n} \sum_{i=1}^{n} \lambda_c(x_i) \rho_{n-1}(t, x_1, ..., x_{i-1}, x_{i+1}, ..., x_n) \\ & - \gamma \rho_n(t, x_1, ..., x_n), \qquad n \geq 0, t > 0, (x_1, ..., x_n) \in [0,1]^n, \end{cases} \tag{5.2.1}$$

We are now going to state our main result and we refer the reader to the next sections for a detailed discussion of our assumptions and for the proof.

Theorem 5.2.1. *For $k \geq 1$ let*

$$\xi_k(x) := \sqrt{2} \cos((k-1)\pi x), x \in [0,1] \quad \text{and} \quad \alpha_k := (k-1)^2 \pi^2,$$

i.e. the eigenfunctions with corresponding eigenvalues of the differential operator $-\mathcal{A} = \partial^2_x$ with homogeneous Neumann boundary conditions (as prescribed in (5.1.2)). We also write Π_N for the orthogonal projection onto the linear span of $\{\xi_1, ..., \xi_N\}$.
If $\{\rho_n\}_{n \geq 0}$ solves (5.2.1)-(5.1.2), then we have the representation

$$\Pi_N^{\otimes n} \rho_n(t, x_1, ..., x_n) = \frac{1}{n!} \sum_{j_1, ..., j_n = 1}^{N} \left(\int_{\mathbb{R}^N} (\partial_{z_{j_1}} \cdots \partial_{z_{j_n}} u_N)(t, z) (2\pi)^{-N/2} e^{-\frac{|z|^2}{2}} dz \right) \cdot \xi_{j_1}(x_1) \ldots \xi_{j_n}(x_n), \tag{5.2.2}$$

where u_N is the solution to the following fourth order Cauchy problem

$$\begin{cases} \partial_t u_N(t,z) = -\sum_{k=1}^{N} \alpha_k (z_k - \partial_{z_k}) \partial_{z_k} u_N(t,z) + \frac{\lambda_d}{2} \partial^2_{z_1} u_N(t,z) \\ \qquad - \frac{\lambda_d}{2} \sum_{j,k=1}^{N} (z_j - \partial_{z_j})(z_k - \partial_{z_k}) \partial_{z_j} \partial_{z_k} u_N(t,z) \\ \qquad + \sum_{k=1}^{N} \mathsf{c}_k (z_k - \partial_{z_k}) u_N(t,z) - \gamma u_N(t,z); \quad t > 0, z \in \mathbb{R}^N; \\ u_N(0,z) = 1, \quad z \in \mathbb{R}^N. \end{cases}$$

and $\mathsf{c}_k := \langle \lambda_c, \xi_k \rangle_{L^2([0,1])}$ for $k \geq 1$.

The paper is organized as follows: In Chapter 5.3, we propose an alternative derivation of equation (5.1.1) than the one presented in Chapter 3 and in papers [del Razo et al., 2022] and also in [del Razo et al., 2023]. We mimic the classical approach utilized to obtain the chemical master equation through an adaptation that includes diffusion of the single particles. Even though the computation is pretty standard, we believe that such derivation helps for a better understanding of the ingredients that describe the problem under investigation. To this aim we will fix a set of transition probabilities (see Assumption 5.3.3 below) and derive through a limit argument the desired equation. We remark that our approach can be readily generalized to include higher order chemical reactions and more complex descriptions of the diffusive motion of the particles (i.e. anisotropic diffusion with drift).

In Chapter 5.2.1 we employ the general method proposed in [Lanconelli, 2023] and summarized in Chapter 3.4 to analytically solve equation (5.2.1)-(5.1.2). This requires the use of Gaussian Malliavin calculus's techniques (summarized in the appendix sections A.8 and A.9 below) and provides a link between the solution to (5.2.1)-(5.1.2) and the solution of a single fourth order linear PDE which describes certain finite dimensional projections of the solution to the original problem. At the end, some comments on the Gaussian features introduced in our problem by the proposed approach are also discussed.

5.3 Alternative Derivation of Equation (5.1.1)

In this section we present a derivation of equation (5.1.1) (here we do not need to confine ourselves to the case of a constant λ_d function as prescribed in the Theorem 5.2.1). We recall that the particles of the system under investigation are subject to the chemical reactions

$$\text{(I)} \quad \varnothing \xrightarrow{\lambda_c(x)} S \qquad \text{(II)} \quad S+S \xrightarrow{\lambda_d(x,y)} \varnothing, \tag{5.3.1}$$

and diffuse in space, between successive reactions, as independent Brownian motions on the interval $[0,1]$ with reflecting boundary conditions (compare with (5.1.2)). In the sequel we will be dealing with probabilities of the form $\mathbb{P}(\mathcal{N}(t)=n, X(t)\in A)$: this represents the probability that the system at time t is made of n many particles and that such particles are located in the region $A\subseteq[0,1]^n$. We are not going to use an extra index in $X(t)$ to stress that it is an n-dimensional vector; this vector will always come with an event of the type $\{\mathcal{N}(t)=n\}$ and hence the number of components of $X(t)$ will be uniquely determined. We mention that an analogous derivation for the chemical master equation with mutual annihilation and creation (without diffusion) can be found in [Erban and Chapman, 2020], Section 1.4.
Now we list a couple of technical assumptions which are necessary for our derivation:

Assumption 5.3.1. *For any $n\geq 1$, $A\in\mathcal{B}([0,1]^n)$ (the Borel sets of $[0,1]^n$) and $t>0$ there exists a symmetric function $\rho_n(t,x_1,...,x_n)$ such that*

$$\mathbb{P}(\mathcal{N}(t)=n, X(t)\in A)=\int_A \rho_n(t,x_1,...,x_n)dx_1\cdots dx_n;$$

we also set

$$\rho_0(t):=\mathbb{P}(\mathcal{N}(t)=0).$$

Notice that the symmetry of the functions ρ_n models the indistinguishability of the particles in the system; moreover, by construction the sequence $\{\rho_n\}_{n\geq 0}$ fulfils the constraint

$$\sum_{n\geq 0}\int_{[0,1]^n}\rho_n(t,x_1,...,x_n)dx_1\cdots dx_n = 1. \tag{5.3.2}$$

Assumption 5.3.2. *The functions* λ_c *and* λ_d *appearing in* (5.3.1) *are non negative, bounded and continuous. Moreover,* $\lambda_d(x,y)=\lambda_d(y,x)$ *for all* $x,y\in[0,1]$*.*

We are now ready to describe the probabilistic structure to be imposed on our system for the formal derivation of equation (5.1.1).

Assumption 5.3.3. *The system under investigation possesses the following properties:*

- Diffusion of particles*: in absence of chemical reactions, particles diffuse in* $[0,1]$ *like independent Brownian motions with variance* $2t$ *and reflecting boundary conditions; more precisely, the transition density* $\{\mathrm{p}_t(x|y)\}_{t\geq 0,x,y\in[0,1]^n}$ *for the motion of* n *many particles solves*

$$\begin{cases}\partial_t \mathrm{p}_t(x|y)=\sum_{j=1}^n\partial^2_{x_i}\mathrm{p}_t(t,x|y), & t>0, x,y\in[0,1]^n;\\ \mathrm{p}_0(x|y)=\delta_y(x), & x,y\in[0,1]^n;\\ \partial_\nu \mathrm{p}_t(x|y)=0, & t\geq 0, x\in\partial[0,1]^n, y\in[0,1]^n.\end{cases}$$

- Reaction (I) + diffusion of particles*: for any* $n\geq 1$*,* $A\in\mathcal{B}([0,1]^n)$ *and* $t,h>0$ *we have*

$$\begin{aligned}\mathbb{P}(\mathcal{N}(t+h)=n, X(t+h)\in A|\mathcal{N}(t)=n-1, X(t)=y)\\ = h\frac{1}{n}\sum_{j=1}^n\int_A\int_{[0,1]}\mathrm{p}_h(x|y\cup_j z)\lambda_c(z)dzdx+\mathcal{O}(h^2),\end{aligned} \tag{5.3.3}$$

  with $y\cup_j z := (y_1,...,y_{j-1},z,y_{j+1},...,y_n)\in[0,1]^n$ *and* $\mathrm{p}_h(x|y\cup_j z)$ *being the transition density between* $y\cup_j z$ *and* x *during the time interval* h*. To explain the contribution of each single term of the identity above, we imagine to split the function* λ_c *as* $\gamma\cdot\pi_c$ *where* $\gamma:=\int_{[0,1]}\lambda_c(z)dz$ *while* π_c *is a probability density function supported on* $[0,1]$*. The chemical reaction (I) adds a new particle, here denoted with* z*, to the system: the rate at which this happens is* γ *while the location for the birth of the particle is distributed according to* π_c*. Moreover, once the creation takes place the outer integral* $\int_A ...dx$ *in* (5.3.3) *describes the diffusion of the* n *particles of the system from the location* $y\cup_j z$ *to the set* A *during the time frame* h*. Lastly, to make particles indistinguishable we symmetrize over the possible positions of* z *in the vector* $y\cup_j z$ *with the term* $\frac{1}{n}\sum_{j=1}^n$*.*

- Reaction (II) + diffusion of particles*: for any $n \geq 0$, $A \in \mathcal{B}([0,1]^n)$ and $t, h > 0$ we have*

$$\begin{aligned}\mathbb{P}(\mathcal{N}(t+h) = n, X(t+h) \in A | \mathcal{N}(t) = n+2, X(t) = y)& \\ = h \sum_{j<k} \lambda_d(y_j, y_k) \int_A \mathrm{p}_h(x|\hat{y}_{j,k})dx + \mathcal{O}(h^2),&\end{aligned} \tag{5.3.4}$$

with $\hat{y}_{j,k} := (y_1, ..., y_{j-1}, y_{j+1}, ..., y_{k-1}, y_{k+1}, ..., y_n) \in [0,1]^n$. The chemical reaction (II) removes two particles from the system while the others diffuse: this is the contribution of $\int_A \mathrm{p}_h(x|\hat{y}_{j,k})dx$ where the particles labelled j and k are those undergoing the chemical reaction through the term $h\sum_{j<k} \lambda_d(y_j, y_k)$. This term is mediated over all the possible couples of particles in the system: the weights of this average, represented by the sum above, are provided by λ_d which measures the likelihood for two particles to react depending on their locations. We also mention that for $n = 0$ the right hand side of (5.3.4) simplifies to $h\lambda_d(x_1, x_2) + \mathcal{O}(h^2)$.

- No reactions + diffusion of particles*: for any $n \geq 1$, $A \in \mathcal{B}([0,1]^n)$ and $t, h > 0$ we have*

$$\begin{aligned}&\mathbb{P}(\mathcal{N}(t+h) = n, X(t+h) \in A | \mathcal{N}(t) = n, X(t) = y) \\ &\quad = \left(1 - h\int_{[0,1]} \lambda_c(z)dz - h\sum_{j<k} \lambda_d(y_j, y_k)\right) \int_A \mathrm{p}_h(x|y)dx + \mathcal{O}(h^2).\end{aligned} \tag{5.3.5}$$

The term inside parenthesis reflects the probability of no reaction happening while the integral formalizes the diffusion of particles.

- Multiple reactions*: for any $n \geq 1$, $A \in \mathcal{B}([0,1]^n)$ and $t, h > 0$ we have*

$$\mathbb{P}(\mathcal{N}(t+h) = n, X(t+h) \in A | \mathcal{N}(t) = k, X(t) = y) = \mathcal{O}(h^2), \tag{5.3.6}$$

whenever $k \notin \{n-1, n, n+2\}$.

We now show how to use Assumption 5.3.1-5.3.2-5.3.3 to get the CDME (5.1.1). Let $n \geq 1$ and $A \in \mathcal{B}([0,1]^n)$; then, according to the law of total probability we can write

$$\begin{aligned}\int_A \rho_n(t+h, x)dx =& \mathbb{P}(\mathcal{N}(t+h) = n, X(t+h) \in A) \\ =& \sum_{k\geq 0} \int_{[0,1]^k} [\mathbb{P}(\mathcal{N}(t+h) = n, X(t+h) \in A | \mathcal{N}(t) = k, X(t) = y) \\ & \qquad \mathbb{P}(\mathcal{N}(t) = k, X(t) \in dy)] \\ =& \sum_{k\geq 0} \int_{[0,1]^k} \mathbb{P}(\mathcal{N}(t+h) = n, X(t+h) \in A | \mathcal{N}(t) = k, X(t) = y)\end{aligned}$$

$$\cdot\, \rho_k(t,y)dy. \tag{5.3.7}$$

Notice that for $k=0$ the corresponding term in the sum above should be interpreted as

$$\mathbb{P}(\mathcal{N}(t+h)=n, X(t+h)\in A|\mathcal{N}(t)=0)\rho_0(t).$$

Now, in view of Assumption 5.3.3 the only transitions of order one in h are those with $k=n+2$, $k=n-1$ and $k=n$ while the others are of order at least two; therefore, we can rewrite (5.3.7) as

$$\begin{aligned}
&\int_A \rho_n(t+h,x)dx\\
=&\sum_{k\geq 0}\int_{[0,1]^k}\mathbb{P}(\mathcal{N}(t+h)=n, X(t+h)\in A|\mathcal{N}(t)=k, X(t)=y)\rho_k(t,y)dy\\
=&\int_{[0,1]^{n+2}}\mathbb{P}(\mathcal{N}(t+h)=n, X(t+h)\in A|\mathcal{N}(t)=n+2, X(t)=y)\rho_{n+2}(t,y)dy\\
&+\int_{[0,1]^{n-1}}\mathbb{P}(\mathcal{N}(t+h)=n, X(t+h)\in A|\mathcal{N}(t)=n-1, X(t)=y)\rho_{n-1}(t,y)dy\\
&+\int_{[0,1]^{n}}\mathbb{P}(\mathcal{N}(t+h)=n, X(t+h)\in A|\mathcal{N}(t)=n, X(t)=y)\rho_{n}(t,y)dy+\mathcal{O}(h^2)\\
=&\int_{[0,1]^{n+2}}\left(\int_A h\sum_{j<k}\lambda_d(y_j,y_k)\mathrm{p}_h(x|\hat{y}_{j,k})dx\right)\rho_{n+2}(t,y)dy\\
&+\int_{[0,1]^{n-1}}\left(\int_A \frac{h}{n}\sum_{j=1}^{n}\int_{[0,1]}\lambda_c(z)\mathrm{p}_h(x|y\cup_j z)dzdx\right)\rho_{n-1}(t,y)dy\\
&+\int_{[0,1]^{n}}\left(\int_A\left(1-h\int_{[0,1]}\lambda_c(z)dz-h\sum_{j<k}\lambda_d(y_j,y_k)\right)\mathrm{p}_h(x|y)dx\right)\rho_n(t,y)dy+\mathcal{O}(h^2)\\
=&h\int_A\left(\sum_{j<k}\int_{[0,1]^{n+2}}\lambda_d(y_j,y_k)\mathrm{p}_h(x|\hat{y}_{j,k})\rho_{n+2}(t,y)dy\right)dx\\
&+h\int_A\left(\frac{1}{n}\sum_{j=1}^{n}\int_{[0,1]^{n-1}}\int_{[0,1]}\lambda_c(z)\mathrm{p}_h(x|y\cup_j z)\rho_{n-1}(t,y)dzdy\right)dx\\
&+\int_A\left(\int_{[0,1]^n}\left(1-h\int_{[0,1]}\lambda_c(z)dz-h\sum_{j<k}\lambda_d(y_j,y_k)\right)\mathrm{p}_h(x|y)\rho_n(t,y)dy\right)dx+\mathcal{O}(h^2)
\end{aligned}$$

$$
\begin{aligned}
=&h\int_A\left(\sum_{j<k}\int_{[0,1]^2}\lambda_d(y_j,y_k)\left(\int_{[0,1]^n}\mathtt{p}_h(x|\hat{y}_{j,k})\rho_{n+2}(t,y)d\hat{y}_{j,k}\right)dy_jdy_k\right)dx\\
&+h\int_A\left(\frac{1}{n}\sum_{j=1}^n\int_{[0,1]^{n-1}}\int_{[0,1]}\lambda_c(z)\mathtt{p}_h(x|y\cup_j z)\rho_{n-1}(t,y)dzdy\right)dx\\
&+\int_A\left(\int_{[0,1]^n}\left(1-h\int_{[0,1]}\lambda_c(z)dz-h\sum_{j<k}\lambda_d(y_j,y_k)\right)\mathtt{p}_h(x|y)\rho_n(t,y)dy\right)dx\\
&+\mathcal{O}(h^2).
\end{aligned}
\tag{5.3.8}
$$

To ease the notation we now introduce the following:

$$
\mathtt{T}_h f(x):=\int_{[0,1]^n}\mathtt{p}_h(x|y)f(y)dy,\quad f\in C_0([0,1]^n),
$$

and recall that for suitably regular f we have

$$
\lim_{h\to 0}\mathtt{T}_h f(x)=f(x),\quad x\in[0,1]^n,
\tag{5.3.9}
$$

and

$$
\lim_{h\to 0}\frac{\mathtt{T}_h f(x)-f(x)}{h}=\sum_{i=1}^n\partial^2_{x_i}f(x)\quad x\in[0,1]^n;
\tag{5.3.10}
$$

we refer to [Kallenberg, 2021] for a precise formulation of those statements. With this notation at hand we can rewrite (5.3.8) as

$$
\begin{aligned}
\int_A\rho_n(t+h,x)dx=&h\int_A\left(\sum_{j<k}\int_{[0,1]^2}\lambda_d(y_j,y_k)(\mathtt{T}_h\rho_{n+2}(t,\cdot,y_j,y_k))(x)dy_jdy_k\right)dx\\
&+h\int_A\frac{1}{n}\sum_{j=1}^n\mathtt{T}_h(\lambda_c\otimes_j\rho_{n-1}(t,\cdot))(x)dx\\
&+\int_A(\mathtt{T}_h\rho_n(t,\cdot))(x)dx-h\int_{[0,1]}\lambda_c(z)dz\int_A(\mathtt{T}_h\rho_n(t,\cdot))(x)dx\\
&-h\sum_{j<k}(\mathtt{T}_h\lambda_d(\cdot_j,\cdot_k)\rho_n(t,\cdot))(x)dx+\mathcal{O}(h^2).
\end{aligned}
$$

Here, the symbol $\otimes_j$ denotes the tensor product that locates the variable of λ_c in the j-th position. We now subtract the quantity $\int_A\rho_n(t,x)dx$ from both sides of the last equality, divide by h and take the limit as h tends to zero. This gives

$$
\begin{aligned}
\int_A\partial_t\rho_n(t,x)dx=&\lim_{h\to 0}\int_A\frac{\rho_n(t+h,x)-\rho_n(t,x)}{h}dx\\
=&\lim_{h\to 0}\int_A\left(\sum_{j<k}\int_{[0,1]^2}\lambda_d(y_j,y_k)(\mathtt{T}_h\rho_{n+2}(t,\cdot,y_j,y_k))(x)dy_jdy_k\right)dx
\end{aligned}
$$

$$
\begin{aligned}
&+ \lim_{h\to 0}\int_A \frac{1}{n}\sum_{j=1}^{n} \mathtt{T}_h(\lambda_c \otimes_j \rho_{n-1}(t,\cdot))(x)dx \\
&+ \lim_{h\to 0}\int_A \frac{(\mathtt{T}_h\rho_n(t,\cdot))(x)-\rho_n(t,x)}{h}dx \\
&- \lim_{h\to 0}\int_{[0,1]} \lambda_c(z)dz \int_A (\mathtt{T}_h\rho_n(t,\cdot))(x)dx \\
&- \lim_{h\to 0}\int_A \sum_{j<k}(\mathtt{T}_h\lambda_d(\cdot_j,\cdot_k)\rho_n(t,\cdot))(x)dx.
\end{aligned}
$$

Now, using (5.3.9) we get

$$
\begin{aligned}
&\lim_{h\to 0}\int_A \left(\sum_{j<k}\int_{[0,1]^2} \lambda_d(y_j,y_k)(\mathtt{T}_h\rho_{n+2}(t,\cdot,y_j,y_k))(x)dy_jdy_k\right)dx \\
&= \int_A \left(\sum_{j<k}\int_{[0,1]^2} \lambda_d(y_j,y_k)\rho_{n+2}(t,x,y_j,y_k)dy_jdy_k\right)dx \\
&= \int_A \left(\frac{(n+2)(n+1)}{2}\int_{[0,1]^2} \lambda_d(y_j,y_k)\rho_{n+2}(t,x,y_j,y_k)dy_jdy_k\right)dx,
\end{aligned}
$$

and

$$
\begin{aligned}
&\lim_{h\to 0}\int_A \frac{1}{n}\sum_{j=1}^{n} \mathtt{T}_h(\lambda_c \otimes_j \rho_{n-1}(t,\cdot))(x)dx \\
&= \int_A \left(\frac{1}{n}\sum_{j=1}^{n}\lambda_c(x_j)\rho_{n-1}(t,x_1,...,x_{j-1},x_{j+1},...,x_n)\right)dx.
\end{aligned}
$$

Moreover, formula (5.3.10) yields

$$
\lim_{h\to 0}\int_A \frac{(\mathtt{T}_h\rho_n(t,\cdot))(x)-\rho_n(t,x)}{h}dx = \int_A \left(\sum_{i=1}^{n}\partial_{x_i}^2\rho_n(t,x)\right)dx,
$$

while formula (5.3.9) gives

$$
\lim_{h\to 0}\int_{[0,1]} \lambda_c(z)dz \int_A (\mathtt{T}_h\rho_n(t,\cdot))(x)dx = \int_{[0,1]} \lambda_c(z)dz \int_A \rho_n(t,x)dx
$$

and

$$
\lim_{h\to 0}\int_A \sum_{j<k}(\mathtt{T}_h\lambda_d(\cdot_j,\cdot_k)\rho_n(t,\cdot))(x)dx = \int_A \sum_{j<k}\lambda_d(x_j,x_k)\rho_n(t,x)dx.
$$

If we combine all the preceding equalities we can conclude that

$$
\int_A \partial_t\rho_n(t,x)dx = \int_A \left(\frac{(n+2)(n+1)}{2}\int_{[0,1]^2} \lambda_d(y_j,y_k)\rho_{n+2}(t,x,y_j,y_k)dy_jdy_k\right)dx
$$

$$
\begin{aligned}
&+\int_A \left(\frac{1}{n}\sum_{j=1}^{n}\lambda_c(x_j)\rho_{n-1}(t,x_1,...,x_{j-1},x_{j+1},...,x_n)\right)dx \\
&+\int_A \left(\sum_{i=1}^{n}\partial^2_{x_i}\rho_n(t,x)\right)dx \\
&-\int_{[0,1]}\lambda_c(z)dz\int_A \rho_n(t,x)dx \\
&-\int_A \sum_{j<k}\lambda_d(x_j,x_k)\rho_n(t,x)dx.
\end{aligned}
$$

Since $A \in \mathcal{B}([0,1]^n)$ is arbitrary, this is equivalent to (5.1.1). This derivation methodology is not specific to the mutual annihilation reaction so the readers are welcomed to derive the CDME of birth-death reaction (2.2.1) and check with expression (3.3.1).

5.4 Analysis of Equation (5.2.1)-(5.1.2) Through an Infinite Dimensional Generating Function Method

In this section we employ the general method proposed in [Lanconelli, 2023] to solve analytically the CDME (5.1.1)-(5.1.2). We mention that this method has lead to an explicit representation for the solution to the general birth-death CDME [Lanconelli et al., 2023]. For the application of that approach in the current framework we need to impose the following technical condition.

Assumption 5.4.1. *The function* $\lambda_d : [0,1]^2 \to [0,+\infty[$ *is constant; this means that equation* (5.1.1) *simplifies to*

$$
\begin{cases}
\partial_t\rho_n(t,x_1,...,x_n) = \displaystyle\sum_{i=1}^{n}\partial^2_{x_i}\rho_n(t,x_1,...,x_n) \\
\qquad + \lambda_d\dfrac{(n+2)(n+1)}{2}\displaystyle\int_{[0,1]^2}\rho_{n+2}(t,x_1,...,x_n,x,y)dxdy \\
\qquad - \lambda_d\dfrac{n(n-1)}{2}\rho_n(t,x_1,...,x_n) \\
\qquad + \dfrac{1}{n}\displaystyle\sum_{i=1}^{n}\lambda_c(x_i)\rho_{n-1}(t,x_1,...,x_{i-1},x_{i+1},...,x_n) \\
\qquad - \gamma\rho_n(t,x_1,...,x_n), \qquad n\geq 0, t>0, (x_1,...,x_n)\in[0,1]^n,
\end{cases}
\tag{5.4.1}
$$

The need for such assumption is related to some technical features of the method used to solve (5.4.1). We refer to Remark 5.4.6 below for details.

Remark 5.4.2. *As pointed out in [del Razo et al., 2022], if we fix the reaction rates to be positive constants so* $\gamma, \lambda_d \in \mathbb{R}^+$ *and integrate equation (5.4.1)-(5.1.2) with respect to* *all degrees of freedom, then this reduces to the classical chemical master equation for the reactions as also shown in Remark 3.2.2.*

$$(I)\quad \varnothing \xrightarrow{\gamma} S \qquad\qquad (II)\quad S+S \xrightarrow{\lambda_d} \varnothing.$$

In fact, identity

$$\mathbb{P}(\mathcal{N}(t)=n)=\int_{[0,1]^n}\rho_n(t,x_1,...,x_n)dx_1\cdots dx_n,$$

(compare with Assumption 5.3.1) together with the boundary conditions in (5.1.2) yield

$$\begin{aligned}\partial_t\mathbb{P}(\mathcal{N}(t)=n)=&\lambda_d\frac{(n+2)(n+1)}{2}\mathbb{P}(\mathcal{N}(t)=n+2)-\lambda_d\frac{n(n-1)}{2}\mathbb{P}(\mathcal{N}(t)=n)\\&+\gamma\mathbb{P}(\mathcal{N}(t)=n-1)-\gamma\mathbb{P}(\mathcal{N}(t)=n),\end{aligned}\tag{5.4.2}$$

which is indeed the desired chemical master equation (see equation (1.28) in the book [Erban and Chapman, 2020]: here, the authors employ the standard generating function method for solving equation (5.4.2)). We also mention that such computation, and hence the link between chemical diffusion master equations and their corresponding chemical master equations, is far from being obvious.

The scheme for solving (5.4.1), as presented in detail in [Lanconelli, 2023] and summarized in Chapter 3.4, is made of several steps that we now discuss in the following preparatory results. Before doing that, we introduce the notation $-\mathcal{A}:=\partial_x^2$ and we recall that in the Appendix A below, one can find a quick review of the Malliavin calculus's tools utilized in the sequel.

Lemma 5.4.3. *If $\{\rho_n\}_{n\geq 0}$ is a classical solution to equation (5.4.1)-(5.1.2), then*

$$\Phi(t):=\sum_{n\geq 0}I_n(\rho_n(t,\cdot))\tag{5.4.3}$$

solves

$$\begin{cases}\partial_t\Phi=d\Gamma(-\mathcal{A})\Phi+\frac{\lambda_d}{2}D_1^2\Phi-\frac{\lambda_d}{2}\mathtt{N}(\mathtt{N}-\mathtt{I})\Phi+D^\star_{\lambda_c}\Phi-\gamma\Phi;\\ \Phi(0)=1,\end{cases}\tag{5.4.4}$$

in $\mathtt{F}^\star$.

Proof. Using the definitions made in sections A.8 and A.9, let $\{\rho_n\}_{n\geq 0}$ be a classical solution to equation (5.4.1)-(5.1.2); this means in particular that $\rho_0\in C^1([0,+\infty[)$ and $\rho_n\in C^{1,2}([0,+\infty[\times[0,1]^n)$ for all $n\geq 1$. Recall also that according to Assumption 5.3.1, for any $n\geq 2$ and $t\geq 0$ the function $\rho_n(t,\cdot)$ is symmetric in its arguments. This allows us to consider the multiple Itô integrals $I_n(\rho_n(t,\cdot))$, formally defined in Appendix A.4, and to interchange the partial derivative ∂_t with the iterated integrals. Furthermore, employing the operators $d\Gamma(-\mathcal{A})$, D_1, $\mathtt{N}$ and $D^\star_{\lambda_c}$, whose definitions and properties can be found in the Appendix A.8 below, and equation (5.4.1), we can write for all $n \geq 1$ and $t \geq 0$ that

$$\begin{aligned}
\partial_t I_n(\rho_n(t,\cdot)) =& I_n(\partial_t \rho_n(t,\cdot))\\
=& d\Gamma(-\mathcal{A}) I_n(\rho_n(t,\cdot)) + \frac{\lambda_d}{2} D_1^2 I_{n+2}(\rho_{n+2}(t,\cdot)) - \frac{\lambda_d}{2}\mathtt{N}(\mathtt{N}-\mathtt{I}) I_n(\rho_n(t,\cdot))\\
&+ D^\star_{\lambda_c} I_{n-1}(\rho_{n-1}(t,\cdot)) - \gamma I_n(\rho_n(t,\cdot)).
\end{aligned}$$

If we now sum over $n \geq 0$ and recall that $\rho_{-1} \equiv 0$ while D_1^2 maps to zero any multiple Itô integral of order less than two, we obtain equation (5.4.4) for the stochastic process defined in (5.4.3). □

Remark 5.4.4. *It is worth to point out that condition (5.3.2) is already encoded in equation (5.4.4). In fact, using the tools introduced in Appendix A.5, A.8.1 and A.9, if* $\{\Phi(t)\}_{t\geq 0}$ *solves (5.4.4), then*

$$\begin{aligned}
\partial_t \langle\langle \Phi, \mathcal{E}(1)\rangle\rangle =& \langle\langle \partial_t\Phi, \mathcal{E}(1)\rangle\rangle\\
=& \langle\langle d\Gamma(-\mathcal{A})\Phi, \mathcal{E}(1)\rangle\rangle\\
&+ \frac{\lambda_d}{2}\langle\langle D_1^2\Phi, \mathcal{E}(1)\rangle\rangle - \frac{\lambda_d}{2}\langle\langle \mathtt{N}(\mathtt{N}-\mathtt{I})\Phi, \mathcal{E}(1)\rangle\rangle\\
&+ \langle\langle D^\star_{\lambda_c}\Phi, \mathcal{E}(1)\rangle\rangle - \gamma\langle\langle \Phi, \mathcal{E}(1)\rangle\rangle.
\end{aligned}$$

Now,

$$\langle\langle d\Gamma(-\mathcal{A})\Phi, \mathcal{E}(1)\rangle\rangle = \langle\langle \Phi, d\Gamma(-\mathcal{A})\mathcal{E}(1)\rangle\rangle = \langle\langle \Phi, \mathcal{E}(1)\diamond\delta(-\mathcal{A}1)\rangle\rangle = 0,$$

while

$$\begin{aligned}
\langle\langle D_1^2\Phi, \mathcal{E}(1)\rangle\rangle - \langle\langle \mathtt{N}(\mathtt{N}-\mathtt{I})\Phi, \mathcal{E}(1)\rangle\rangle =& \langle\langle \Phi, D_1^\star D_1^\star\mathcal{E}(1)\rangle\rangle - \langle\langle \Phi, \mathtt{N}(\mathtt{N}-\mathtt{I})\mathcal{E}(1)\rangle\rangle\\
=& \langle\langle \Phi, \mathcal{E}(1)\diamond\delta(1)\diamond\delta(1)\rangle\rangle - \langle\langle \Phi, \mathtt{N}^2\mathcal{E}(1) - \mathtt{N}\mathcal{E}(1)\rangle\rangle\\
=& \langle\langle \Phi, \mathcal{E}(1)\diamond\delta(1)\diamond\delta(1)\rangle\rangle - \langle\langle \Phi, \mathcal{E}(1)\diamond\delta(1)\diamond\delta(1)\rangle\rangle\\
=& 0.
\end{aligned}$$

Here, in the last equality we utilized the identities

$$\mathtt{N}\mathcal{E}(1) = \mathcal{E}(1)\diamond\delta(1) \quad \text{and} \quad \mathtt{N}^2\mathcal{E}(1) = \mathcal{E}(1)\diamond\delta(1)\diamond\delta(1) + \mathcal{E}(1)\diamond\delta(1).$$

Lastly,

$$\begin{aligned}
\langle\langle D^\star_{\lambda_c}\Phi, \mathcal{E}(1)\rangle\rangle - \gamma\langle\langle \Phi, \mathcal{E}(1)\rangle\rangle =& \langle\langle \Phi, D_{\lambda_c}\mathcal{E}(1)\rangle\rangle - \gamma\langle\langle \Phi, \mathcal{E}(1)\rangle\rangle\\
=& \int_{[0,1]} \lambda_c(x)dx \cdot \langle\langle \Phi, \mathcal{E}(1)\rangle\rangle - \gamma\langle\langle \Phi, \mathcal{E}(1)\rangle\rangle\\
=& 0.
\end{aligned}$$

This proves that $\partial_t \langle\langle \Phi(t), \mathcal{E}(1)\rangle\rangle = 0$*; since* $\Phi(0) = 1$ *(recall the initial condition in* (5.4.4) *which in turn follows from* (5.1.2)*) we deduce that* $\langle\langle \Phi(0), \mathcal{E}(1)\rangle\rangle = 1$ *and hence*

$$\langle\langle \Phi(t), \mathcal{E}(1)\rangle\rangle = 1, \qquad \textit{for all } t \geq 0. \tag{5.4.5}$$

On the other hand, by definition of dual pairing we can write

$$\langle\langle \Phi(t), \mathcal{E}(1)\rangle\rangle = \sum_{n\geq 0} \int_{[0,1]^n} \rho_n(t, x_1, ..., x_n) dx_1 \cdots dx_n,$$

which together with (5.4.5) *implies* (5.3.2)*. Notice that a similar calculation can be carried also when* λ_d *is not constant; in this case the operator* $\Phi \mapsto \mathtt{N}(\mathtt{N} - \mathtt{I})\Phi$ *should be replaced with* $\Phi \mapsto \delta^2(\lambda(\cdot,\cdot)D^2\Phi)$*. This shows that condition* (5.3.2) *is part of equation* (5.4.1) *also in the absence of Assumption* 5.4.1*.*

The usefulness of transforming the CDME (5.4.1)-(5.1.2) into the abstract problem (5.4.4) becomes apparent when we consider suitable finite dimensional projections of the stochastic process $\{\Phi(t)\}_{t\geq 0}$. To this aim, we set for $k \geq 1$

$$\xi_k(x) = \sqrt{2}\cos((k-1)\pi x), x \in [0,1] \quad \text{and} \quad \alpha_k = (k-1)^2\pi^2 \tag{5.4.6}$$

to be the eigenfunctions with corresponding eigenvalues of the differential operator $\mathcal{A}$ defined as: $-\mathcal{A} := \partial_x^2$ with homogeneous Neumann boundary conditions (as prescribed in (5.1.2)). As also done in Chapter 4, we also write Π_N for the orthogonal projection onto the linear span of $\{\xi_1, ..., \xi_N\}$.

Lemma 5.4.5. *If* $\{\Phi(t)\}_{t\geq 0}$ *solves* (5.4.4) *in* $\mathtt{F}^\star$*, then*

$$\Phi_N(t) := \Gamma(\Pi_N)\Phi(t), \quad t \geq 0 \tag{5.4.7}$$

solves

$$\begin{cases} \partial_t \Phi_N = d\Gamma(-\mathcal{A})\Phi_N + \frac{\lambda_d}{2} D_1^2 \Phi_N - \frac{\lambda_d}{2}\mathtt{N}(\mathtt{N}-\mathtt{I})\Phi_N + D^\star_{\Pi_N \lambda_c}\Phi_N - \gamma\Phi_N; \\ \Phi_N(0) = 1, \end{cases} \tag{5.4.8}$$

in $\mathtt{F}^\star$*.*

Proof. First of all note we direct the readers to Chapter A.9 for the definition of generalized random variables F^* and other tools utilized. Bearing this in mind, using (5.4.7) and (5.4.4) we can write

$$\begin{aligned} \partial_t \Phi_N &= \partial_t \Gamma(\Pi_N)\Phi = \Gamma(\Pi_N)\partial_t \Phi \\ &= \Gamma(\Pi_N)\left(d\Gamma(-\mathcal{A})\Phi + \frac{\lambda_d}{2} D_1^2 \Phi - \frac{\lambda_d}{2}\mathtt{N}(\mathtt{N}-\mathtt{I})\Phi + D^\star_{\lambda_c}\Phi - \gamma\Phi \right). \end{aligned} \tag{5.4.9}$$

The proof consists in showing that our assumptions allow for the commutation between the operator $\Gamma(\Pi_N)$ and each of the following: $d\Gamma(-\mathcal{A})$, D_1^2, $\mathtt{N}(\mathtt{N}-\mathtt{I})$ and $D^\star_{\lambda_d}$. Let us start with the commutation between $\Gamma(\Pi_N)$ and $d\Gamma(-\mathcal{A})$: for any smooth $h \in L^2([0,1])$ we have

$$\begin{aligned}\langle\langle \Gamma(\Pi_N) d\Gamma(-\mathcal{A})\Phi, \mathcal{E}(h)\rangle\rangle =& \langle\langle d\Gamma(-\mathcal{A})\Phi, \mathcal{E}(\Pi_N h)\rangle\rangle\\ =& \langle\langle \Phi, d\Gamma(-\mathcal{A})\mathcal{E}(\Pi_N h)\rangle\rangle\\ =& \langle\langle \Phi, \mathcal{E}(\Pi_N h) \diamond \delta(-\mathcal{A}\Pi_N h)\rangle\rangle\\ =& \langle\langle \Phi, \mathcal{E}(\Pi_N h) \diamond \delta(\Pi_N(-\mathcal{A})h)\rangle\rangle\\ =& \langle\langle \Phi, \Gamma(\Pi_N)(\mathcal{E}(h) \diamond \delta(-\mathcal{A}h))\rangle\rangle\\ =& \langle\langle \Gamma(\Pi_N)\Phi, \mathcal{E}(h) \diamond \delta(-\mathcal{A}h)\rangle\rangle\\ =& \langle\langle d\Gamma(-\mathcal{A})\Gamma(\Pi_N)\Phi, \mathcal{E}(h)\rangle\rangle\\ =& \langle\langle d\Gamma(-\mathcal{A})\Phi_N, \mathcal{E}(h)\rangle\rangle.\end{aligned}$$

Comparing the first and last members of this chain of equalities we deduce that

$$\Gamma(\Pi_N) d\Gamma(-\mathcal{A})\Phi = d\Gamma(-\mathcal{A})\Phi_N, \quad \text{in } \mathtt{F}^\star.$$

It is important to observe how in the fourth equality above the commutation between $-\mathcal{A}$ and Π_N is made possible by having chosen to project onto the space generated by the eigenfunctions of $-\mathcal{A}$.
We now study the commutation between $\Gamma(\Pi_N)$ and D_1^2:

$$\begin{aligned}\langle\langle \Gamma(\Pi_N) D_1^2\Phi, \mathcal{E}(h)\rangle\rangle =& \langle\langle D_1^2\Phi, \mathcal{E}(\Pi_N h)\rangle\rangle\\ =& \langle\langle D_1 D_1\Phi, \mathcal{E}(\Pi_N h)\rangle\rangle\\ =& \langle\langle \Phi, D_1^\star D_1^\star\mathcal{E}(\Pi_N h)\rangle\rangle\\ =& \langle\langle \Phi, \mathcal{E}(\Pi_N h) \diamond \delta(1) \diamond \delta(1)\rangle\rangle\\ =& \langle\langle \Phi, \Gamma(\Pi_N)(\mathcal{E}(h) \diamond \delta(1) \diamond \delta(1))\rangle\rangle\\ =& \langle\langle \Gamma(\Pi_N)\Phi, \mathcal{E}(h) \diamond \delta(1) \diamond \delta(1)\rangle\rangle\\ =& \langle\langle D_1 D_1 \Gamma(\Pi_N)\Phi, \mathcal{E}(h)\rangle\rangle\\ =& \langle\langle D_1^2 \Gamma(\Pi_N)\Phi, \mathcal{E}(h)\rangle\rangle.\end{aligned}$$

In the fifth equality above we employed the identity $\Pi_N 1 = \Pi_1 1 = 1$ since the first eigenfunction of $-\mathcal{A}$ is precisely 1. We therefore can conclude that

$$\Gamma(\Pi_N) D_1^2\Phi = D_1^2\Phi_N, \quad \text{in } \mathtt{F}^\star.$$

We proceed with the commutation between $\Gamma(\Pi_N)$ and $\mathtt{N}(\mathtt{N}-\mathtt{I})$:

$$\begin{aligned}\langle\langle \Gamma(\Pi_N)\mathtt{N}(\mathtt{N}-\mathtt{I})\Phi, \mathcal{E}(h)\rangle\rangle &= \langle\langle \mathtt{N}(\mathtt{N}-\mathtt{I})\Phi, \mathcal{E}(\Pi_N h)\rangle\rangle\\ &= \langle\langle \Phi, \mathcal{E}(\Pi_N h) \diamond \delta(\Pi_N h) \diamond \delta(\Pi_N h)\rangle\rangle\\ &= \langle\langle \Phi, \Gamma(\Pi_N)(\mathcal{E}(h) \diamond \delta(h) \diamond \delta(h))\rangle\rangle\\ &= \langle\langle \Phi_N, \mathcal{E}(h) \diamond \delta(h) \diamond \delta(h)\rangle\rangle\\ &= \langle\langle \Phi_N, \mathtt{N}(\mathtt{N}-\mathtt{I})\mathcal{E}(h)\rangle\rangle\end{aligned}$$

$$= \langle\langle \mathtt{N}(\mathtt{N}-\mathtt{I})\Phi_N, \mathcal{E}(h)\rangle\rangle.$$

This yields

$$\Gamma(\Pi_N)\mathtt{N}(\mathtt{N}-\mathtt{I})\Phi = \mathtt{N}(\mathtt{N}-\mathtt{I})\Phi_N, \quad \text{in } \mathtt{F}^\star.$$

Lastly,

$$\begin{aligned}\langle\langle \Gamma(\Pi_N)D^\star_{\lambda_c}\Phi, \mathcal{E}(h)\rangle\rangle =& \langle\langle D^\star_{\lambda_c}\Phi, \mathcal{E}(\Pi_N h)\rangle\rangle \\ =& \langle\langle \Phi, \mathcal{E}(\Pi_N h)\rangle\rangle \int_0^1 \Pi_N h(x)\lambda_c(x)dx \\ =& \langle\langle \Gamma(\Pi_N)\Phi, \mathcal{E}(h)\rangle\rangle \int_0^1 h(x)\Pi_N\lambda_c(x)dx \\ =& \langle\langle \Phi_N, D_{\Pi_N\lambda_c}\mathcal{E}(h)\rangle\rangle \\ =& \langle\langle D^\star_{\Pi_N\lambda_c}\Phi_N, \mathcal{E}(h)\rangle\rangle,\end{aligned}$$

and hence

$$\Gamma(\Pi_N)D^\star_{\lambda_c}\Phi = D^\star_{\Pi_N\lambda_c}\Phi_N, \quad \text{in } \mathtt{F}^\star.$$

An implementation of all derived identities in (5.4.9) leads directly to (5.4.8). □

Remark 5.4.6. *The previous lemma is a key ingredient of our method since it allows for finite dimensional projections of the solution to equation (5.4.4). In particular, it is the possibility of commuting* $d\Gamma(-\mathcal{A})$ *and* $\mathtt{N}(\mathtt{N}-\mathtt{I})$ *with* $\Gamma(\Pi_N)$ *that implies the desired result. It is worth to mention that such possibility exists because of assumption 5.4.1, thus motivating this strong simplification. In fact, without such assumption we would not be able to commute* $\Gamma(\Pi_N)$ *with the operator* $\Phi \mapsto \delta^2(\lambda(\cdot,\cdot)D^2\Phi)$ *which is what one should work with, in the place of* $\mathtt{N}(\mathtt{N}-\mathtt{I})$*, for non constant* λ_d*. One may also wonder whether changing the projection space related to* Π_N *could solve this issue (maybe defining a finite dimensional space described by the function* λ_d*): however, this modification would imply the loss of commutativity between* $\Gamma(\Pi_N)$ *and* $d\Gamma(-\mathcal{A})$*.*

Lemma 5.4.7. *For any* $N \geq 1$ *there exists a function* $u_N : [0+\infty[\times\mathbb{R}^N$ *such that*

$$\Phi_N(t) = u_N(t, I_1(\xi_1), ..., I_1(\xi_N)), \quad \mathbb{P}\text{-a.s.}$$

Furthermore, the function u_N *solves (weakly) the following fourth order linear problem:*

$$\begin{cases}\partial_t u_N(t,z) = -\sum_{k=1}^N \alpha_k\partial_k^\star\partial_k u_N(t,z) + \frac{\lambda_d}{2}\partial_1^2 u_N(t,z) \\ \qquad -\frac{\lambda_d}{2}\sum_{j,k=1}^N \partial_j^\star\partial_k^\star\partial_j\partial_k u_N(t,z) \\ \qquad + \sum_{k=1}^N \mathtt{c}_k\partial_k^\star u_N(t,z) - \gamma u_N(t,z); \quad t>0, z\in\mathbb{R}^N; \\ u_N(0,z) = 1, \quad z\in\mathbb{R}^N.\end{cases} \tag{5.4.10}$$

Here, for any $k \in \{1,...,N\}$ *the symbol* ∂_k *is a shorthand notation for* ∂_{z_k} *while* $\partial_k^\star$ *stands for the differential operator* $-\partial_k + z_k$ *(which is nothing else that the Gaussian divergence). Moreover,* $\mathtt{c}_k := \langle\lambda_c, \xi_k\rangle_{L^2([0,1])}$*.*

Proof. It is well known (see for instance Theorem 4.9 in [Janson, 1997]) that the second quantization operator $\Gamma(\Pi_N)$ corresponds to the conditional expectation with respect to the sigma-algebra generated by the random variables $I_1(\xi_1)$,..., $I_1(\xi_N)$; therefore, according to (5.4.7) we can write

$$\Phi_N(t)=\Gamma(\Pi_N)\Phi(t)=\mathbb{E}[\Phi(t)|\sigma(I_1(\xi_1),...,I_1(\xi_N))]=u_N(t,I_1(\xi_1),...,I_1(\xi_N)).$$

Here, the function $u_N : [0+\infty[\times\mathbb{R}^N$ is measurable and its existence in guaranteed by Doob's lemma (see Lemma 1.13 in [Kallenberg, 2021]). We now replace $\Phi_N(t)$ with $u_N(t,I_1(\xi_1),...,I_1(\xi_N))$ in (5.4.8) and decompose the Malliavin calculus's operators along the orthonormal bases $\{\xi_k\}_{k\geq 1}$. More precisely:

$$\begin{aligned}
d\Gamma(-\mathcal{A})[u_N(t,I_1(\xi_1),...,I_1(\xi_N))] =&\delta\left(-\mathcal{A}D[u_N(t,I_1(\xi_1),...,I_1(\xi_N))]\right)\\
=&\delta\left(-\mathcal{A}\sum_{k\geq 1}D_{\xi_k}u_N(t,I_1(\xi_1),...,I_1(\xi_N))\xi_k\right)\\
=&\delta\left(-\mathcal{A}\sum_{k=1}^{N}\partial_k u_N(t,I_1(\xi_1),...,I_1(\xi_N))\xi_k\right)\\
=&\delta\left(-\sum_{k=1}^{N}\alpha_k\partial_k u_N(t,I_1(\xi_1),...,I_1(\xi_N))\xi_k\right)\\
=&-\sum_{k=1}^{N}\alpha_k\partial_k u_N(t,I_1(\xi_1),...,I_1(\xi_N))I_1(\xi_k)\\
&+\sum_{k=1}^{N}\alpha_k\partial_k^2 u_N(t,I_1(\xi_1),...,I_1(\xi_N))\\
=&-\sum_{k=1}^{N}\alpha_k\partial_k^{\star}\partial_k u_N(t,I_1(\xi_1),...,I_1(\xi_N));
\end{aligned}$$

Here, in the second-to-last equality we employed identity (1.56) from [Nualart, 2006]. We proceed now with

$$D_1^2u_N(t,I_1(\xi_1),...,I_1(\xi_N))=\partial_1^2u_N(t,I_1(\xi_1),...,I_1(\xi_N)),$$

and

$$\begin{aligned}
\mathtt{N}(\mathtt{N}-\mathtt{I})u_N(t,I_1(\xi_1),...,I_1(\xi_N)) =&(\mathtt{N}^2-\mathtt{N})u_N(t,I_1(\xi_1),...,I_1(\xi_N))\\
=&\sum_{j=1}^{N}\partial_j^{\star}\partial_j\left(\sum_{k=1}^{N}\partial_k^{\star}\partial_k u_N(t,I_1(\xi_1),...,I_1(\xi_N))\right)\\
&-\sum_{k=1}^{N}\partial_k^{\star}\partial_k u_N(t,I_1(\xi_1),...,I_1(\xi_N))
\end{aligned}$$

$$= \sum_{j,k=1}^{N} \partial_j^\star \partial_k^\star \partial_j \partial_k u_N(t, I_1(\xi_1), ..., I_1(\xi_N)).$$

In the last equality we employed the commutation relation $\partial_j \partial_k^\star = \partial_k^\star \partial_j + \delta_{jk}\mathtt{I}$ where δ_{jk} stands for the Kronecker symbol. Lastly,

$$\begin{aligned} D^\star_{\Pi_N \lambda_c} u_N(t, I_1(\xi_1), ..., I_1(\xi_N)) &= \sum_{k\geq 1} D^\star_{\xi_k} u_N(t, I_1(\xi_1), ..., I_1(\xi_N)) \langle \Pi_N \lambda_c, \xi_k \rangle_{L^2([0,1])} \\ &= \sum_{k=1}^{N} \partial_k^\star u_N(t, I_1(\xi_1), ..., I_1(\xi_N)) \langle \Pi_N \lambda_c, \xi_k \rangle_{L^2([0,1])} \\ &= \sum_{k=1}^{N} \partial_k^\star u_N(t, I_1(\xi_1), ..., I_1(\xi_N)) \mathsf{c}_k. \end{aligned}$$

Collecting all identities derived above we see how equation (5.4.8) is equivalent to (5.4.10). □

We are now ready to state the main result of the present section.

Theorem 5.4.8. *Let $\{\rho_n\}_{n\geq 0}$ be a classical solution to the CDME (5.4.1)-(5.1.2). Then, for any $N \geq 1$ we have the representation*

$$\Pi_N^{\otimes n} \rho_n(t, x_1, ..., x_n) = \frac{1}{n!} \sum_{j_1,...,j_n=1}^{N} \mathbb{E}[(\partial_{j_1} \cdots \partial_{j_n} u_N)(t, I_1(\xi_1), ..., I_1(\xi_n))] \xi_{j_1}(x_1) \cdots \xi_{j_n}(x_n), \tag{5.4.11}$$

for all $n \geq 1$, $t \geq 0$, $(x_1, ..., x_n) \in [0,1]^n$ and with u_N solution to the Cauchy problem (5.4.10).

Proof. If $\{\rho_n\}_{n\geq 0}$ is a classical solution to the CDME (5.4.1)-(5.1.2), then according to Lemma 5.4.3 the stochastic process $\{\Phi(t)\}_{t\geq 0}$ defined in (5.4.3) solves equation (5.4.4) in $\mathtt{F}^\star$. Moreover, Lemma 5.4.5 shows that the finite dimensional projection of $\{\Phi(t)\}_{t\geq 0}$ introduced in (5.4.7) solves the auxiliary problem (5.4.8). Notice that by construction the kernels of the Wiener Itô chaos expansion of $\{\Phi_N(t)\}_{t\geq 0}$ are $\{\Pi_N^{\otimes} \rho_n\}_{n\geq 0}$ (since this is the action of $\Gamma(\Pi_N)$ on $\{\Phi(t)\}_{t\geq 0}$).
On the other hand, according to the Stroock-Taylor formula (see Exercise 1.2.6 in [Nualart, 2006] and Chapter A.9) the Wiener Itô chaos expansion of $\{\Phi_N(t)\}_{t\geq 0}$ can also be represented as

$$\Pi_N^{\otimes} \rho_n(t, x_1, ..., x_n) = \frac{1}{n!} \mathbb{E}[D_{x_1} \cdots D_{x_n} \Phi_N(t)]. \tag{5.4.12}$$

From Lemma 5.4.7 the process $\{\Phi_N(t)\}_{t\geq 0}$ can be written as $\{u_N(t, I_1(\xi_1), ..., I_1(\xi_n))\}_{t\geq 0}$ where u_N solution to the Cauchy problem (5.4.10). Therefore, substituting this into

(5.4.12) and computing the Malliavin derivatives yields

$$\begin{aligned}\Pi_N^{\otimes}\rho_n(t,x_1,...,x_n) =&\frac{1}{n!}\mathbb{E}[D_{x_1}\cdots D_{x_n}u_N(t,I_1(\xi_1),...,I_1(\xi_n))]\\ =&\frac{1}{n!}\sum_{j_1,...,j_n=1}^{N}\mathbb{E}[(\partial_{j_1}\cdots\partial_{j_n}u_N)(t,I_1(\xi_1),...,I_1(\xi_n))]\xi_{j_1}(x_1)\cdots\xi_{j_n}(x_n),\end{aligned}$$

which is the formula we wanted to prove. □

5.5 Some Comments on the PDE (5.4.10)

The generalization of the generating function method utilized in this section has introduced some new Gaussian features to the original problem (5.4.1)-(5.1.2). At a formal level, the infinite dimensional nature of the system of Fokker-Planck equations under investigation combined with the Fock space structure of the sequence $\{\rho_n\}_{n\geq 0}$ leads naturally to the use of Gaussian stochastic analysis's techniques.
We now try to rewrite the representation formula (5.4.11) in a Gaussian-free manner. To this aim, we present the following technical result.

Lemma 5.5.1. *Let $f\in C^1(\mathbb{R}^N)$ be, together with all its first order partial derivatives, polynomially bounded at infinity. Then, setting*

$$\tilde{f}(z):=\int_{\mathbb{R}^N}f(y)(2\pi)^{-N/2}e^{-|z-y|^2/2}dy,\quad z\in\mathbb{R}^N,$$

we have for all $k\in\{1,...,N\}$ and $z\in\mathbb{R}^N$ that

$$\widetilde{\partial_k f}(z)=\partial_k\tilde{f}(z)\quad \text{and}\quad \widetilde{\partial_k^{\star}f}(z)=z_k\tilde{f}(z)\tag{5.5.1}$$

Proof. It is a direct verification. □

Proposition 5.5.2. *If u_N solves the PDE (5.4.10), then $v_N:=\tilde{u}_N$ solves*

$$\begin{cases}\partial_t v_N(t,z)=-\sum_{k=1}^N\alpha_k z_k\partial_k v_N(t,z)+\frac{\lambda_d}{2}\partial_1^2 v_N(t,z)\\ \qquad -\frac{\lambda_d}{2}\sum_{j,k=1}^N z_j z_k\partial_j\partial_k v_N(t,z)\\ \qquad +\sum_{k=1}^N \mathsf{c}_k z_k v_N(t,z)-\gamma v_N(t,z);\quad t>0,z\in\mathbb{R}^N;\\ v_N(0,z)=1,\quad z\in\mathbb{R}^N.\end{cases}\tag{5.5.2}$$

Proof. Follows immediately from (5.5.1). □

The PDE (5.5.2) represents a version of (5.4.10) in which the Gaussian features inherited from our approach have been removed. Equation (5.5.2) has certainly the advantage over

(5.4.10) of being of second order (contrary to the fourth order of the latter); moreover, if we consider the case $N = 1$ and remember that $\xi_1 \equiv 1$ and $\alpha_1 = 0$ we obtain

$$\begin{cases} \partial_t v_1(t,z) = \frac{\lambda_d}{2}(1 - z_1^2)\partial_1^2 v_1(t,z) + \gamma(z_1 - 1)v_1(t,z); \quad t > 0, z \in \mathbb{R}; \\ v_1(0,z) = 1, \quad z \in \mathbb{R}. \end{cases} \tag{5.5.3}$$

This is exactly the equation you obtain via the classical generating function method applied to the CME (5.4.2), which is the diffusion-free analogue of our system (5.4.1)-(5.1.2). See [Erban and Chapman, 2020] for a detailed study of (5.5.3). Therefore, from this point of view equation (5.5.2) is the natural extension of (5.5.3) to a model that includes diffusion of the particles.

Even though equation (5.5.2) possesses some desirable properties, its investigation from both analytical and numerical points of view presents some important obstacles. First of all, if we use the function v_N solution to (5.5.2) in the place of u_N solution to (5.4.10), then the representation formula (5.4.11) takes the form

$$\Pi_N^{\otimes n}\rho_n(t,x_1,...,x_n) = \frac{1}{n!}\sum_{j_1,...,j_n=1}^{N}(\partial_{j_1}\cdots\partial_{j_n}v_N)(t,0,...,0)\xi_{j_1}(x_1)\cdots\xi_{j_n}(x_n), \tag{5.5.4}$$

as it follows immediately by the definition of v_N and Lemma 5.5.1. This means that the natural domain for solving (5.5.2) would be a neighborhood of the origin instead of the whole space; this can be seen already in the case $N = 1$, i.e. equation (5.5.3), where z_1 should be taken in $[-1,1]$ in order to avoid a sign change in the leading second order term. However, it is very hard to find a reasonable argument for assigning a boundary value to the problem (5.5.2) (this issue is also discussed in [McQuarrie, 1967b]).

A second main difficulty in analyzing equation (5.5.2) is due to its intrinsic ill-posedness. In fact, if for simplicity we take $N = 2$ and focus on the second order (i.e. leading) term of the differential operator appearing in the right hand side of (5.5.2), we see that the matrix describing its coefficients is a multiple of

$$A(z_1,z_2) = \begin{bmatrix} 1 - z_1^2 & -z_1 z_2 \\ -z_1 z_2 & -z_2^2 \end{bmatrix}.$$

Checking the positive semi-definiteness of the matrix A (recall that where have an initial condition for solving equation (5.5.2)) we see that

$$\begin{aligned} \langle A(z_1,z_2)\theta,\theta\rangle =& (1 - z_1^2)\theta_1^2 - 2z_1z_2\theta_1\theta_2 - z_2^2\theta_2^2 \\ =& \theta_1^2 - (z_1\theta_1 + z_2\theta_2)^2 \end{aligned}$$

and the last quantity cannot be non negative for any choice of $(\theta_1,\theta_2) \in \mathbb{R}^2$ unless $z_2 = 0$ (to see this take $\theta_1 = 0$). Therefore, there is no open neighborhood of the origin for the space variable z where the matrix A is positive semi-definiteness. This entails the ill-posedness of the PDE (5.5.2).

The discussion presented above highlights some potential advantages in embedding the CDME (5.4.1)-(5.1.2) into the Gaussian framework utilized in this section for deriving the representation formula (5.4.11).

Chapter 6

Branching Brownian Motion from a CDME Perspective

Abstract

Aim of this note is to analyse branching Brownian motion within the class of models introduced in the recent paper [del Razo et al., 2022] and called chemical diffusion master equations. These models provide a description for the probabilistic evolution of chemical reaction kinetics associated with spatial diffusion of individual particles. We derive an infinite system of Fokker-Planck equations that rules the probabilistic evolution of the single particles generated by the branching mechanism and analyse its properties using Malliavin Calculus techniques, following the ideas proposed in [Lanconelli, 2023]. Another key ingredient of our approach is the McKean representation for the solution of the Fisher-Kolmogorov-Petrovskii-Piskunov equation and a stochastic counterpart of that equation. We also derive the reaction-diffusion partial differential equation solved by the average concentration field of the branching Brownian system of particles.

6.1 Introduction and Statement of the Main Results

Let $\{X_k(t), k \in \{1, ..., \mathtt{n}(t)\}\}_{t\geq 0}$ be a (binary) branching Brownian motion. That means, at time zero a single particle $\{X(t)\}_{t\geq 0}$ starting at the origin begins to perform Brownian motion in $\mathbb{R}$; after an exponential time τ of parameter one, the particle splits into two identical, independent copies of itself that start Brownian motion at $X(\tau)$. This process is repeated ad infinitum, producing a collection of $\mathtt{n}(t)$ particles $\{X_1(t), X_2(t), ..., X_{\mathtt{n}(t)}(t)\}_{t\geq 0}$ (we refer the reader to [Bovier, 2015] and the references quoted there for more details on the subject). For $t \geq 0$, $n \geq 1$ and $A \in \mathcal{B}(\mathbb{R}^n)$ we set

$$\int_A \rho_n(t, y_1, ..., y_n) dy_1 \cdots dy_n := \mathbb{P}\left(\{\mathtt{n}(t) = n\} \cap \{(X_1(t), ..., X_n(t)) \in A\}\right); \qquad (6.1.1)$$

notice that by construction the sequence $\{\rho_n\}_{n\geq 1}$ fulfils the constraint

$$\sum_{n\geq 1}\int_{\mathbb{R}^n}\rho_n(t,y_1,...,y_n)dy_1\cdots dy_n = 1. \tag{6.1.2}$$

Furthermore, for all $n\geq 2$ and $t\geq 0$ the functions

$$(y_1,...,y_n)\mapsto\rho_n(t,y_1,...,y_n)$$

are symmetric in their arguments: this formalizes the indistinguishability of the different Brownian particles generated by the branching mechanism.
Our first main result reads as follows.

Theorem 6.1.1. *The sequence $\{\rho_n\}_{n\geq 1}$ solves the system of equations*

$$\begin{cases}\partial_t\rho_n(t,y_1,...,y_n) = \frac{1}{2}\sum_{k,l=1}^{n}\partial^2_{y_k y_l}\rho_n(t,y_1,...,y_n)+\sum_{k=1}^{n-1}\rho_k\hat{\otimes}\rho_{n-k}(t,y_1,...,y_n)\\ \qquad\qquad\qquad\qquad -\rho_n(t,y_1,...,y_n), \quad \textit{for } n\geq 1, t>0, y_1,...,y_n\in\mathbb{R};\\ \rho_1(0,y_1)=\delta_0(y_1), \quad y_1\in\mathbb{R};\\ \rho_n(0,y_1,...,y_n)=0, \quad y_1,...,y_n\in\mathbb{R};\end{cases} \tag{6.1.3}$$

here, δ_0 stands for the Dirac delta function concentrated at the origin while $\hat{\otimes}$ denotes symmetric tensor product with respect to the variables $(y_1,...,y_n)$. Moreover, we have the representation

$$\rho_n(t,y_1,...,y_n) = g_n(t,x;x-y_1,...,x-y_n), \quad t\geq 0, x,y_1,...,y_n\in\mathbb{R} \tag{6.1.4}$$

where $\{g_n\}_{n\geq 1}$ is a sequence of functions with

$$\begin{aligned} g_n : [0,+\infty[\times\mathbb{R}\times\mathbb{R}^n &\to \mathbb{R}\\ (t,x,y_1,...,y_n) &\mapsto g_n(t,x;y_1,...,y_n)\end{aligned}$$

and defined recursively as

$$\begin{cases} g_1(t,x;y_1) := e^{-t}\mathtt{p}_t(x-y_1), \quad t\geq 0, x, y_1\in\mathbb{R};\\ g_n(t,x;y_1,...,y_n) := e^{-t}\int_0^t\int_{\mathbb{R}}\mathtt{p}_{t-s}(x-z)e^s\sum_{k=1}^{n-1}g_k\hat{\otimes}g_{n-k}(s,z;y_1,...,y_n)dzds,\\ \qquad\qquad\qquad\qquad n\geq 2, t\geq 0 \textit{ and } x,y_1,...,y_n\in\mathbb{R}.\end{cases}$$

The symbol $\mathtt{p}_t(x-z)$ stands for the one dimensional heat kernel $(2\pi t)^{-\frac{1}{2}}e^{-\frac{(x-z)^2}{2t}}$.

Remark 6.1.2. *If we view branching Brownian motion as a system of particles undergoing Brownian diffusion and splitting chemical reactions (as described above), then following [del Razo et al., 2022],[del Razo et al., 2023] (see also [Doi, 1976]) we can interpret system (6.1.3) within the class of chemical diffusion master equations. Equation (6.1.3) has been previously derived in [Adke and Moyal, 1963] and further developed in [Adke, 1964] but not treated as presented here.*

Now, let $\{\rho_n\}_{n\geq 1}$ be solution to (6.1.3) and consider for $0 \leq k \leq n$ the quantity

$$p^{\varepsilon}_{k,n-k}(t,x) := \binom{n}{k} \int_{B_\varepsilon(x)^k \times B^c_\varepsilon(x)^{n-k}} \rho_n(t, y_1, ..., y_n) dy_1 ... dy_n. \tag{6.1.5}$$

This represents the probability of having n particles at time t with exactly k of the them in the ball centred at $x \in \mathbb{R}$ and radius $\varepsilon > 0$; moreover, writing

$$\mathcal{X}^{\varepsilon}(t,x) := \sum_{n\geq 1} \sum_{k=0}^{n} k p^{\varepsilon}_{k,n-k}(t,x) \tag{6.1.6}$$

we obtain the average number of particles that are located at time t in the ball $B_\varepsilon(x)$. Lastly, the average concentration of particles at x is obtained through the limit

$$c(t,x) := \lim_{\varepsilon\to 0} \frac{\mathcal{X}^{\varepsilon}(t,x)}{\mathtt{vol}(B_\varepsilon(x))},$$

and combining (6.1.5) with (6.1.6) one finds that $\{c(t,x)\}_{t\geq 0, x\in\mathbb{R}}$, which we call *average concentration field*, can be directly related to the sequence $\{\rho_n\}_{n\geq 1}$ via the formula

$$c(t,x) = \sum_{n\geq 1} n \int_{\mathbb{R}^{n-1}} \rho_n(t, y_1, ..., y_{n-1}, x) dy_1 ... dy_{n-1}, \quad t \geq 0, x \in \mathbb{R}; \tag{6.1.7}$$

(for such derivation we refer to [del Razo et al., 2022]). We are now ready to state our second main result.

Theorem 6.1.3. *The average concentration field* (6.1.7) *associated with the system* (6.1.3) *solves the reaction-diffusion partial differential equation*

$$\begin{cases} \partial_t c(t,x) = \frac{1}{2}\partial_x^2 c(t,x) + c(t,x), & t > 0, x \in \mathbb{R}; \\ c(0,x) = \delta_0(x), & x \in \mathbb{R}. \end{cases} \tag{6.1.8}$$

The paper is organized as follows: Chapter 6.1.1 contains the proof of Theorem 6.1.1 which is essentially based on the McKean representation for the solution to the Fisher-Kolmogorov-Petrovskii-Piskunov equation and its connection to a certain stochastic partial differential equation. Here, we also collect some notions and results from Malliavin Calculus needed for the proof of our main theorems: the implementation of these techniques represents one of the principal novelties of our contribution; then, in Chapter 6.1.2 we describe the proof of Theorem 6.1.3 which is inspired by some ideas from [Lanconelli, 2023].

6.1.1 Proof of Theorem 6.1.1

It is well known [McKean, 1975, Bovier, 2015] that, for a continuous function $f : \mathbb{R} \to [0,1]$ and branching Brownian motion $\{X_k(t) : k \leq \mathtt{n}(t)\}_{t\geq 0}$, the function

$$(t,x) \mapsto u(t,x) := \mathbb{E}\left[\prod_{k=1}^{\mathtt{n}(t)} f(x - X_k(t))\right] \tag{6.1.9}$$

is solution to the Fisher-Kolmogorov-Petrovskii-Piskunov equation as seen in [Fisher, 1937] and [Kolmogorov et al., 1937].

$$\begin{cases} \partial_t u(t,x) = \frac{1}{2}\partial_{xx}u(t,x) + u(t,x)^2 - u(t,x), & t>0, x\in\mathbb{R}; \\ u(0,x) = f(x), & x\in\mathbb{R}. \end{cases} \tag{6.1.10}$$

According to such representation and in view of (6.1.1) we can write by means of the Law of Total Probability that

$$\begin{aligned} u(t,x) =& \mathbb{E}\left[\prod_{k=1}^{\mathtt{n}(t)} f(x - X_k(t))\right] \\ =& \sum_{n\geq 1}\int_{\mathbb{R}^n} \mathbb{E}\left[\prod_{k=1}^{\mathtt{n}(t)} f(x - X_k(t)) \middle| \mathtt{n}(t) = n, X(t) = y\right]\rho_n(t,y)dy \\ =& \sum_{n\geq 1}\int_{\mathbb{R}^n} \prod_{k=1}^{n} f(x-y_k)\rho_n(t,y)dy \\ =& \sum_{n\geq 1}\int_{\mathbb{R}^n} \prod_{k=1}^{n} f(y_k)\rho_n(t,x\mathtt{1}_n - y)dy \\ =& \sum_{n\geq 1}\int_{\mathbb{R}^n} f^{\otimes n}(y)\rho_n(t,x\mathtt{1}_n - y)dy \\ =& \langle\langle \hat{U}(t,x), \mathcal{E}(f)\rangle\rangle, \end{aligned} \tag{6.1.11}$$

where for $n\geq 1$ we used the notation $\mathtt{1}_n := (1,1,...,1)\in\mathbb{R}^n$ and set

$$\hat{U}(t,x) := \sum_{n\geq 1} I_n(\rho_n(t,x\mathtt{1}_n - \cdot)), \quad t\geq 0, x\in\mathbb{R}. \tag{6.1.12}$$

In (6.1.12) the notation I_n stands for n-th order multiple Itô integral with respect to an auxiliary two sided Brownian motion, say $\{B_y\}_{y\in\mathbb{R}}$ as also defined in Chapter A.4. Moreover, in (6.1.11) the brackets $\langle\langle\cdot,\cdot\rangle\rangle$ denote dual pairing between the generalized random variable $\hat{U}(t,x)$ and the *stochastic exponential* $\mathcal{E}(f)$, which is the smooth random variable defined by in expression (A.8.1). For more details on smooth and generalized random variables we refer the reader to [Holden et al., 1996] and [Kuo, 1996].

We now want to relate the expression in (6.1.12) with the solution to a Wick-type stochastic partial differential equation investigated in [Levajković et al., 2018]. In the sequel, the symbol $\diamond$ will denote the so-called *Wick product* defined in Chapter A.9.

The transformation

$$X\mapsto \mathcal{S}(X)(f) := \langle\langle X, \mathcal{E}(f)\rangle\rangle = \sum_{n\geq 0}\int_{\mathbb{R}^n} h_n(x) f^{\otimes n}(x)dx, \quad f\in C_0^\infty(\mathbb{R}),$$

is injective and called $\mathcal{S}$-transform of X for $X\in\mathtt{F}^*$ as described in Appendix A.9.

Lemma 6.1.4. *Let* $\{U(t,x)\}_{t\geq 0, x\in\mathbb{R}}$ *be the unique solution to*

$$\begin{cases} \partial_t U(t,x) = \frac{1}{2}\partial_x^2 U(t,x) + U(t,x)^{\diamond 2} - U(t,x), & t>0, x\in\mathbb{R}; \\ U(0,x) = W_x, & x\in\mathbb{R}; \end{cases} \tag{6.1.13}$$

here, W_x *denotes the white noise at* x*, i.e.* $W_x = I_1(\delta_0(x-\cdot))$ *(see (A.5.11)). Then,*

$$U(t,x) = \sum_{n\geq 1} I_n(g_n(t,x;\cdot)), \quad t\geq 0, x\in\mathbb{R}$$

where $\{g_n\}_{n\geq 1}$ *is the sequence of functions*

$$\begin{aligned} g_n : [0,+\infty[\times\mathbb{R}\times\mathbb{R}^n &\to \mathbb{R} \\ (t,x,y_1,...,y_n) &\mapsto g_n(t,x;y_1,...,y_n) \end{aligned}$$

solving the system of partial differential equations

$$\begin{cases} \partial_t g_n(t,x;y) = \frac{1}{2}\partial_x^2 g_n(t,x;y) + \sum_{k=1}^{n-1} g_k \hat{\otimes} g_{n-k}(t,x;y) \\ \qquad\qquad -g_n(t,x;y), \quad n\geq 1, t>0, x\in\mathbb{R}, y\in\mathbb{R}^n; \\ g_1(0,x;y_1) = \delta_0(x-y_1), \quad x,y_1\in\mathbb{R}; \\ g_n(0,x;y) = 0, \quad n\geq 2, x\in\mathbb{R}, y\in\mathbb{R}^n. \end{cases} \tag{6.1.14}$$

Moreover, for $f\in C_0^\infty(\mathbb{R})$ *the function*

$$(t,x)\mapsto (\mathcal{S}U(t,x))(f) = \langle\langle U(t,x), \mathcal{E}(f)\rangle\rangle$$

solves equation (6.1.10).

Proof. For the notion of solution to the problem (6.1.13) we refer the reader to the paper of [Levajković et al., 2018]. Projecting equation (6.1.13) onto chaos spaces of different orders yields a system of partial differential equations solved by the sequence of kernels $\{g_n\}_{n\geq 1}$ of $U(t,x)$; more precisely, recalling the definition of Wick product and the fact that the initial condition in (6.1.13) is made of a first order Wiener chaos one easily see that (6.1.14) corresponds to the aforementioned system of partial differential equations. On the other hand, thanks to the interplay between Wick product and S-transform, i.e.

$$\langle\langle U(t,x)^{\diamond 2}, \mathcal{E}(f)\rangle\rangle = \langle\langle U(t,x), \mathcal{E}(f)\rangle\rangle^2, \quad t\geq 0, x\in\mathbb{R}, f\in C_0^\infty(\mathbb{R}),$$

and the identity

$$\langle\langle W_x, \mathcal{E}(f)\rangle\rangle = f(x), \quad x\in\mathbb{R}, f\in C_0^\infty(\mathbb{R}),$$

we see that an application of the S-transform to both sides of (6.1.13) reduces this problem to (6.1.10). □

Remark 6.1.5. *The triangular structure of system (6.1.14) allows for an explicit recursive representation of its solution; namely,*

$$\begin{cases} g_1(t,x;y_1) := e^{-t}\mathtt{p}_t(x-y_1), \quad t\geq 0, x, y_1 \in \mathbb{R}; \\ g_n(t,x;y_1,...,y_n) := e^{-t}\int_0^t\int_{\mathbb{R}} \mathtt{p}_{t-s}(x-z)e^s\sum_{k=1}^{n-1} g_k\hat{\otimes}g_{n-k}(s,z;y_1,...,y_n)dzds, \\ \qquad\qquad\qquad\qquad n\geq 2, t\geq 0 \ \textit{and}\ x, y_1,...,y_n\in\mathbb{R}. \end{cases}$$

Now, employing the conclusion of Lemma 6.1.4 in combination with (6.1.11) we can affirm that

$$\langle\langle \hat{U}(t,x), \mathcal{E}(f)\rangle\rangle = \langle\langle U(t,x), \mathcal{E}(f)\rangle\rangle \quad \text{for all } t\geq 0,\ x\in\mathbb{R} \text{ and } f\in C_0^\infty(\mathbb{R});$$

from the invertibility of the S-transform and uniqueness of chaos expansion's kernels we then deduce

$$\rho_n(t, x\mathtt{1}_n - y) = g_n(t,x;y), \qquad \text{for all } n\geq 1, t\geq 0, x\in\mathbb{R}, y\in\mathbb{R}^n$$

and thus

$$\begin{aligned} \rho_n(t,y_1,...,y_n) =& \rho_n(t, x-(x-y_1),...,x-(x-y_n)) \\ =& g_n(t,x;x-y_1,...,x-y_n), \quad n\geq 1, t\geq 0, x, y_1,...,y_n\in\mathbb{R}, \end{aligned}$$

which corresponds to (6.1.4). Lastly, recalling that the sequence $\{g_n\}_{n\geq 1}$ solves the system of equations (6.1.14) we have

$$\begin{aligned} \partial_t\rho_n(t,x\mathtt{1}_n - y) =& \partial_t g_n(t,x;y) \\ =& \frac{1}{2}\partial_x^2 g_n(t,x;y) + \sum_{k=1}^{n-1} g_k\hat{\otimes}g_{n-k}(t,x;y) - g_n(t,x;y) \\ =& \frac{1}{2}\partial_x^2(\rho_n(t,x\mathtt{1}_n - y)) + \sum_{k=1}^{n-1}\rho_k\hat{\otimes}\rho_{n-k}(t,x\mathtt{1}_n - y) - \rho_n(t,x\mathtt{1}_n - y) \\ =& \frac{1}{2}\sum_{j,k=1}^{n}\partial^2_{y_jy_k}\rho_n(t,x\mathtt{1}_n - y) + \sum_{k=1}^{n-1}\rho_k\hat{\otimes}\rho_{n-k}(t,x\mathtt{1}_n - y) - \rho_n(t,x\mathtt{1}_n - y); \end{aligned}$$

if we now replace $x\mathtt{1}_n - y$ with y we obtain the desired system (6.1.3), completing the proof of Theorem 6.1.1.

Remark 6.1.6. *One can see the interplay between the different Brownian particles generated by the branching mechanism in the diffusion term*

$$\frac{1}{2}\sum_{k,l=1}^{n}\partial^2_{y_ky_l}\rho_n(t,y_1,...,y_n).$$

This is due to the fact that the newly created particles do not emerge at an independent random location but enter to the system at the same exact location of the parent particle. Such feature is in contrast with the models considered in chapters 4 and 5, which are also investigated in [del Razo et al., 2022] and [del Razo et al., 2023] where diffusion is described by a simple Laplace operator.

6.1.2 Proof of Theorem 6.1.3

Inspired by the ideas presented in [Lanconelli, 2023] and further developed in the paper [Lanconelli et al., 2023] and [Lanconelli and Perçin, 2024a] we now rewrite the system of equations (6.1.3) as a single abstract equation containing Malliavin Calculus operators. For details on the subject the reader is referred to Appendix A.5, A.6, A.7 and A.8. For even more detailed information one can refer to the books [Hu, 2017], [Janson, 1997] and [Nualart, 2006]; here, we recall few basic definitions and properties needed for proving our result. In the sequel, we denote by $\{D_x\Phi\}_{x\in\mathbb{R}}$ the *Malliavin derivative* of $\Phi = \sum_{n\geq 0} I_n(h_n)$ defined as

$$D_x\Phi := \sum_{n\geq 1} nI_{n-1}(h_n(\cdot, x)), \quad x \in \mathbb{R};$$

notice that

$$D_x\mathcal{E}(f) = f(x)\mathcal{E}(f), \qquad \text{for all } f \in C_0^\infty(\mathbb{R}).$$

where $\mathcal{E}(f)$ being the stochastic exponential as defined in expression (A.8.1). Moreover, for a possibly unbounded $A : L^2(\mathbb{R}) \to L^2(\mathbb{R})$ we define its *differential second quantization operator* as

$$d\Gamma(A)\Phi := \sum_{n\geq 1} I_n\left(\sum_{i=1}^{n} A_i h_n\right),$$

where A_i stands for the operator A acting on the i-th variable of h_n as explained in Chapter A.8.1. The following useful identities hold true as also explained in sections A.5, A.8 and A.9:

$$\langle\langle d\Gamma(A)\Phi, 1\rangle\rangle = 0; \quad \langle\langle d\Gamma(A)\Phi, \Psi\rangle\rangle = \langle\langle \Phi, d\Gamma(A^\star)\Psi\rangle\rangle;$$
$$d\Gamma(A)\mathcal{E}(f) = \mathcal{E}(f) \diamond I_1(Af); \quad D_x(\Phi \diamond \Psi) = D_x\Phi \diamond \Psi + \Phi \diamond D_x\Psi.$$

Lemma 6.1.7. *Let $\{\rho_n\}_{n\geq 1}$ be solution to (6.1.3). Then, the generalized stochastic process*

$$\Phi(t) := \sum_{n\geq 0} I_n(\rho_n(t, \cdot)), \quad t \geq 0, \tag{6.1.15}$$

solves the abstract equation

$$\begin{cases} \partial_t\Phi(t) = \frac{1}{2}d\Gamma(\partial)^2\Phi(t) + \Phi(t)^{\diamond 2} - \Phi(t), & t > 0; \\ \Phi(0) = W_0. \end{cases} \tag{6.1.16}$$

Proof. We have

$$\partial_t\Phi(t) = \partial_t \sum_{n\geq 0} I_n(\rho_n(t, \cdot))$$

$$
\begin{aligned}
&= \sum_{n\geq 0} I_n(\partial_t \rho_n(t,\cdot)) \\
&= \sum_{n\geq 0} I_n\left(\frac{1}{2}\sum_{k,l=1}^{n} \partial^2_{y_k y_l}\rho_n(t,\cdot)\right) + \sum_{n\geq 0} I_n\left(\sum_{k=1}^{n-1} \rho_k \hat{\otimes} \rho_{n-k}(t,\cdot)\right) \\
&\quad - \sum_{n\geq 0} I_n(\rho_n(t,\cdot)) \\
&= \frac{1}{2}\sum_{n\geq 0} d\Gamma(\partial)^2 I_n\left(\rho_n(t,\cdot)\right) + \sum_{n\geq 0} I_n(\rho_n(t,\cdot)) \diamond \sum_{n\geq 0} I_n(\rho_n(t,\cdot)) \\
&\quad - \sum_{n\geq 0} I_n(\rho_n(t,\cdot)) \\
&= \frac{1}{2} d\Gamma(\partial)^2 \Phi(t) + \Phi(t)^{\diamond 2} - \Phi(t).
\end{aligned}
$$

Here, we utilized (6.1.3) and the definitions of differential second quantization operator and Wick product. Moreover,

$$\Phi(0) = \sum_{n\geq 0} I_n(\rho_n(0,\cdot)) = I_1(\delta_0) = W_0.$$

□

Remark 6.1.8. *Notice that using the notation introduced in the previous lemma condition (6.1.2) reads*

$$\langle\langle \Phi(t), \mathtt{E}(1)\rangle\rangle = 1, \qquad \text{for all } t \geq 0.$$

The usefulness of switching from system (6.1.3) to equation (6.1.16) becomes evident in the following result where a compact representation for the average concentration field is proposed.

Lemma 6.1.9. *The average concentration field (6.1.7) enjoys the representation*

$$c(t,x) = \langle\langle D_x\Phi(t), \mathtt{E}(1)\rangle\rangle, \quad t \geq 0, x \in \mathbb{R}. \tag{6.1.17}$$

Proof. From (6.1.15) we can write

$$D_x\Phi(t) = D_x \sum_{n\geq 0} I_n(\rho_n(t,\cdot)) = \sum_{n\geq 1} n I_{n-1}(\rho_n(t,\cdot,x));$$

therefore,

$$\langle\langle D_x\Phi(t), \mathtt{E}(1)\rangle\rangle = \sum_{n\geq 1} n \int_{\mathbb{R}^{n-1}} \rho_n(t, y_1, ..., y_{n-1}, x) dy_1 ... dy_{n-1},$$

and since the last member above agrees with (6.1.7) the validity of formula (6.1.17) is proven. □

We are now ready to prove Theorem 6.1.3. By means of the two previous lemmas we get

$$\begin{aligned}\partial_t c(t,x) =&\partial_t\langle\langle D_x\Phi(t),\mathtt{E}(1)\rangle\rangle\\ =&\langle\langle \partial_t D_x\Phi(t),\mathtt{E}(1)\rangle\rangle\\ =&\langle\langle D_x\partial_t\Phi(t),\mathtt{E}(1)\rangle\rangle\\ =&\langle\langle D_x\left(\frac{1}{2}d\Gamma(\partial)^2\Phi(t)+\Phi(t)^{\diamond 2}-\Phi(t)\right),\mathtt{E}(1)\rangle\rangle\\ =&\frac{1}{2}\langle\langle D_x d\Gamma(\partial)^2\Phi(t),\mathtt{E}(1)\rangle\rangle+\langle\langle D_x\Phi(t)^{\diamond 2},\mathtt{E}(1)\rangle\rangle-\langle\langle D_x\Phi(t),\mathtt{E}(1)\rangle\rangle. \qquad (6.1.18)\end{aligned}$$

Moreover,

- the following commutation relation holds:

  $$D_x d\Gamma(\partial)=\left(d\Gamma(\partial)+\frac{d}{dx}\right)D_x. \qquad (6.1.19)$$

  In fact, checking its validity on stochastic exponentials we get

  $$d\Gamma(\partial)D_x\mathtt{E}(h)=d\Gamma(\partial)\mathtt{E}(h)h(x)=h(x)\mathtt{E}(h)\diamond I_1(h')$$

  and

  $$D_x d\Gamma(\partial)\mathtt{E}(h)=D_x\mathtt{E}(h)\diamond I_1(h')=\mathtt{E}(h)h(x)\diamond I_1(h')+\mathtt{E}(h)h';$$

  thus,

  $$\begin{aligned}D_x d\Gamma(\partial)\mathtt{E}(h)&=d\Gamma(\partial)D_x\mathtt{E}(h)+\mathtt{E}(h)h'\\ &=d\Gamma(\partial)D_x\mathtt{E}(h)+\frac{d}{dx}D_x\mathtt{E}(h);\end{aligned}$$

- iterating (6.1.19) twice one gets

  $$D_x d\Gamma(\partial)^2=\left(d\Gamma(\partial)^2+2d\Gamma(\partial)\frac{d}{dx}+\frac{d^2}{dx^2}\right)D_x; \qquad (6.1.20)$$

- for all $\Phi=\sum_{n\geq 0}I_n(h_n)$ we have

  $$\langle\langle d\Gamma(\partial)\Phi,\mathtt{E}(1)\rangle\rangle=0. \qquad (6.1.21)$$

  In fact, using the properties of differential second quantization operators we can write

  $$\langle\langle d\Gamma(\partial)\Phi,\mathtt{E}(1)\rangle\rangle=\langle\langle\Phi,d\Gamma(-\partial)\mathtt{E}(1)\rangle\rangle=\langle\langle\Phi,\mathtt{E}(1)\diamond I_1(0)\rangle\rangle=0.$$

By virtue of (6.1.20) and (6.1.21) the first term in (6.1.18) can be simplified to

$$\begin{aligned}\frac{1}{2}\langle\langle D_x d\Gamma(\partial)^2\Phi(t), \mathtt{E}(1)\rangle\rangle &= \frac{1}{2}\langle\langle \frac{d^2}{dx^2} D_x\Phi(t), \mathtt{E}(1)\rangle\rangle \\ &= \frac{1}{2}\frac{d^2}{dx^2}\langle\langle D_x\Phi(t), \mathtt{E}(1)\rangle\rangle \\ &= \frac{1}{2}\frac{d^2}{dx^2}c(t,x).\end{aligned}$$

The second term in (6.1.18), exploiting the chain rule for the Malliavin derivative and Wick product, becomes

$$\begin{aligned}\langle\langle D_x\Phi(t)^{\diamond 2}, \mathtt{E}(1)\rangle\rangle &= 2\langle\langle \Phi(t)\diamond D_x\Phi(t), \mathtt{E}(1)\rangle\rangle \\ &= 2\langle\langle \Phi(t), \mathtt{E}(1)\rangle\rangle\langle\langle D_x\Phi(t), \mathtt{E}(1)\rangle\rangle \\ &= 2\langle\langle D_x\Phi(t), \mathtt{E}(1)\rangle\rangle \\ &= 2c(t,x),\end{aligned}$$

where we also utilized the observation in Remark 6.1.8. Combining those identities in (6.1.18) we conclude that

$$\partial_t c(t,x) = \frac{1}{2}\partial_x^2 c(t,x) + c(t,x).$$

Moreover,

$$c(0,x) = \langle\langle D_x\Phi(0), \mathtt{E}(1)\rangle\rangle = \langle\langle D_x W_0, \mathtt{E}(1)\rangle\rangle = \delta_0(x).$$

The proof of Theorem 6.1.3 is now complete.

Appendix A

Stochastic Processes and Malliavin Calculus

Before introducing the main tools of our research, first it is necessary to start with introducing preliminaries of stochastic calculus:

A.1 Stochastic Processes and Brownian Motion

In this section, the main concepts of the stochastic calculus will be introduced from the beginning, because the sections 4, 5 and 6 use these concepts thoroughly.

A.1.1 Stochastic Processes

A *continuous-time stochastic process* $\{X_t\}_{t\geq 0}$ is a collection of random variables defined within a common probability space $(\Omega, \mathcal{F}, \mathbb{P})$. These random variables are indexed by the non-negative real number t, which represents *time*. Our understanding is, X_t is the value of a system at time t, where the system's evolution is random. Note that:

- for each fixed $t \geq 0$, the mapping $\omega \mapsto X_t(\omega)$ is a random variable, and
- for each fixed $\omega \in \Omega$, the mapping $t \mapsto X_t(\omega)$ represents a possible path or trajectory of the stochastic process $\{X_t\}_{t\geq 0}$.

A.1.2 Brownian Motion

The most famous stochastic process in the literature is the *Brownian motion.*

Definition A.1.1. *As defined in [Karatzas and Shreve, 1991], a continuous-time stochastic process* $\{B_t\}_{t\geq 0}$*, defined on a probability space* $(\Omega, \mathcal{F}, \mathbb{P})$*, is termed (standard)* Brownian motion *or a* Wiener process *if it meets the following criteria:*

1. *The process starts at zero almost surely:* $\mathbb{P}(B_0 = 0) = 1$.
2. *For any* $0 \leq s < t$*, the increments* $B_t - B_s$ *are normally distributed with mean zero and variance* $t - s$*:* $B_t - B_s \sim \mathtt{N}(0, t-s)$*. This implies the process has* stationary increments*, as the distribution of* $B_t - B_s$ *depends only on the time difference* $t - s$*.*
3. *For any* $0 \leq t_1 < t_2 < \cdots < t_n$*, the increments*

$$B_{t_1}, B_{t_2} - B_{t_1}, \ldots, B_{t_n} - B_{t_{n-1}}$$

are mutually independent, indicating that the process has independent increments*.*

4. *The process has continuous paths almost surely:* $\mathbb{P}(t \mapsto B_t \text{ is continuous}) = 1$.

Remark A.1.2. *From the definition of Brownian motion, we can derive the following properties:*

- *For any* $t > 0$*, the random variable* $B_t = B_t - B_0$ *is normally distributed with mean 0 and variance* t *(i.e.,* $B_t \sim \mathtt{N}(0, t)$*). Additionally, for any* $s, t > 0$*, the covariance between* B_s *and* B_t *is* $\mathtt{cov}(B_s, B_t) = \min(s, t)$*.*
- Translation invariance*: If* $t_0 > 0$ *is fixed, then the process defined by* $\tilde{B}_t := B_{t+t_0} - B_{t_0}$ *for* $t \geq 0$ *is also a Brownian motion.*
- Scaling invariance*: For any* $\lambda > 0$*, the process defined by* $\hat{B}_t := \frac{B_{\lambda t}}{\sqrt{\lambda}}$ *for* $t \geq 0$ *is still a Brownian motion.*

A.1.3 Measurability, Martingale Property and Filtrations

A fundamental concept in probability theory is the *measurability* of random variables. This concept ensures that a random variable is compatible with the underlying probability space and allows us to assign probabilities to events in a meaningful way.

Definition A.1.3. *Let* $(\Omega, \mathcal{F}, \mathbb{P})$ *be a probability space, where* Ω *is the sample space,* $\mathcal{F}$ *is a sigma-algebra on* Ω*, and* $\mathbb{P}$ *is a probability measure. A function* $X : \Omega \to \mathbb{R}$ *is called a* random variable *(or* $\mathcal{F}$-measurable*) if it satisfies the following condition:*

$$X^{-1}(B) \in \mathcal{F} \quad \text{for every } B \in \mathcal{B}(\mathbb{R})$$

where $\mathcal{B}(\mathbb{R})$ stands for the Borel σ-algebra of the real line, which is countable intersection, union and complement of all open intervals. This definition implies that for any Borel set $B \in \mathcal{B}(\mathbb{R})$, the preimage of B under X, denoted by $X^{-1}(B)$, is an event in $\mathcal{F}$. In other words, we can measure the probability of X taking values in B using the measure $\mathbb{P}$ that is already assigned for events in $\mathcal{F}$.

A *filtration* $\{\mathcal{F}_t\}_{t\geq 0}$ on the probability space $(\Omega, \mathcal{F}, \mathbb{P})$ is a sequence of σ-algebras that are increasing and contained within $\mathcal{F}$. In other words, we have:

$$\mathcal{F}_s \subseteq \mathcal{F}_t \subseteq \mathcal{F} \quad \text{for all } 0 \leq s < t.$$

A continuous-time stochastic process $\{X_t\}_{t\geq 0}$ is said to be *adapted* to the filtration $\{\mathcal{F}_t\}_{t\geq 0}$ if each X_t is measurable with respect to $\mathcal{F}_t$ for every $t \geq 0$ in the sense of definition A.1.3.

Definition A.1.4. *The natural filtration $\{\mathcal{F}_t^B\}_{t\geq 0}$ associated with a Brownian motion $\{B_t\}_{t\geq 0}$ is defined as:*

$$\mathcal{F}_t^B := \sigma\left(B_s \mid 0 \leq s \leq t\right), \quad t \geq 0.$$

This means that $\mathcal{F}_t^B$ is the smallest σ-algebra generated by the events of the form $\{B_s \in A\}$, where A is an interval in $\mathbb{R}$ and $s \in [0,t]$. By construction, this definition leads that the Brownian motion $\{B_t\}_{t\geq 0}$ is measurable with respect to its natural filtration $\mathcal{F}_t^B$ and therefore it is adapted.

In the field Stochastic Differential Equations (SDEs), it is common to work with larger σ-algebras than $\mathcal{F}_t^B$. If they also preserve the features listed below of the natural filtration of the Brownian motion, then we call it *admissible filtration.*

Definition A.1.5. *Consider a Brownian motion $\{B_t\}_{t\geq 0}$. A filtration $\{\mathcal{F}_t\}_{t\geq 0}$ is deemed* admissible *for this Brownian motion if it satisfies the following conditions:*

1. *For every $t \geq 0$, the sigma-algebra $\mathcal{F}_t^B \subseteq \mathcal{F}_t$.*
2. *The increment $B_t - B_s$ is independent of the sigma-algebra $\mathcal{F}_s$ for all $0 \leq s \leq t$.*

Because the term *measurability* is already introduced, it is wise to spend some words on the conditional expectation:

Definition A.1.6. *Consider a random variable X in $\mathbb{L}^2(\Omega, \mathcal{F}, \mathbb{P})$ and $\mathcal{G}$ being a sub-sigma-algebra of $\mathcal{F}$, the* conditional expectation of X given $\mathcal{G}$, *denoted $\mathbb{E}[X \mid \mathcal{G}]$, is defined as the unique element in $\mathbb{L}^2(\Omega, \mathcal{G}, \mathbb{P})$ such that*

$$\mathbb{E}[|X - \mathbb{E}[X \mid \mathcal{G}]|^2] \leq \mathbb{E}[|X - Y|^2], \quad \textit{for all } Y \in \mathbb{L}^2(\Omega, \mathcal{G}, \mathbb{P}).$$

In words, with all the information available in $\mathcal{G}$, the element in space $\mathbb{L}^2(\Omega, \mathcal{G}, \mathbb{P})$ that approximates X the best is $\mathbb{E}[X \mid \mathcal{G}]$. We say it *approximates* because: $\mathbb{L}^2(\Omega, \mathcal{G}, \mathbb{P}) \subseteq \mathbb{L}^2(\Omega, \mathcal{F}, \mathbb{P})$. This leads to being $\mathcal{G}$-measurable imposes stricter conditions than being $\mathcal{F}$-measurable. So $\mathbb{E}[X \mid \mathcal{G}]$ will act most similar to X in $\mathcal{G}$ in the sense that it will minimize the quadratic distance from X. In the following, we will denote the space $\mathbb{L}^2(\Omega, \mathcal{F}, \mathbb{P})$ simply as $\mathbb{L}^2(\Omega)$.

Remark A.1.7. *Here some important properties of conditional expectation are listed:*

1. *If $\mathcal{G}$ is the trivial sigma-algebra $\{\varnothing, \Omega\}$, then $\mathbb{E}[X \mid \mathcal{G}] = \mathbb{E}[X]$.*
2. *For constants $\alpha, \beta, \gamma \in \mathbb{R}$, we have $\mathbb{E}[\alpha X + \beta Y + \gamma \mid \mathcal{G}] = \alpha \mathbb{E}[X \mid \mathcal{G}] + \beta \mathbb{E}[Y \mid \mathcal{G}] + \gamma$.*
3. *If X is already $\mathcal{G}$-measurable, then $\mathbb{E}[X \mid \mathcal{G}] = X$.*
4. *If X is independent of $\mathcal{G}$, then $\mathbb{E}[X \mid \mathcal{G}] = \mathbb{E}[X]$.*

5. *If $\mathcal{H}$ is a sub-sigma-algebra of $\mathcal{G}$, then $\mathbb{E}[\mathbb{E}[X \mid \mathcal{G}] \mid \mathcal{H}] = \mathbb{E}[X \mid \mathcal{H}]$.*
6. *If X is $\mathcal{G}$-measurable, then $\mathbb{E}[XY \mid \mathcal{G}] = X\mathbb{E}[Y \mid \mathcal{G}]$.*

A.2 The Itô Integral

Before introducing the formal definition of the Itô integral and Itô Calculus, one should spend some words on why a new formal definition is necessary.

A.2.1 The Stieltjes Integral and $\int_a^b X_t dB_t$

The aim of this section is to introduce the idea to formalize the integrals in the form $\int_a^b X_t dB_t$ where $\{X_t\}_{t\in[a,b]}$ is a continuous time stochastic process and $\{B_t\}_{t\in[a,b]}$ is the Brownian motion.

First, it will be shown that why the *Stieltjes integral* definition **can't** be used. Consider the following case:

$$\sum_{j=0}^{N-1} f(t_j^\star)(F(t_{j+1}) - F(t_j)), \tag{A.2.1}$$

where $F : [a, b] \to \mathbb{R}$ is a specified function. The formula (A.2.1) serves as the foundation for defining the *Stieltjes integral* $\int_a^b f(t)dF(t)$, which is properly defined when the function $F : [a, b] \to \mathbb{R}$ has *bounded variation*, meaning

$$\lim_{n\to+\infty} \sum_{j=0}^{N_n-1} |F(t_{j+1}^{(n)}) - F(t_j^{(n)})| < +\infty.$$

where the limit is taken along a partition of the interval $[a, b]$ $\{\pi_n\}_{n\geq 1}$, with the property that:

$$\lim_{n\to+\infty} |\pi_n| = 0;$$

the positive number

$$|\pi_n| := \max_{j\in\{0,\dots,N_n-1\}} (t_{j+1}^{(n)} - t_j^{(n)})$$

is called the *mesh* of the partition π_n, and it measures how finely the partition π_n divides the interval $[a, b]$ because we didn't constrain ourselves to divide the interval equally. In corollary A.2.2, it will be obvious why we can't utilize the Stieltjes integral theory but in order to demonstrate this fact, we go on with the procedure.

To fit $\int_a^b X_t dB_t$ within the sense of Stieltjes integral, one would fix the random element $\omega \in \Omega$ and interpret the path $t \mapsto X_t(\omega)$ as the function $t \mapsto f(t)$ and the path $t \mapsto B_t(\omega)$ as the function $t \mapsto F(t)$.

Theorem A.2.1. *Let* $\{B_t\}_{t\geq 0}$ *be a Brownian motion and* $\{\pi_n\}_{n\geq 1}$ *be any sequence of finite partitions of the interval* $[a,b]$ *satisfying*

$$\lim_{n\to+\infty} |\pi_n| = 0.$$

Then,

$$\lim_{n\to+\infty} \sum_{j=1}^{N_n} \left(B_{t_j^{(n)}} - B_{t_{j-1}^{(n)}}\right)^2 = b - a \quad \text{in } \mathbb{L}^2(\Omega). \tag{A.2.2}$$

Which in words state that the quadratic variation of Brownian motion $\{B_t\}_{t\geq 0}$ *defined in interval* $[a,b]$ *is:* $b-a$*. If, in addition,*

$$\sum_{n\geq 1} |\pi_n| < +\infty, \tag{A.2.3}$$

then the convergence in (A.2.2) holds almost surely.

Proof. For simplicity, let us denote

$$S_2^{\pi_n}(B,[a,b]) := \sum_{j=1}^{N_n} \left(B_{t_j^{(n)}} - B_{t_{j-1}^{(n)}}\right)^2,$$

and recall that to prove convergence in $\mathbb{L}^2(\Omega)$, we must verify that

$$\lim_{n\to+\infty} \mathbb{E}\left[\left(S_2^{\pi_n}(B,[a,b]) - (b-a)\right)^2\right] = 0.$$

Observe that

$$\begin{aligned}
\mathbb{E}\left[S_2^{\pi_n}(B,[a,b])\right] =& \mathbb{E}\left[\sum_{j=1}^{N_n} \left(B_{t_j^{(n)}} - B_{t_{j-1}^{(n)}}\right)^2\right] \\
=& \sum_{j=1}^{N_n} \mathbb{E}\left[\left(B_{t_j^{(n)}} - B_{t_{j-1}^{(n)}}\right)^2\right] \\
=& \sum_{j=1}^{N_n} (t_j^{(n)} - t_{j-1}^{(n)}) \\
=& b - a.
\end{aligned}$$

Therefore,

$$\begin{aligned}
&\mathbb{E}\left[\left(S_2^{\pi_n}(B,[a,b]) - (b-a)\right)^2\right] \\
&= \mathbb{E}\left[\left(S_2^{\pi_n}(B,[a,b]) - \mathbb{E}\left[S_2^{\pi_n}(B,[a,b])\right]\right)^2\right] \\
&= \mathbb{V}\left[S_2^{\pi_n}(B,[a,b])\right]
\end{aligned}$$

$$
\begin{aligned}
&= \mathbb{V}\left[\sum_{j=1}^{N_n}\left(B_{t_j^{(n)}} - B_{t_{j-1}^{(n)}}\right)^2\right] \\
&= \sum_{j=1}^{N_n}\mathbb{V}\left[\left(B_{t_j^{(n)}} - B_{t_{j-1}^{(n)}}\right)^2\right] \\
&= \sum_{j=1}^{N_n}\mathbb{E}\left[\left(B_{t_j^{(n)}} - B_{t_{j-1}^{(n)}}\right)^4\right] - \mathbb{E}\left[\left(B_{t_j^{(n)}} - B_{t_{j-1}^{(n)}}\right)^2\right]^2 \\
&= \sum_{j=1}^{N_n} 3\left(t_j^{(n)} - t_{j-1}^{(n)}\right)^2 - \left(t_j^{(n)} - t_{j-1}^{(n)}\right)^2 \\
&= 2\sum_{j=1}^{N_n}\left(t_j^{(n)} - t_{j-1}^{(n)}\right)^2 \\
&\leq 2|\pi_n|(b-a).
\end{aligned}
$$

Hence,

$$\lim_{n\to+\infty}\mathbb{E}\left[\left(S_2^{\pi_n}(B,[a,b]) - (b-a)\right)^2\right] \leq \lim_{n\to+\infty} 2|\pi_n|(b-a) = 0.$$

This proves the convergence in $\mathbb{L}^2(\Omega)$. Moreover, if we assume (A.2.3), then by the Chebyshev-Markov inequality we can write, for any $\varepsilon > 0$, that

$$
\begin{aligned}
\mathbb{P}\left(\left|S_2^{\pi_n}(B,[a,b]) - (b-a)\right| > \varepsilon\right) \leq& \frac{\mathbb{E}\left[\left(S_2^{\pi_n}(B,[a,b]) - (b-a)\right)^2\right]}{\varepsilon^2} \\
\leq& \frac{2|\pi_n|(b-a)}{\varepsilon^2}.
\end{aligned}
$$

Therefore,

$$\sum_{n\geq 1}\mathbb{P}\left(\left|S_2^{\pi_n}(B,[a,b]) - (b-a)\right| > \varepsilon\right) \leq \frac{2(b-a)}{\varepsilon^2}\sum_{n\geq 1}|\pi_n|,$$

and the right hand side is finite by assumption. Hence, the Borel-Cantelli lemma implies that

$$\mathbb{P}\left(\limsup_n\left\{\left|S_2^{\pi_n}(B,[a,b]) - (b-a)\right| > \varepsilon\right\}\right) = 0.$$

The last equality holds for any $\varepsilon > 0$, implying that $S_2^{\pi_n}(B,[a,b])$ converges to $b-a$ almost surely, as n tends to infinity. □

Corollary A.2.2. *For any $a < b$ we have,*

$$\mathbb{P}\left(t \mapsto B_t \text{ is of bounded variation on } [a,b]\right) = 0.$$

Proof. Let $\{\pi_n\}_{n\geq 1}$ be any sequence of finite partitions of the interval $[a,b]$ satisfying

$$\sum_{n\geq 1} |\pi_n| < +\infty,$$

and consider the inequality

$$\sum_{j=1}^{N_n} \left(B_{t_j^{(n)}} - B_{t_{j-1}^{(n)}}\right)^2 \leq \max_{1\leq j\leq N_n} \left|B_{t_j^{(n)}} - B_{t_{j-1}^{(n)}}\right| \cdot \sum_{j=1}^{N_n} \left|B_{t_j^{(n)}} - B_{t_{j-1}^{(n)}}\right|. \tag{A.2.4}$$

According to the previous theorem, we know that the left hand side of (A.2.4) converges to $b-a$, almost surely. On the other hand, the term

$$\max_{1\leq j\leq N_n} \left|B_{t_j^{(n)}} - B_{t_{j-1}^{(n)}}\right|$$

goes to zero almost surely, as n tends to infinity, since the Brownian paths are continuous and hence uniformly continuous on any compact interval $[a,b]$. Since $b-a$ is positive, passing to the limit as n goes to infinity in (A.2.4), we necessarily get

$$\lim_{n\to+\infty} \sum_{j=1}^{N_n} \left|B_{t_j^{(n)}} - B_{t_{j-1}^{(n)}}\right| = +\infty, \quad \text{almost surely.}$$

This is equivalent to saying that Brownian paths are of unbounded variation with probability one and due to this reason the Stieltjes integral theory can't be applied to it. ☐

Intiuitively this shows how wild the Brownian motion is oscillating. From the previous corollary we deduce that, with probability one, the integral

$$\int_a^b X_t dB_t$$

cannot be formalized as a Stieltjes integral (due to the unbounded variation of the Brownian paths). Moreover due to Brownian motion's wild behaviour, it should also be mentioned that:

Remark A.2.3. *Let $\{B_t\}_{t\geq 0}$ be a Brownian motion. Then,*

$$\mathbb{P}(t \mapsto B_t \text{ is nowhere differentiable}) = 1.$$

Therefore in order to define this integral type we will use another formalization is necessary.

A.2.2 The Itô Integral

In this section, one possible new way to define rigorously integrals of the type $\int_0^T X_t dB_t$ will be introduced. Consider $\{B_t\}_{t\geq 0}$ as a Brownian motion defined on the probability space $(\Omega, \mathcal{F}, \mathbb{P})$ with admissible filtration $\{\mathcal{F}_t\}_{t\geq 0}$.

Definition A.2.4. *We define $\mathcal{S}(\Omega \times [0,T])$ as the set of* simple processes *and the class of stochastic processes $\{X_t\}_{t\in[0,T]}$ of the form*

$$X_t := \sum_{j=0}^{N-1} \eta_j \mathbf{1}_{[t_j,t_{j+1})}(t) = \begin{cases} \eta_0, & \text{if } t \in [0,t_1); \\ \eta_1, & \text{if } t \in [t_1,t_2); \\ & \vdots \\ \eta_{N-1}, & \text{if } t \in [t_{N-1},T], \end{cases} \tag{A.2.5}$$

where $0 = t_0 < t_1 < \cdots < t_{n-1} < t_N = T$ and, for all $j \in \{0,\ldots,N-1\}$, the random variable η_j belongs to $\mathbb{L}^2(\Omega)$ and is $\mathcal{F}_{t_j}$-measurable.

The stochastic process X_t is called simple because it takes values of N many discrete random variables $\{\eta_0,\ldots,\eta_{N-1}\}$ where N is the number of partitioned subintervals of interval $[0,T]$. Observe that the elements of $\mathcal{S}(\Omega\times[0,T])$ are stochastic processes which are $\{\mathcal{F}_t\}_{t\geq0}$ adapted. This is due to the fact that, according to (A.2.5), if $t \in [t_j,t_{j+1})$, then $X_t = \eta_j$; therefore, X_t is $\mathcal{F}_{t_j}$-measurable and to greater reason $\mathcal{F}_t$-measurable, since $t_j \leq t$ and $\mathcal{F}_{t_j} \subseteq \mathcal{F}_t$. Moreover, because if $\{X_t\}_{t\in[0,T]}$ and $\{Y_t\}_{t\in[0,T]}$ belong to $\mathcal{S}(\Omega\times[0,T])$, then $\{\alpha X_t + \beta Y_t\}_{t\in[0,T]}$ is also a member of $\mathcal{S}(\Omega\times[0,T])$, for all $\alpha,\beta\in\mathbb{R}$, therefore it can be said that $\mathcal{S}(\Omega\times[0,T])$ is a vector space.

We now define the Itô integral of a simple stochastic process . Let $\{X_t\}_{t\in[0,T]}$ be an element of $\mathcal{S}(\Omega\times[0,T])$ of the form (A.2.5). For such stochastic process we define:

$$\int_0^T X_t dB_t := \sum_{j=0}^{N-1} \eta_j \left(B_{t_{j+1}} - B_{t_j}\right) \tag{A.2.6}$$

and call the random variable $\int_0^T X_t dB_t$ the *Itô integral* of $\{X_t\}_{t\in[0,T]}$.

Proposition A.2.5. *The random variable $\int_0^T X_t dB_t$ belongs to $\mathbb{L}^2(\Omega)$ with the moments:*

$$\mathbb{E}\left[\int_0^T X_t dB_t\right] = 0$$

and

$$\mathbb{E}\left[\left(\int_0^T X_t dB_t\right)^2\right] = \mathbb{E}\left[\int_0^T X_t^2 dt\right]. \tag{A.2.7}$$

Moreover, if $\{X_t\}_{t\in[0,T]}$ and $\{Y_t\}_{t\in[0,T]}$ belong to $\mathcal{S}(\Omega\times[0,T])$, then

$$\int_0^T (\alpha X_t + \beta Y_t) dB_t = \alpha \int_0^T X_t dB_t + \beta \int_0^T Y_t dB_t,$$

for all $\alpha, \beta \in \mathbb{R}$.

Proof. First the membership of $\int_0^T X_t dB_t$ to $\mathbb{L}^2(\Omega)$ should be proven by checking that its second moment is finite. By definition of Itô integral we can write

$$\begin{aligned}
\mathbb{E}\left[\left(\int_0^T X_t dB_t\right)^2\right] =&\mathbb{E}\left[\left(\sum_{j=0}^{N-1} \eta_j \left(B_{t_{j+1}} - B_{t_j}\right)\right)^2\right] \\
=&\mathbb{E}\left[\left(\sum_{j=0}^{N-1} \eta_j \left(B_{t_{j+1}} - B_{t_j}\right)\right) \cdot \left(\sum_{k=0}^{N-1} \eta_k \left(B_{t_{k+1}} - B_{t_k}\right)\right)\right] \\
=&\mathbb{E}\left[\sum_{j,k=0}^{N-1} \eta_j \eta_k \left(B_{t_{j+1}} - B_{t_j}\right)\left(B_{t_{k+1}} - B_{t_k}\right)\right] \\
=&\mathbb{E}\left[\sum_{j=0}^{N-1} \eta_j^2 \left(B_{t_{j+1}} - B_{t_j}\right)^2\right] \\
&+ 2\mathbb{E}\left[\sum_{j<k} \eta_j \eta_k \left(B_{t_{j+1}} - B_{t_j}\right)\left(B_{t_{k+1}} - B_{t_k}\right)\right] \\
=&\sum_{j=0}^{N-1} \mathbb{E}\left[\eta_j^2 \left(B_{t_{j+1}} - B_{t_j}\right)^2\right] \\
&+ 2\sum_{j<k} \mathbb{E}\left[\eta_j \eta_k \left(B_{t_{j+1}} - B_{t_j}\right)\left(B_{t_{k+1}} - B_{t_k}\right)\right] \\
=&\sum_{j=0}^{N-1} \mathbb{E}\left[\mathbb{E}\left[\eta_j^2 \left(B_{t_{j+1}} - B_{t_j}\right)^2 \middle| \mathcal{F}_{t_j}\right]\right] \\
&+ 2\sum_{j<k} \mathbb{E}\left[\mathbb{E}\left[\eta_j \eta_k \left(B_{t_{j+1}} - B_{t_j}\right)\left(B_{t_{k+1}} - B_{t_k}\right) \middle| \mathcal{F}_{t_k}\right]\right] \\
=&\sum_{j=0}^{N-1} \mathbb{E}\left[\eta_j^2 \mathbb{E}\left[\left(B_{t_{j+1}} - B_{t_j}\right)^2 \middle| \mathcal{F}_{t_j}\right]\right] \\
&+ 2\mathbb{E}\left[\sum_{j<k} \eta_j \eta_k \left(B_{t_{j+1}} - B_{t_j}\right) \mathbb{E}\left[B_{t_{k+1}} - B_{t_k} \middle| \mathcal{F}_{t_k}\right]\right] \\
=&\sum_{j=0}^{N-1} \mathbb{E}\left[\eta_j^2 \mathbb{E}\left[\left(B_{t_{j+1}} - B_{t_j}\right)^2\right]\right] \\
&+ 2\mathbb{E}\left[\sum_{j<k} \eta_j \eta_k \left(B_{t_{j+1}} - B_{t_j}\right) \mathbb{E}\left[B_{t_{k+1}} - B_{t_k}\right]\right]
\end{aligned}$$

$$= \sum_{j=0}^{N-1} \mathbb{E}\left[\eta_j^2\right](t_{j+1}-t_j).$$

Here, we utilized the properties 5 ,3 and 4 of conditional expectations in remark A.1.7 together with the fact that the random variable $B_{t_{j+1}} - B_{t_j}$ is independent of the σ-algebra $\mathcal{F}_{t_j}$, for all $j \in \{0, ..., N-1\}$. Comparing the first and last members of the previous chain of equalities we get

$$\mathbb{E}\left[\left(\int_0^T X_t dB_t\right)^2\right] = \sum_{j=0}^{N-1} \mathbb{E}\left[\eta_j^2\right](t_{j+1}-t_j), \tag{A.2.8}$$

which proves the membership of $\int_0^T X_t dB_t$ to $\mathbb{L}^2(\Omega)$, since from the start all η_j's are assumed to be in $\mathbb{L}^2(\Omega)$ as well, then the last sum is finite. Moreover,

$$\begin{aligned}
\mathbb{E}\left[\int_0^T X_t^2 dt\right] =& \mathbb{E}\left[\int_0^T \left(\sum_{j=0}^{N-1} \eta_j \mathbf{1}_{[t_j,t_{j+1}[}(t)\right)^2 dt\right] \\
=& \mathbb{E}\left[\int_0^T \sum_{j,k=0}^{N-1} \eta_j\eta_k \mathbf{1}_{[t_j,t_{j+1}[}(t)\mathbf{1}_{[t_k,t_{k+1}[}(t)dt\right] \\
=& \sum_{j,k=0}^{N-1} \mathbb{E}[\eta_j\eta_k] \int_0^T \mathbf{1}_{[t_j,t_{j+1}[}(t)\mathbf{1}_{[t_k,t_{k+1}[}(t)dt \\
=& \sum_{j=0}^{N-1} \mathbb{E}[\eta_j^2](t_{j+1}-t_j).
\end{aligned} \tag{A.2.9}$$

This yields, together with (A.2.8), identity (A.2.7). The expectation is computed as follows:

$$\begin{aligned}
\mathbb{E}\left[\int_0^T X_t dB_t\right] =& \mathbb{E}\left[\sum_{j=0}^{N-1} \eta_j \left(B_{t_{j+1}} - B_{t_j}\right)\right] \\
=& \sum_{j=0}^{N-1} \mathbb{E}\left[\eta_j \left(B_{t_{j+1}} - B_{t_j}\right)\right] \\
=& \sum_{j=0}^{N-1} \mathbb{E}[\eta_j]\mathbb{E}\left[B_{t_{j+1}} - B_{t_j}\right] \\
=& 0,
\end{aligned}$$

since η_j and $B_{t_{j+1}} - B_{t_j}$ are independent and Brownian increments has 0 expactation. Lastly, the linearity of the Itô integral is an immediate consequence of the definition. □

We now want to extend the definition of Itô integral to a wider class of integrands than $\mathcal{S}(\Omega \times [0,T])$. Inspired by identity (A.2.7) we introduce the following family of stochastic processes.

Definition A.2.6. *We define*

$$\mathbb{L}^2_{ad}(\Omega \times [0,T]) := \Big\{ \{X_t\}_{t\in[0,T]} \text{ is an } \{\mathcal{F}_t\}_{t\in[0,T]}\text{-adapted stochastic process such that } \mathbb{E}\left[\int_0^T X_t^2 dt\right] < +\infty \Big\}$$

Example A.2.7. *One key example is the stochastic process* $\{B_t\}_{t\in[0,T]}$*. That belongs to* $\mathbb{L}^2_{ad}(\Omega \times [0,T])$*, since, it is* $\{\mathcal{F}_t\}_{t\in[0,T]}$*-adapted and*

$$\mathbb{E}\left[\int_0^T B_t^2 dt\right] = \int_0^T \mathbb{E}\left[B_t^2\right] dt = \int_0^T t dt = T^2/2.$$

It should also be noted that the space $\mathbb{L}^2_{ad}(\Omega \times [0,T])$ is a vector space because of (A.2.9) and it contains $\mathcal{S}(\Omega \times [0,T])$.

Theorem A.2.8. *Any element of* $\mathbb{L}^2_{ad}(\Omega \times [0,T])$ *can be approximated by a sequence of elements of* $\mathcal{S}(\Omega \times [0,T])$*. This means,* $\forall \ \{X_t\}_{t\in[0,T]} \in \mathbb{L}^2_{ad}(\Omega \times [0,T]) \ \exists$ *a sequence* $\{X_t^{(n)}\}_{t\in[0,T]}$ *of elements of* $\mathcal{S}(\Omega \times [0,T])$ *such that*

$$\lim_{n\to+\infty} \mathbb{E}\left[\int_0^T |X_t^{(n)} - X_t|^2 dt\right] = 0. \tag{A.2.10}$$

In addition, if $\{X_t\}_{t\in[0,T]} \in \mathbb{L}^2_{ad}(\Omega \times [0,T])$ *is such that the function*

$$(s,t) \in [0,T]^2 \mapsto \mathbb{E}[X_s X_t]$$

is continuous, then one can directly find the $X_t^{(n)}$ *as:*

$$X_t^{(n)} := \sum_{j=0}^{N_n-1} X_{t_j^{(n)}} \mathbf{1}_{\left[t_j^{(n)}, t_{j+1}^{(n)}\right)}(t), \quad t \in [0,T],$$

where $\pi_n := \{t_0^{(n)}, t_1^{(n)}, \cdots, t_{N_n}^{(n)}\}$ *is a sequence of partitions of the interval* $[0,T]$ *such that* $|\pi_n| \to 0$*, as* $n \to +\infty$*.*

Proof. See Lemma 4.3.3 in [Kuo, 2006]. □

Example A.2.9. *As shown in example A.2.7, the stochastic process* $\{B_t\}_{t\in[0,T]}$ *belongs to* $\mathbb{L}^2_{ad}(\Omega \times [0,T])$*; moreover from 1'st property listed in remark A.1.2 it is known that:*

$$(s,t) \in [0,T]^2 \mapsto \mathbb{E}[B_s B_t] = \min\{s,t\}$$

which is a continuous function. Therefore, according to the previous theorem we may take

$$X_t^{(n)} := \sum_{j=0}^{N_n-1} B_{t_j^{(n)}} \mathbf{1}_{\left[t_j^{(n)}, t_{j+1}^{(n)}\right[}(t), \quad t \in [0,T],$$

as sequence of simple processes approximating $\{B_t\}_{t\in[0,T]}$*.*

With all that has been introduced up to know, we are ready to define the Itô integral of a stochastic process from the class $\mathbb{L}^2_{ad}(\Omega \times [0,T])$. Let $\{X_t\}_{t\in[0,T]} \in \mathbb{L}^2_{ad}(\Omega \times [0,T])$ and consider a sequence $\{\{X_t^{(n)}\}_{t\in[0,T]}\}_{n\geq 1}$ of elements of $\mathcal{S}(\Omega \times [0,T])$ such that

$$\lim_{n\to+\infty} \mathbb{E}\left[\int_0^T |X_t^{(n)} - X_t|^2 dt\right] = 0. \tag{A.2.11}$$

For each $n \geq 1$ the Itô integral

$$\int_0^T X_t^{(n)} dB_t$$

is a well defined element in $\mathbb{L}^2(\Omega)$, since $\{X_t^{(n)}\}_{t\in[0,T]}$ is a simple process. We now prove that the sequence of random variables $\left\{\int_0^T X_t^{(n)} dB_t\right\}_{n\geq 1}$ converges in $\mathbb{L}^2(\Omega)$, as n tends to infinity. First of all we observe that, for $n, m \in \mathbb{N}$, we have

$$\begin{aligned}\mathbb{E}\left[\left(\int_0^T X_t^{(n)} dB_t - \int_0^T X_t^{(m)} dB_t\right)^2\right] =& \mathbb{E}\left[\left(\int_0^T X_t^{(n)} - X_t^{(m)} dB_t\right)^2\right]\\ =& \mathbb{E}\left[\int_0^T \left(X_t^{(n)} - X_t^{(m)}\right)^2 dt\right],\end{aligned} \tag{A.2.12}$$

as a consequence of Proposition A.2.5. Moreover, the convergence of $\{\{X_t^{(n)}\}_{t\in[0,T]}\}_{n\geq 1}$ to $\{X_t\}_{t\in[0,T]}$ in the sense (A.2.11) implies that $\{\{X_t^{(n)}\}_{t\in[0,T]}\}_{n\geq 1}$ is a Cauchy sequence, i.e.

$$\lim_{n,m\to+\infty} \mathbb{E}\left[\int_0^T |X_t^{(n)} - X_t^{(m)}|^2 dt\right] = 0.$$

Therefore, from (A.2.12) we get that

$$\begin{aligned}&\lim_{n,m\to+\infty} \mathbb{E}\left[\left(\int_0^T X_t^{(n)} dB_t - \int_0^T X_t^{(m)} dB_t\right)^2\right]\\ &= \lim_{n,m\to+\infty} \mathbb{E}\left[\int_0^T \left(X_t^{(n)} - X_t^{(m)}\right)^2 dt\right] = 0,\end{aligned}$$

entailing that $\left\{\int_0^T X_t^{(n)} dB_t\right\}_{n\geq 1}$ is a Cauchy sequence in $\mathbb{L}^2(\Omega)$. The completeness of this space yields the convergence of the sequence $\left\{\int_0^T X_t^{(n)} dB_t\right\}_{n\geq 1}$ towards a unique element in $\mathbb{L}^2(\Omega)$.

Definition A.2.10. *Let* $\{X_t\}_{t\in[0,T]}$ *be a stochastic process in* $\mathbb{L}^2_{ad}(\Omega \times [0,T])$*. Then, the* Itô integral *of* $\{X_t\}_{t\in[0,T]}$ *is defined as*

$$\int_0^T X_t dB_t := \lim_{n\to+\infty} \int_0^T X_t^{(n)} dB_t, \qquad \textit{in } \mathbb{L}^2(\Omega),$$

where $\{\{X_t^{(n)}\}_{t\in[0,T]}\}_{n\geq 1}$ *is a sequence of simple stochastic processes converging to* $\{X_t\}_{t\in[0,T]}$ *in the sense* (A.2.11).

Remark A.2.11. *The value of the Itô integral* $\int_0^T X_t dB_t$ *does not depend on the particular sequence* $\{\{X_t^{(n)}\}_{t\in[0,T]}\}_{n\geq 1}$ *of simple stochastic processes utilized to approximate* $\{X_t\}_{t\in[0,T]}$*. More precisely: if* $\{\{\hat{X}_t^{(n)}\}_{t\in[0,T]}\}_{n\geq 1}$ *is another sequence of simple stochastic processes approximating* $\{X_t\}_{t\in[0,T]}$*, then*

$$\lim_{n\to+\infty}\int_0^T \hat{X}_t^{(n)} dB_t = \lim_{n\to+\infty}\int_0^T X_t^{(n)} dB_t = \int_0^T X_t dB_t, \qquad \text{in } \mathbb{L}^2(\Omega).$$

The properties of Itô integrals with integrands in the class $\mathbb{L}^2_{ad}(\Omega\times[0,T])$ coincide with those proved for integrands in the class $\mathcal{S}(\Omega\times[0,T])$ due to their relation as shown below:

Theorem A.2.12. *Let* $\{X_t\}_{t\in[0,T]}$ *and* $\{Y_t\}_{t\in[0,T]}$ *be stochastic processes in* $\mathbb{L}^2_{ad}(\Omega\times[0,T])$*. Then:*

- $\int_0^T X_t dB_t \in \mathbb{L}^2(\Omega)$,

  $$\mathbb{E}\left[\int_0^T X_t dB_t\right] = 0$$

  and

  $$\mathbb{E}\left[\left(\int_0^T X_t dB_t\right)^2\right] = \mathbb{E}\left[\int_0^T X_t^2 dt\right]. \qquad \text{Itô isometry} \tag{A.2.13}$$

  More generally,

  $$\mathbb{E}\left[\int_0^T X_t dB_t \int_0^T Y_t dB_t\right] = \mathbb{E}\left[\int_0^T X_t Y_t dt\right]. \tag{A.2.14}$$

- $\int_0^T(\alpha X_t+\beta Y_t)dB_t = \alpha\int_0^T X_t dB_t + \beta\int_0^T Y_t dB_t$*, for all* $\alpha,\beta\in\mathbb{R}$*.*

Corollary A.2.13. *Let* $f\in L^2([0,T])$*, i.e.* $f:[0,T]\to\mathbb{R}$ *is a deterministic function such that* $\int_0^T f^2(t)dt$ *is finite. Then,* $f\in\mathbb{L}^2_{ad}(\Omega\times[0,T])$ *and* $\int_0^T f(t)dB_t$ *is a Gaussian random variable with mean zero and variance* $\int_0^T f^2(t)dt$*. If* g *is another function from* $L^2([0,T])$*, then* $\int_0^T f(t)dB_t$ *and* $\int_0^T g(t)dB_t$ *are independent if and only if* $\int_0^T f(t)g(t)dt = 0$*.*

Proof. Because the function f is a deterministic function, it is certainly adapted. Moreover, the membership of f to $L^2([0,T])$ guarantees the finiteness of $\mathbb{E}\left[\int_0^T f(t)^2 dt\right] =$

$\int_0^T f(t)^2 dt$. This proves that $f \in \mathbb{L}^2_{ad}(\Omega \times [0,T])$. We now take a sequence a deterministic simple functions

$$f^{(n)}(t) := \sum_{j=0}^{N_n-1} a_j^{(n)} \mathbf{1}_{\left[t_j^{(n)}, t_{j+1}^{(n)}\right)}(t), \quad t \in [0,T],$$

approximating f in the sense

$$\lim_{n\to+\infty} \mathbb{E}\left[\int_0^T |f^{(n)}(t) - f(t)|^2 dt\right] = \lim_{n\to+\infty} \int_0^T |f^{(n)}(t) - f(t)|^2(t)dt = 0,$$

and define

$$\int_0^T f(t)dB_t := \lim_{n\to\infty} \int_0^T f^{(n)}(t)dB_t = \lim_{n\to\infty} \sum_{j=0}^{N_n-1} a_j^{(n)} \left(B_{t_{j+1}^{(n)}} - B_{t_{j+1}^{(n)}}\right), \quad \text{in } \mathbb{L}^2(\Omega).$$

Observe that, for each $n \geq 1$, the random variable

$$\int_0^T f^{(n)}(t)dB_t = \sum_{j=0}^{N_n-1} a_j^{(n)} \left(B_{t_{j+1}^{(n)}} - B_{t_{j+1}^{(n)}}\right)$$

is Gaussian, being a linear combination of independent Gaussian random variables. Because in $\mathbb{L}^2(\Omega)$ the limits of sequences of Gaussian random variables are also Gaussian, we conclude that $\int_0^T f(t)dB_t$ is Gaussian. The statement concerning its mean and variance is a consequence of Theorem A.2.12. Moreover, the Gaussian random variables $\int_0^T f(t)dB_t$ and $\int_0^T g(t)dB_t$ are independent if and only if their covariance is zero; formula (A.2.14) completes the proof. ☐

A.2.3 Extension of the Itô Integral

This section aims to extend the definition of Itô integral to a larger class of integrands. The next definition introduces this new family of stochastic processes.

Definition A.2.14. *We set*

$$\mathcal{L}_{ad}(\Omega; L^2([0,T])) := \Big\{ \{X_t\}_{t\in[0,T]} \textit{ is an } \{\mathcal{F}_t\}_{t\in[0,T]}\textit{-adapted stochastic process such that } \mathbb{P}\left(\int_0^T X_t^2 dt < +\infty\right) = 1 \Big\}$$

In words: an adapted stochastic process belongs to $\mathcal{L}_{ad}(\Omega; L^2([0,T]))$ if the path $t \in [0,T] \mapsto X_t$ is square integrable, almost surely.

Remark A.2.15. *Any adapted stochastic process with almost surely continuous paths belongs to* $\mathcal{L}_{ad}(\Omega; L^2([0,T]))$*; in fact, continuous functions on the compact interval* $[0,T]$ *are bounded and hence square integrable:*

$$\int_0^T X_t^2 dt \leq \int_0^T \sup_{t\in[0,T]} |X_t|^2 dt = T \sup_{t\in[0,T]} |X_t|^2 < +\infty,$$

almost surely.

Example A.2.16. *In particular, the stochastic process* $\left\{e^{B_t^2/2T}\right\}_{t\in[0,T]}$ *doesn't belong to* $\mathbb{L}^2_{ad}(\Omega \times [0,T])$ *since it fails the condition* $\mathbb{E}\left[\int_0^T (e^{B_t^2/2T})^2 dt\right] < \infty$ *but belongs to* $\mathcal{L}_{ad}(\Omega; L^2([0,T]))$ *since it has continuous sample paths.*

We have

$$\mathbb{L}^2_{ad}(\Omega \times [0,T]) \subset \mathcal{L}_{ad}(\Omega; L^2([0,T])).$$

Because, the condition

$$\mathbb{E}\left[\int_0^T X_t^2 dt\right] < +\infty$$

means that the non negative random variable $\int_0^T X_t^2 dt$ has finite expectation and hence it is necessarily finite almost surely, i.e.

$$\mathbb{P}\left(\int_0^T X_t^2 dt < +\infty\right) = 1.$$

Remark A.2.17. *It is usually easier to check the membership of a stochastic process to* $\mathcal{L}_{ad}(\Omega; L^2([0,T]))$ *than to* $\mathbb{L}^2_{ad}(\Omega \times [0,T])$*.*

Theorem A.2.18. *Any element of* $\mathcal{L}_{ad}(\Omega; L^2([0,T]))$ *can be approximated by a sequence of elements of* $\mathcal{S}(\Omega \times [0,T])$*. More precisely, for any* $\{X_t\}_{t\in[0,T]} \in \mathcal{L}_{ad}(\Omega; L^2([0,T]))$ *there exists a sequence* $\{X_t^{(n)}\}_{t\in[0,T]}$ *of elements of* $\mathcal{S}(\Omega \times [0,T])$ *such that*

$$\lim_{n\to+\infty} \int_0^T |X_t^{(n)} - X_t|^2 dt = 0 \quad \textit{in probability,} \tag{A.2.15}$$

i.e. for any $\varepsilon > 0$ *we have*

$$\lim_{n\to+\infty} \mathbb{P}\left(\int_0^T |X_t^{(n)} - X_t|^2 dt > \varepsilon\right) = 0.$$

Proof. See Lemma 5.3.1 in [Kuo, 2006]. □

We are now ready to define the Itô integral of a stochastic process from the class $\mathcal{L}_{ad}(\Omega; L^2([0,T]))$. Namely, let $\{X_t\}_{t\in[0,T]} \in \mathcal{L}_{ad}(\Omega; L^2([0,T]))$ and consider a sequence $\{\{X_t^{(n)}\}_{t\in[0,T]}\}_{n\geq 1}$ of elements of $\mathcal{S}(\Omega \times [0,T])$ such that (A.2.15) holds true. For each $n \geq 1$ the Itô integral

$$\int_0^T X_t^{(n)} dB_t$$

is a well defined element of $\mathbb{L}^2(\Omega)$. Similar to what has been done for the space $\mathbb{L}^2_{ad}(\Omega \times [0,T])$, one can prove that the sequence of random variables $\left\{\int_0^T X_t^{(n)} dB_t\right\}_{n\geq 1}$ converges in probability; this limit will be the Itô integral of $\{X_t\}_{t\in[0,T]}$.

Definition A.2.19. *Let* $\{X_t\}_{t\in[0,T]}$ *be a stochastic process in* $\mathcal{L}_{ad}(\Omega; L^2([0,T]))$. *Then, the* Itô integral *of* $\{X_t\}_{t\in[0,T]}$ *is defined as*

$$\int_0^T X_t dB_t := \lim_{n\to+\infty} \int_0^T X_t^{(n)} dB_t, \qquad \textit{in probability,}$$

where $\{\{X_t^{(n)}\}_{t\in[0,T]}\}_{n\geq 1}$ *is a sequence of simple stochastic processes converging to* $\{X_t\}_{t\in[0,T]}$ *in the sense (A.2.15).*

Remark A.2.20. *The Itô integral of a stochastic process from the class* $\mathcal{L}_{ad}(\Omega; L^2([0,T]))$ *doesn't in general possess those nice properties we proved for Itô integrals of processes from* $\mathbb{L}^2_{ad}(\Omega \times [0,T])$. *In particular, the expectations* $\mathbb{E}[\int_0^T X_s dB_s]$ *and* $\mathbb{E}[(\int_0^T X_s dB_s)^2]$ *are not defined when the integrand belongs to* $\mathcal{L}_{ad}(\Omega; L^2([0,T]))$.

A.3 Itô Formula

The Fundamental Theorem of Calculus (FTC) states that, if $F : [0,T] \to \mathbb{R}$ and $\varphi : \mathbb{R} \to \mathbb{R}$ are continuously differentiable functions, then for any $0 \leq a < b \leq T$ we have

$$\varphi(F(b)) - \varphi(F(a)) = \int_a^b \varphi'(F(t))F'(t)dt.$$

Moreover, if $F : [0,T] \to \mathbb{R}$ is a function of bounded variation, then

$$\varphi(F(b)) - \varphi(F(a)) = \int_a^b \varphi'(F(t))dF(t),$$

where the integral is interpreted in the Stieltjes' sense.

It is natural to wonder whether the FTC holds for F being a Brownian motion and integral interpreted in the Itô's sense. More precisely, given a continuously differentiable function $\varphi : \mathbb{R} \to \mathbb{R}$, does identity

$$\varphi(B_b) - \varphi(B_a) = \int_a^b \varphi'(B_t)dB_t \tag{A.3.1}$$

hold true, almost surely?

Let us check the validity of formula (A.3.1) for $\varphi(x) = x^2$; in this case, we would get

$$B_b^2 - B_a^2 = \int_a^b 2B_t dB_t. \tag{A.3.2}$$

But when we take the expectation of both sides, what happens is:

$$b - a = \mathbb{E}\left[B_b^2 - B_a^2\right] \neq \mathbb{E}\left[\int_a^b 2B_t dB_t\right] = 0.$$

(note that the integrand $\{2B_t \mathbf{1}_{[a,b]}(t)\}_{t\in[0,T]}$ belongs to $\mathbb{L}^2_{ad}(\Omega \times [0,T])$ which implies $\int_a^b 2B_t dB_t \in \mathbb{L}^2(\Omega)$ and $\mathbb{E}\left[\int_a^b 2B_t dB_t\right] = 0$). This entails the fallacy of formula (A.3.2) and hence of (A.3.1), which is expected because like stated earlier in order to define the Stieltjes' integral above the F function was assumed to have bounded variation but we already know this is not the case for B_t via corollary A.2.2. Then the next question is, if there is a similar identity to the FTC but for Itô calculus? The answer to this question is the theorem A.3.2 below. First we define Itô processes:

Definition A.3.1. *We say $\{X_t\}_{t\in[a,b]}$ is an Itô process when it has the form:*

$$\begin{aligned} X_t &= x + \int_0^t \mu_s ds + \int_0^t \sigma_s dB_s, \quad t \in [0,T], \\ &\text{or} \\ dX_t &= \mu_t dt + \sigma_t dB_t, \quad X_0 = x. \end{aligned} \tag{A.3.3}$$

in differential notation. Where $x \in \mathbb{R}$, $\{\mu_t\}_{t\in[0,T]}$ is an adapted stochastic process such that $\mathbb{P}\left(\int_0^T |\mu_t| dt < +\infty\right) = 1$, and $\{\sigma_t\}_{t\in[0,T]}$ belongs to $\mathcal{L}_{ad}(\Omega; L^2([0,T]))$.

Theorem A.3.2 (Itô formula for Itô processes)**.** *Let X_t be an Itô process as explained above and $\varphi : [0,T] \times \mathbb{R} \to \mathbb{R}$ be continuously differentiable in the first variable t and twice continuously differentiable in the second variable x. Then, for any $0 \leq a < b \leq T$ we have*

$$\begin{aligned} \varphi(b, X_b) - \varphi(a, X_a) &= \int_a^b (\partial_x \varphi)(t, X_t)\sigma_t dB_t \\ &+ \int_a^b \left[(\partial_t \varphi)(t, X_t) + \frac{1}{2}(\partial_{xx}\varphi)(t, X_t)\sigma_t^2 + (\partial_x \varphi)(t, X_t)\mu_t\right] dt, \end{aligned} \tag{A.3.4}$$

or, in the equivalent differential form,

$$\begin{aligned} d\varphi(t, X_t) &= (\partial_x \varphi)(t, X_t)\sigma_t dB_t \\ &+ \left[(\partial_t \varphi)(t, X_t) + \frac{1}{2}(\partial_{xx}\varphi)(t, X_t)\sigma_t^2 + (\partial_x \varphi)(t, X_t)\mu_t\right] dt. \end{aligned} \tag{A.3.5}$$

Proof. See section 7 of [Kuo, 2006]. ☐

Remark A.3.3. *It is customary, and very convenient, to rewrite equation (A.3.5) as the symbolic expression*

$$d\varphi(t, X_t) = (\partial_t \varphi)(t, X_t)dt + (\partial_x \varphi)(t, X_t)dX_t + \frac{1}{2}(\partial_{xx}\varphi)(t, X_t)\,(dX_t)^2\,. \tag{A.3.6}$$

This shows the equivalence between (A.3.5) and (A.3.6). The heuristic reason behind identities, which is given in table A.1 can be described as follows: the quadratic variation of the Brownian motion $\{B_t\}_{t\in[0,T]}$ *on the interval* $[a, b] \subset [0, T]$ *is* $b - a$*; hence, for an infinitesimal intervals of time* dt *we can write*

$$(dB_t)^2 := (B_{t+dt} - B_t)^2 \approx dt.$$

This formally gives $dB_t \approx (dt)^{1/2}$*; moreover, since all the terms of the type* $(dt)^\alpha$*, with* $\alpha > 1$*, are negligible compared to* dt*, we get* $dB_t dt = 0$*.*

$\times$	dt	dB_t
dt	0	0
dB_t	0	dt

Table A.1: Product rules for dt and dB_t in Itô calculus in differential form.

A.4 Iterated Itô Integrals

In the previous section we were able to define the Itô integral for a stochastic process $X_t \in \mathcal{L}_{ad}(\Omega; L^2([0, T]))$, where if one fixes the chance parameter $\omega \in \Omega$ the mapping is $t \to X_t(\omega)$ is a function only depending on t. In this section we will improve the definition of the Itô integral so that we will able to define iterated integrals for the processes that has the mapping $(x_1, \ldots, x_n) \to X_{x_1,\ldots,x_n}(\omega)$, when the chance parameter is fixed. In other words, the question is: how to define the Iterated Itô integrals when the integrand depends on multiple variables $(x_1, \ldots, x_n)$? The answer to this question and properties of iterated Itô integrals will be given based on the article [Lanconelli, 2023].

Definition A.4.1. *For a function* $h_n \in L^2_s([0, T]^n)$ *for* $n \geq 1$*, namely for a function* h_n *that is symmetric in its variables and square integrable along the domain* $[0, T]^n$*, the iterated Itô integral is defined as:*

$$I_n(h_n) := n! \int_0^T \int_0^{x_1} \cdots \int_0^{x_{n-1}} h_n(x_1, \ldots, x_n) dB_{x_n} \ldots dB_{x_2} dB_{x_1}. \tag{A.4.1}$$

Remark A.4.2. *One can easily see if* $n = 1$*, then we are in the setting of Corollary A.2.13. So indeed this iterated Itô integral definition is a generalizaiton of the previous section.*

Corollary A.4.3. *The properties of the iterated Itô integral are given below:*

- *Since in definition A.4.1 n is assumed to be greater or equal than 1, it should also be pointed out that for $h_0 \in \mathbb{R}$, $I_0(h_0) := h_0$ for convention.*
- *for $n \geq 1$, $\mathbb{E}[I_n(h_n)] = 0$.*
- *$n \neq m$, $\mathbb{E}[I_n(h_n)I_m(h_m)] = 0$, also called the* orthogonality *of the iterated Itô integrals.*
- *for $n \geq 1$, $\mathbb{E}\left[(I_n(h_n))^2\right] = n!|h_n|^2_{L^2([0,T]^n)}$.*

A.5 The Wiener-Itô Chaos Expansion and Wick Product

Because they will be utilized later in the following sections the *Wiener-Itô chaos expansion* and the *Wick Product* will be introduced in this section. The introduction will follow the steps as in book [Nunno et al., 2009] in section 5.

A.5.1 The White Noise Probability Space

In this section we will formally define the white noise probability space, which is the backbone in introducing the idea of Wiener-Itô chaos expansion. Let $\mathcal{S} = \mathcal{S}(\mathbb{R}^d)$ be the Schwartz space of rapidly decreasing smooth $C^\infty(\mathbb{R}^d)$ real functions on $\mathbb{R}^d$. This space is characterized to be extremely regular so that the functions that belongs to the space and their derivatives will go to 0 faster than any order of polynomial. Namely if $f \in \mathcal{S}$, then:

$$||f||_{K,\alpha} := \sup_{x \in \mathbb{R}^d} \left\{ (1 + |x|^K) \left| \frac{\partial^{|\alpha|}}{\partial^{\alpha_1}_{x_1} \dots \partial^{\alpha_d}_{x_d}} f(x) \right| \right\} < \infty$$

for all $K \in \mathbb{R}$ and any set of multi-indexes $\alpha := (\alpha_1, \dots, \alpha_d)$ with $\alpha_j = 0, 1, \dots$ $(j = 1, \dots, d)$). Lastly $|\alpha| := \alpha_1 + \dots + \alpha_d$.

Then we define the dual space of $\mathcal{S}$, so called the space of *tempered distributions*, $\Omega := \mathcal{S}'(\mathbb{R}^d)$. This space will instead be composed of *wilder* functions, of those properties we are interested in. Since we already have the Ω, it makes sense to define the σ-algebra as: $\mathcal{F} := \mathcal{B}(\mathcal{S}'(\mathbb{R}^d))$ and the probability measure $\mathcal{P}$.

Theorem A.5.1. *The Bochner-Minlos theorem*

There exists a unique probability measure $\mathbb{P}$ on $\mathcal{B}(\mathcal{S}'(\mathbb{R}^d))$ with the following property:

$$\int_{\Omega = \mathcal{S}'} e^{i\langle \omega, \phi \rangle} \mathbb{P}(d\omega) = e^{\frac{-1}{2}||\phi||^2}, \quad \phi \in \mathcal{S}.$$

where $||\phi||^2 := \int_{\mathbb{R}} |\phi(x)|^2 dx$ and $\langle \omega, \phi \rangle = \omega(\phi)$ is the action of $\omega \in \mathcal{S}'(\mathbb{R}^d)$ on $\phi \in \mathcal{S}(\mathbb{R}^d)$.

Proof. See the reference in the book [Nunno et al., 2009] for the Bochner-Minlos-Sazonov theorem in the beginning of section 5.1. $\square$

with the aid of the The Bochner-Minlos theorem, now the triplet $(\mathcal{S}'(\mathbb{R}^d), \mathcal{B}(\mathcal{S}'(\mathbb{R}^d)), \mathbb{P})$ is called the white noise probability space.

Definition A.5.2. *The (smoothed) white noise process is the measurable mapping*

$$\hat{\mathcal{W}} : \mathcal{S}(\mathbb{R}^d) \times \mathcal{S}'(\mathbb{R}^d) \longrightarrow \mathbb{R}$$

given by:

$$\hat{\mathcal{W}}(\phi, \omega) = \hat{\mathcal{W}}_\phi(\omega) = \langle \omega, \phi \rangle, \quad \phi \in \mathcal{S}(\mathbb{R}^d),\ \omega \in \mathcal{S}'(\mathbb{R}^d).$$

As seen from the same book [Nunno et al., 2009], just before section 5.2, one can define the d-parameter Wiener process $W(t)$, $t \in \mathbb{R}$ starting from the smothed white noise as:

$$\hat{\mathcal{W}}_\phi(\omega) = \langle \omega, \phi \rangle = \int_{\mathbb{R}^d} \phi(x) dB(x, \omega); \quad \omega \in \mathcal{S}'(\mathbb{R}^d).$$

A.5.2 Chaos Expansion in Terms of Hermite Polynomials

Our aim in this section is to introduce a way to expand any square integrable random variable, namely for any $X \in \mathbb{L}^2(\Omega)$, in terms of, linear combination of some functions H_αs which are constructed by *Hermite functions*.

In order to do so, we start with introducing the *Hermite polynomials* $h_n(x)$ are defined by:

$$h_n(x) := (-1)^n e^{x^2/2} \frac{d^n}{dx^n} \big(e^{-x^2/2}\big), \quad n = 0, 1, 2, \dots.$$

The explicit representations of first few terms are given by

$$h_0(x) = 1,\ h_1(x) = x,\ h_2(x) = x^2 - 1,\ h_3(x) = x^3 - 3x \tag{A.5.1}$$

Definition A.5.3. *The* Hermite functions*, which should not be confused with the* Hermite polynomials*, are defined by:*

$$\xi_n(x) = \frac{\pi^{-1/4}}{\sqrt{(n-1)!}} e^{-x^2/2} h_{n-1}(\sqrt{2}x), \quad n = 1, 2, \dots. \tag{A.5.2}$$

Remark A.5.4. *Some important properties of the Hermite functions are provided below:*

- *It is a known fact that the collection* $\{\xi_n\}_{n=1}^\infty$ *constitutes an orthonormal basis for* $L^2(\mathbb{R})$.
- *Due to the term* $e^{-x^2/2}$ *present in expression* (A.5.2), $\xi_n \in (S(\mathbb{R}))$ *for all* n. *This states that both* $\mathcal{S}(\mathbb{R}) \subseteq L^2(\mathbb{R})$ *and* $\mathcal{S}(\mathbb{R})$ *is dense in* $L^2(\mathbb{R})$.

- *It is another fact that* $\sup_{x\in\mathbb{R}} |\xi_n(x)| = \mathcal{O}(n^{-1/12})$.

Since our aim is to expand any random variable in $\mathbb{L}^2(\Omega)$, first we should define an orthogonal basis for it. Recall $\langle \omega, \xi_n\rangle := \hat{\mathcal{W}}_{\xi_n}(\omega) = \int_{\mathbb{R}} \xi_n(x) dB(x,\omega)$, $\omega \in \Omega$. Let $\mathcal{J}$ denote the set of all finite multi-indices $\boldsymbol{\alpha} = (\alpha_1, \dots, \alpha_m)$, $m = 1, 2, \dots$ of non-negative integers α_i. If $\boldsymbol{\alpha} \in \mathcal{J}$ and $\boldsymbol{\alpha} \neq 0$, we define

$$H_{\boldsymbol{\alpha}}(\omega) := \prod_{j=1}^{m} h_{\alpha_j}(\langle \omega, \xi_j\rangle) = I_m(\xi_1^{\otimes \alpha_1} \hat{\otimes} \dots \hat{\otimes} \xi_m^{\otimes \alpha_m}) = I_m(\xi^{\hat{\otimes}\boldsymbol{\alpha}}), \quad \omega \in \Omega. \tag{A.5.3}$$

where the last equality is proven by Itô in [ITO, 1951]. By convention $H_0 := 1$, moreover it should be noted that:

$$\mathbb{E}\left[H_{\boldsymbol{\alpha}}\right] = \mathbb{E}\left[I_m(\xi^{\hat{\otimes}\boldsymbol{\alpha}})\right] = 0 \quad \text{for } \boldsymbol{\alpha} = 0. \tag{A.5.4}$$

The symbols $\otimes$ and $\hat{\otimes}$ denote the regular and symmetrized tensor product respectively. Namely:

$$f(x_1) \otimes g(x_2) := f(x_1)g(x_2) = (f \otimes g)(x_1, x_2)$$

and

$$f(x_1)\hat{\otimes} g(x_2) := 1/2[f(x_1)g(x_2) + f(x_2)g(x_1)] = (f\hat{\otimes} g)(x_1, x_2).$$

It turns out, the family $\{H_{\boldsymbol{\alpha}}\}_{\boldsymbol{\alpha}\in\mathcal{J}}$ is an orthogonal basis for $\mathbb{L}^2(\Omega)$. So we are ready to introduce the main theorem of this section:

Theorem A.5.5. *The Wiener-Itô chaos expansion theorem*

Because the family $\{H_{\boldsymbol{\alpha}}\}_{\boldsymbol{\alpha}\in\mathcal{J}}$ *is an orthogonal basis for* $\mathbb{L}^2(\Omega)$*. For all measurable* $X \in \mathbb{L}^2(\Omega)$*, there exists a unique set of constants* $c_{\boldsymbol{\alpha}} \in \mathbb{R}$ *such that:*

$$X = \sum_{\boldsymbol{\alpha} in \mathcal{J}} c_{\boldsymbol{\alpha}} H_{\boldsymbol{\alpha}} \tag{A.5.5}$$

Moreover the isometry holds:

$$||X||^2_{\mathbb{L}^2(\Omega)} = \sum_{\boldsymbol{\alpha}\in\mathcal{J}} \boldsymbol{\alpha}! c^2_{\boldsymbol{\alpha}}$$

As an example take one dimensional $B(x,\omega)$, we know Brownian motion $\in \mathbb{L}^2(\Omega)$ since its second moment exists. Therefore by the above theorem there should be an unique expansion. Using the definition of smoothed white noise, the brownian motion can be defined as:

$$B(x,\omega) := \langle \omega, \psi\rangle$$

where $\psi := \mathbb{1}_{[0,x]}(y)$. Because $\psi(y) \in L^2(\mathbb{R})$, one can expand it using the Hermite functions:

$$\begin{aligned} B(x,\omega) &:= \langle \omega, \psi \rangle \\ &= \int_{\mathbb{R}} \mathbb{1}_{[0,x]}(y) dB(y) \\ &= \int_{\mathbb{R}} \sum_{n\geq 1} \Big(\mathbb{1}_{[0,x]}, \xi_n \Big)_{L^2(\mathbb{R})} \xi_n(y) dB(y) \\ &= \sum_{n\geq 1} \left(\int_0^x \xi_n(y) dy \right) \int_{\mathbb{R}} \xi_n(y) dB(y) \\ &= \sum_{n\geq 1} \left(\int_0^x \xi_n(y) dy \right) H_{\epsilon^{(n)}}, \quad \textit{let } c_n := \int_0^x \xi_n(y) dy \\ &= \sum_{n\geq 1} c_n H_{\boldsymbol{\epsilon}^{(n)}} \end{aligned} \tag{A.5.6}$$

where $\boldsymbol{\epsilon}^{(n)} := (0, 0, \dots, 0, 1, 0, \dots, 0)$ where the n'th entry is 1 and the rest is zero. Due to the intrinsic relation of iterated Itô integrals and the Hermite polynomials the chaos expansion theorem stated above can be reformulated. This new formulation will be the main tool utilized in this thesis.

Theorem A.5.6. *The Wiener-Itô chaos expansion theorem, with iterated Itô integrals*

Let $(\Omega, \mathcal{B}, \mathbb{P})$ be the Wiener space of the interval $[0, T]$ and X be an element in $\mathbb{L}^2(\Omega)$, then as stated in [Lanconelli, 2023], X can be uniquely expressed by

$$X := \sum_{n\geq 0} I_n(f_n), \text{ for some } f_n \ s.t. \ f_n \in L^2_s([0,T]^n) \ \forall n. \tag{A.5.7}$$

Moreover there is the isometry:

$$||X||^2_{\mathbb{L}^2(\Omega)} = \sum_{n\geq 0} n! ||f_n||^2_{L^2(\mathbb{R})}$$

Proof. See section 9.7 in [Karatzas and Shreve, 1991] for the main theorem. For the isometry part, it is evident from the corollary A.4.3. □

Remark A.5.7. *The two chaos expansion theorems are actually the same. Their connection can be explained by the following reasoning:*

- *Because Hermite functions $\{\xi_n(x)\}_{n\geq 1}$ is an orthonormal basis for $L^2(\mathbb{R})$.*
- *This means that for a set of multi-indices $\boldsymbol{\alpha} = (\alpha_1, \dots, \alpha_m) \in \mathcal{J}$ which satisfy that: $|\boldsymbol{\alpha}| := \alpha_1 + \dots + \alpha_m = n$, then $\xi_1^{\otimes \alpha_1} \hat{\otimes} \xi_2^{\otimes \alpha_2} \hat{\otimes} \dots \hat{\otimes} \xi_m^{\otimes \alpha_m}$ forms and orthogonal basis for the space $L^2(\mathbb{R}^n)$.*

- *In other words, one can expand any function $f \in L_s^2(\mathbb{R})$ as:*

$$f_n = \sum_{\boldsymbol{\alpha}\in\mathcal{J},\, s.t.\, |\boldsymbol{\alpha}|=n} c_\alpha \xi_1^{\otimes\alpha_1}\hat{\otimes}\xi_2^{\otimes\alpha_2}\hat{\otimes}\dots\hat{\otimes}\xi_m^{\otimes\alpha_m}, \quad n = 0, 1, 2, \dots$$

- *Due to the definition provided in expression (A.5.3), $H_{\boldsymbol{\alpha}} := I_m(\xi^{\hat{\otimes}\boldsymbol{\alpha}})$. Which ensures the connection between two theorems.*

A.5.3 The Hida Spaces of Stochastic Test Functions and Stochastic Distributions

In this section we will define analogous spaces of $\mathcal{S}(\mathbb{R}^d)$ and $\mathcal{S}'(\mathbb{R}^d)$ that we have defined in the previous section in relation with $L^2(\mathbb{R}^d)$. Now we need the stochastic versions of these two spaces.

Definition A.5.8. *For a $f := \sum_{\boldsymbol{\alpha}\in\mathcal{J}} c_\alpha H_{\boldsymbol{\alpha}} \in \mathbb{L}^2(\Omega)$ belongs to the so called* Hida test function Hilbert space $(\mathcal{S})_k$ *if:*

$$||f||_k^2 := \sum_{\boldsymbol{\alpha}\in\mathcal{J}} \alpha! c_{\boldsymbol{\alpha}}^2 \Big(\prod_{j=1}^{m} (2j)^{\alpha_j}\Big)^k, \quad \forall\, k \in \mathbb{R} < \infty.$$

Based on this result, the Hida test function space $(\mathcal{S})$ *as the space*

$$(\mathcal{S}) = \bigcap_{k\in\mathbb{R}} (\mathcal{S})_k,$$

where $f_n \longrightarrow f$ as $n \to \infty$ in $(\mathcal{S})$ if and only if $||f_n - f||_k \longrightarrow 0$ as $n \to \infty$, for all k.

Definition A.5.9. *The Hida distribution space $(\mathcal{S})^*$*

i. Let $q \in \mathbb{R}$. The formal sum $F = \sum_{\boldsymbol{\alpha}\in\mathcal{J}} b_{\boldsymbol{\alpha}} H_{\boldsymbol{\alpha}}$ belongs to the Hida distribution Hilbert space $(\mathcal{S})_{-q}$ if:

$$||F||_{-q}^2 := \sum_{\boldsymbol{\alpha}\in\mathcal{J}} \boldsymbol{\alpha}! b_{\boldsymbol{\alpha}}^2 \Big(\prod_{j=1}^{m} (2j)^{\alpha_j}\Big)^{-q} < \infty.$$

We define the Hida distribution space $(\mathcal{S})^*$ *as:*

$$(\mathcal{S})^* = \bigcup_{q\in\mathbb{R}} (\mathcal{S})_{-q},$$

where $F_n \longrightarrow F$ as $n \to \infty$ in $(\mathcal{S})^*$ if and only if there exists q, such that $||F_n - F||_{-q} \longrightarrow 0$ as $n \to \infty$.

ii. For $F = \sum_{\boldsymbol{\alpha} \in \mathcal{J}} b_{\boldsymbol{\alpha}} H_{\boldsymbol{\alpha}} \in (\mathcal{S})^*$*, the generalized expectation is defined as:*

$$\mathbb{E}[F] = b_0.$$

Note that if $F \in \mathbb{L}^2(\Omega)$ *then the generalized expectation coincides with the usual expectation due to the fact that* $\mathbb{E}[H_{\boldsymbol{\alpha}}] = 0$ *for all* $\boldsymbol{\alpha} \neq 0$*.*

Remark A.5.10. *Due to the definitions above note the relation holds true:*

$$(\mathcal{S}) \subseteq (\mathcal{S})_k \subseteq \mathcal{L}^2(\Omega) \subseteq (\mathcal{S})_{-q} \subseteq (\mathcal{S})^*$$

Proof. It is direct verification from the definitions. □

The usage of Hida test spaces and Hida distributions in stochastic analysis are similar to Schwartz space and tempered distributions space in functional analysis. The logic is to see define a more generalized feature of derivative and see how the elements of the wilder set will behave, when they are acted on the regular set elements. One example is given below:

Consider the step function

$$\mathbb{1}_{[t \geq 0]} = \begin{cases} 0, & \text{if } t < 0, \\ 1, & \text{if } t \geq 0. \end{cases}$$

that the derivative can't be defined in the normal sense because of the discontinuity at $t = 0$. However we can define the action of $\mathbb{1}_{[t \geq 0]}$ on any regular function belongs to $\mathcal{S}(\mathbb{R})$ as $\langle \mathbb{1}_{[t \geq 0]}, \phi \rangle$ for any $\phi \in \mathcal{S}(\mathbb{R})$:

$$\langle \mathbb{1}_{[t \geq 0]}, \phi \rangle := \int_{\mathbb{R}} \mathbb{1}_{[t \geq 0]} \phi(t) dt,$$

so that $\mathbb{1}_{[t \geq 0]} \in \mathcal{S}'(\mathbb{R})$. Because the actual derivative of $\mathbb{1}_{[t \geq 0]}$ does not exists we go on to define the so called *distributional derivative* as follows:

$$\langle \frac{d}{dt} \mathbb{1}_{[t \geq 0]}, \phi \rangle := -\langle \mathbb{1}_{[t \geq 0]}, \frac{d}{dt} \phi \rangle \tag{A.5.8}$$

Note that if $\mathbb{1}_{[t \geq 0]}$ was also differentiable then the expression (A.5.8) is again valid, but because now we define it for functions that can't be differentiated traditionally, it is a generalization of traditional derivative. We use identity (A.5.8) to go on as:

$$\begin{aligned} \int_{\mathbb{R}} \frac{d}{dt} \mathbb{1}_{[t \geq 0]} \phi(t) dt &= - \int_{\mathbb{R}} \mathbb{1}_{[t \geq 0]} \phi'(t) dt \\ &= - \int_0^{\infty} \phi'(t) dt \\ &= \phi(0) \\ &= \int_{\mathbb{R}} \delta_0(t) \phi(t) dt \end{aligned} \tag{A.5.9}$$

So we see that $\frac{d}{dt}\mathbb{1}_{[t\geq 0]}$ behaves as $\delta_0(t)$ when applied on a function belonging to a Schwartz space. This is why although the derivative of $\mathbb{1}_{[t\geq 0]}$ is not defined at $t=0$, its distributional derivative is a dirac delta function centered around 0.

One of our aims in this section with the Hida test function space and the family of hida distributions is doing the same for Brownian motion. Although it is known by remark A.2.3 that Brownian motion is nowhere differentiable, we will be able to define a distributional derivative of it in the following sense. Define the singular white noise process as:

$$\hat{\mathcal{W}}(x) := \sum_{n\geq 1} \xi_n(x) H_{\epsilon^{(n)}}, \tag{A.5.10}$$

where the function $\hat{\mathcal{W}}(x) \in (\mathcal{S})^*$ and bearing in mind the remark A.5.4, it can be checked via,

$$||\hat{\mathcal{W}}(x)||^2_{-q} := \sum_{n\geq 1} \xi_n^2(x)\,(2n)^{-q} \leq \sum_{n\geq 1} \sup_{x\in\mathbb{R}} |\xi_n^2(x)|(2n)^{-q} \leq C \sum_{n\geq 1} \frac{1}{n^{q+1/6}} < \infty.$$

for any $q \geq 2$.

Note the relation of this definition to the definition of Brownian motion in the white noise probability space in (A.5.6). The explicit relation is given by:

$$\hat{\mathcal{W}}(x) = \sum_{n\geq 1} \frac{d}{dx} \int_0^x \xi_n(y) dy H_{\epsilon^{(n)}} = \frac{d}{dx} B(x,\omega)$$

So white noise really acts like a form of derivative of Brownian motion. An equal way of defining it is by realizing:

$$\begin{aligned}
\hat{\mathcal{W}}(x) &= \sum_{n\geq 1} \frac{d}{dx} \int_0^x \xi_n(y) dy H_{\epsilon^{(n)}} \\
&= \sum_{n\geq 1} \frac{d}{dx} \int_{\mathbb{R}} \mathbb{1}_{[0,x]}(y) \xi_n(y) dy H_{\epsilon^{(n)}} \\
&= \sum_{n\geq 1} \int_{\mathbb{R}} \frac{d}{dx} \mathbb{1}_{[0,x]}(y) \xi_n(y) dy H_{\epsilon^{(n)}} \\
&= \sum_{n\geq 1} \int_{\mathbb{R}} -\frac{d}{dx} \mathbb{1}_{[0,\infty)}(y-x) \xi_n(y) dy H_{\epsilon^{(n)}} \quad \text{since } \mathbb{1}_{[0,x]} = \mathbb{1}_{[0,\infty)} - \mathbb{1}_{[x,\infty)} \\
&= \sum_{n\geq 1} \int_{\mathbb{R}} \frac{d}{dy} \mathbb{1}_{[y-x\geq 0]} \xi_n(y) dy H_{\epsilon^{(n)}} \\
&= \sum_{n\geq 1} \int_{\mathbb{R}} \delta_x(y) \xi_n(y) dy H_{\epsilon^{(n)}} \quad \text{as done in (A.5.9)} \\
&= \mathcal{W}_{\delta_x}(\omega) = \langle \omega, \delta_x \rangle
\end{aligned}$$

using the definition of white noise in A.5.10. Note that an alternative expression for the singular white noise $\hat{\mathcal{W}}(x)$ can be given using the last identity above, using the smothed white noise with $\lim_{n\to\infty}\phi_n = \delta_x$ where $\phi_n \in (\mathcal{S})\ \forall n$ so that

$$\hat{\mathcal{W}}(x) = \langle \omega, \delta_x \rangle = \lim_{n\to\infty} \langle \omega, \phi_n \rangle = \lim_{n\to\infty} \int_{\mathbb{R}} \phi_n(x) dB_x = \int_{\mathbb{R}} \delta_x dB_x. \tag{A.5.11}$$

So this is how you singularize the smothed white noise.

A.5.4 The Wick Product

One key advantage of working in spaces $(\mathcal{S})$ and $(\mathcal{S})^*$ is, the existence of a well defined product operator unlike of spaces $\mathcal{S}(\mathbb{R}^d)$ and $\mathcal{S}'(\mathbb{R}^d)$. This natural product is called the *Wick product* and it is a fundamental study of stochastic differential equations, both ODE and PDE. In the following we formally let $d = 1$ for simplicity but any idea can be further generalized to d-dimensions.

Definition A.5.11. *If* $X := \sum_\alpha c_\alpha H_\alpha \in (\mathcal{S})^*$ *and* $Y := \sum_\beta b_\beta H_\beta \in (\mathcal{S})^*$, *then the Wick product,* $X \diamond Y$ *of* X *and* Y *is defined by:*

$$X \diamond Y := \sum_{\alpha,\beta} c_\alpha b_\beta H_{\alpha+\beta} = \sum_\gamma \left(\sum_{\alpha+\beta=\gamma} c_\alpha b_\beta \right) H_\gamma$$

when one refers $z_\gamma := \left(\sum_{\alpha+\beta=\gamma} c_\alpha b_\beta\right)$ it is easy to see that

$$\text{If } X, Y \in (\mathcal{S})^* \Rightarrow X \diamond Y := \sum_\gamma z_\gamma H_\gamma \in (\mathcal{S})^*$$

$$\text{If } X, Y \in (\mathcal{S}) \Rightarrow X \diamond Y := \sum_\gamma z_\gamma H_\gamma \in (\mathcal{S})^*.$$

However as also explained in the book [Nunno et al., 2009], if $X, Y \in \mathbb{L}^2(\Omega) \not\Rightarrow X \diamond Y \in \mathbb{L}^2(\Omega)$ in general. One key example of Wick product is the wick product of 2 smooth white noises. Let $X = \hat{\mathcal{W}}_\phi(\omega)$ and $Y = \hat{\mathcal{W}}_\psi(\omega)$ in the above definition where $\phi, \psi \in \mathcal{S}(\mathbb{R}^x)$. Then

$$\hat{\mathcal{W}}_\phi(\omega) \diamond \hat{\mathcal{W}}_\psi(\omega) = \sum_{k,l} c_k b_l H_{\boldsymbol{\epsilon}^{(k)}+\boldsymbol{\epsilon}^{(l)}}$$

because

$$H_{\boldsymbol{\epsilon}^{(k)}+\boldsymbol{\epsilon}^{(l)}} = \begin{cases} H_{\boldsymbol{\epsilon}^{(k)}} \cdot H_{\boldsymbol{\epsilon}^{(l)}}, & \text{if } k \neq l, \\ H^2_{\boldsymbol{\epsilon}^{(k)}} - 1, & \text{if } k = l. \end{cases}$$

due to the definition of $H_{\boldsymbol{\alpha}}$ from expression (A.5.3).

Corollary A.5.12. *Here some properties of the Wick product will be listed:*

- *If* X *and* Y *are deterministic, then* $X \diamond Y = X \cdot Y$.

- *$X \diamond Y = Y \diamond X$. (commutative law).*
- *$X \diamond (Y \diamond Z) = (X \diamond Y) \diamond Z$ (associative law).*
- *$X \diamond (Y + Z) = (X \diamond Y) + (X \diamond Z)$ (distirbutive law).*
- *In general $X \cdot (Y \diamond Z) \neq (X \cdot Y) \diamond Z$.*
- *When $X := \sum_\alpha c_\alpha H_\alpha \in \mathbb{L}^2(\Omega)$ and $Y := \sum_\beta b_\beta H_\beta \in \mathbb{L}^2(\Omega)$, then*
  $$\mathbb{E}[X \diamond Y] = c_\alpha b_\beta = \mathbb{E}[X]\mathbb{E}[Y],$$
  due to the fact that $\mathbb{E}[H_\alpha] = 0$ as explained in equation (A.5.4). Note that this identity does not assume independence *of X and Y.*

Due to the commutation relation, one can define the Wick powers as

$$X^{\diamond n} := X \diamond \cdots \diamond X \quad (n\,times) \quad \text{for} \quad X \in (\mathcal{S})^*, \quad n \in \{1, 2, \dots\}$$

and by convention $X^{\diamond 0} = 1$. Going on with the same mentality, The Wick exponential of $X \in (\mathcal{S})^*$ is defined as:

$$\exp^\diamond(X) := \sum_{n \geq 0} \frac{1}{n!} X^{\diamond n}. \tag{A.5.12}$$

Proposition A.5.13. *It should be noted that, the wick exponential can be represented fully analytically without using any Wick product at all as:*

$$\exp^\diamond\{B_t\} := \exp\left\{B_t - \frac{t}{2}\right\}$$

Proof. Using the definition of Wick exponential given in expression (A.5.12) and letting $X := B_t$ one can write:

$$\begin{aligned}
\exp^\diamond\{B_t\} &= \sum_{n=0}^{\infty} \frac{1}{n!} B_t^{\diamond n} = \sum_{n=0}^{\infty} \frac{1}{n!} \left(I_1(1)\right)^{\diamond n} \\
&= \sum_{n=0}^{\infty} \frac{1}{n!} \Big(h_1(I_1(1))\Big)^{\diamond n} = \sum_{n=0}^{\infty} \frac{1}{n!} H_{\boldsymbol{\epsilon_1}}^{\diamond n} \\
&= \sum_{n=0}^{\infty} \frac{1}{n!} H_{\boldsymbol{n\epsilon_1}} = \sum_{n=0}^{\infty} \frac{1}{n!} h_n\big(I_1(1)\big) \\
&= \exp\{I_1(1) - \frac{t}{2}\} = \exp\left\{B_t - \frac{t}{2}\right\}
\end{aligned}$$

where the first equality in the last line is given by the *generating formula for Hermite polynomials*:

$$\exp\left\{tx - \frac{t^2}{2}\right\} := \sum_{n=0}^{\infty} \frac{t^n}{n!} h_n(x).$$

□

It turns out the Proposition A.5.13 can be further generalized to cases other than B_t. The theorem below explains it:

Theorem A.5.14. *Let $\phi \in L^2(\mathbb{R}^d)$. Then*

$$\exp^{\diamond}\left\{\int_{\mathbb{R}^d} \phi(x)dB_x\right\} = \exp\left\{\int_{\mathbb{R}^d} \phi(x)dB_x - \frac{1}{2}\int_{\mathbb{R}^d} \phi^2(x)dx\right\}$$

Proof. See section 5.3.4 in [Nunno et al., 2009] for the derivation. ☐

Most of the time the Wick product acts similar to a regular algebra, for example

$$(X+Y)^{\diamond 2} = X^{\diamond 2} + 2X \diamond Y + Y^{\diamond 2},$$

and similarly:

$$\exp^{\diamond}(X+Y) = \exp^{\diamond}(X) \diamond \exp^{\diamond}(Y).$$

Lastly another crucial property of Wick product is called the chain rule of Wick product:

$$\frac{d}{dt} f^{\diamond}(X(t)) = (f')^{\diamond}(X(t)) \diamond \frac{d}{dt} X(t)$$

Using all these properties, the main advantage of Wick product in stochastic calculus is how it regularizes the stochastic calculus to classic calculus once you know the properties of it.

Theorem A.5.15. *Let X_t be an Itô integrable process. Then:*

$$\int_{\mathbb{R}^d} X_t dB_t = \int_{\mathbb{R}^d} X_t \diamond \hat{\mathcal{W}}(t)dt$$

where $\hat{\mathcal{W}}$ is the White noise process defined in expression (A.5.10).

By the theorem A.5.15 one can see how the usage of Wick product and the white noise process can be utilized to transform an Itô integral to a Lebesgue integral of $X_t \diamond \hat{\mathcal{W}}(t) \in (\mathcal{S})^*$. One example where theorem A.5.15 is very useful is the following: Consider $d = 1$ and $X_t = B_t$, then

$$\int_0^T B_t dB_t = \frac{1}{2}\left(B^2(T) - T\right)$$

when one applies Itô formula as given in expression (A.3.2) to the function $\varphi(t, B_t) := B_t^2$. However one can also utilize the wick product to reach to the correct outcome as:

$$\int_0^T B_t dB_t = \int_0^T B_t \diamond B_t' dt = \frac{1}{2} B^{\diamond 2}(T) = \frac{1}{2}\left(B^2(T) - T\right)$$

Since the natural emergence and usefulness of Wick product is already mentioned lastly it needs to eb said that. Due to the connections of theorems A.5.5 and A.5.6, for any $X \in \mathbb{L}(\Omega)$ we can already define the Wick product in terms of iterated Itô integrals. However it is more useful to define it in full generality in the following section:

A.5.5 Wick Product for Iterated Itô Integrals Defined in Spaces $\mathcal{G}$ and $\mathcal{G}^*$

Definition A.5.16. *Let $k \in \mathbb{R}$. Then the space $\mathcal{G}_k$ consists of all expansions as:*

$$X = \sum_{n \geq 0} I_n(f_n),$$

such that:

$$||X||_{\mathcal{G}_k} = \left(\sum_{n \geq 0} n! e^{2kn} ||f_n||^2_{L^2(R^n)} \right)^{1/2} < \infty. \tag{A.5.13}$$

$\forall k \in \mathbb{R}$ and for every:

$$X = \sum_{n \geq 0} I_n(f_n), \quad Y = \sum_{n \geq 0} I_n(g_n),$$

the space $\mathcal{G}_k$ is a Hilbert space with the inner product defined as:

$$(X, Y)_{\mathcal{G}_k} := \sum_{n \geq 0} n! e^{2kn} (f_n, g_n)_{L^2(\mathbb{R}^n)}.$$

As one can see from the expression (A.5.13), as the k value increases, the space $\mathcal{G}_k$ includes *more regular* random variables and with smaller or even negative k values, the included random variables become *wilder*.

Definition A.5.17. *Because of the relation $k_1 \leq k_2 \Rightarrow \mathcal{G}_{k_2} \subseteq \mathcal{G}_{k_1}$ (which is evident from expression (A.5.13) above). We define:*

$$\mathcal{G} := \bigcap_{k > 0} \mathcal{G}_k$$

Now we are going to define the so called *dual space* of $\mathcal{G}$, the $\mathcal{G}^*$. Because the space $\mathcal{G}$ is made of highly regular random variables in the sense of the norm in expression (A.5.13), the dual space will include all kinds of irregular random variables in the following sense:

Definition A.5.18. *$\mathcal{G}^*$ is defined as:*

$$\mathcal{G}^* := \bigcup_{k < 0} \mathcal{G}_k.$$

Note that due to the union present, the set $\mathcal{G}^*$ will include wilder and wilder random variables with each increasing k. All these facts will be summarized in the remark below:

Remark A.5.19. *Note that for an element $Y \in \mathcal{G}^*$, it can be represented as the formal sum:*

$$Y = \sum_{n \geq 0} I_n(g_n),$$

where $g_n \in L^2_s(\mathbb{R}^n)$ and we know for some $k \in \mathbb{R}$, $||Y||_{\mathcal{G}_k} < \infty$ whereas a random variable $X \in \mathcal{G}$ satisfies $||X||_{\mathcal{G}_k}$ for all $k \in \mathbb{R}$.

The following relation can be proven:

$$(\mathcal{S}) \subset \mathcal{G} \subset \mathbb{L}(\Omega) \subset \mathcal{G}^* \subset (\mathcal{S})^*.$$

and similarly again spaces $\mathcal{G}$ and $\mathcal{G}^*$ are closed under Wick product.

Although the space $\mathcal{G}^*$ is not big enough to include the singular white noise $\hat{\mathcal{W}}$, still it is very useful to include solutions to stochastic differential equations.

In these new spaces the Wick product is defined as:

Definition A.5.20. *Consider* $X := \sum_{n\geq 0} I_n(f_n) \in \mathcal{G}^*$ *and* $Y := \sum_{m\geq 0} I_m(g_m) \in \mathcal{G}$. *Then the Wick product can be alternatively defined as:*

$$X \diamond Y := \sum_{n+m=0}^{\infty} I_{n+m}(f_n \hat{\otimes} g_m)$$

A.6 The Malliavin Derivative

The Malliavin derivative is a way of taking the derivative of a stochastic process with respect to the chance parameter ω. After a series of definitions it will be more apparent.

A.6.1 The Brownian Functional

Definition A.6.1. *A random variable* F *is called a Brownian functional if* $F \in F_T^B$.

This alternatively means that the random variable F is a measurable function of Brownian sample paths. So if the entire Brownian path is known, then the value of this random variable F is also known. Some examples of Brownian functionals are given below:

- $F_1 := \phi(B_{t_1}, \dots, B_{t_n})$, where $0 \leq t_1 \leq \dots \leq t_n \leq T$ and $\phi : \mathbb{R}^n \to \mathbb{R}$ is a measurable function;
- $F_2 := \int_0^T \psi(s, B_s)ds$, where $\psi : [0,T] \times \mathbb{R} \to \mathbb{R}$ is a measurable function such that $\mathbb{P}(\int_0^T |\psi(s, B_s)|ds < +\infty) = 1$;
- $F_3 := \int_0^T \chi(s, B_s)dB_s$, where $\chi : [0,T] \times \mathbb{R} \to \mathbb{R}$ is a measurable function such that $\mathbb{P}(\int_0^T |\chi(s, B_s)|^2 ds < +\infty) = 1$;
- $F_4 := \sup_{t\in[0,T]} |B_t|$.

The most important Brownian functionals for our purposes are the *strong solutions of stochastic differential equations* (SDEs) with deterministic initial condition:

$$\begin{aligned} dX_t &= b(t, X_t)dt + \sigma(t, X_t)dB_t, \quad 0 < t \leq T, \\ X_0 &= x \in \mathbb{R}. \end{aligned}$$

This is due to the fact that, a strong solution of an SDE $\{X_t\}_{t\in[0,T]}$ is by definition an $\{F_t^B\}_{t\geq 0}$ adapted stochastic process $\forall t \in [0,T]$. Because $F_t^B \subseteq F_T^B$, we have for any fixed $t \in [0,T]$, X_t is a Brownian functional.

Definition A.6.2. *A* smooth *Brownian functional is defined as:*

$$F := \varphi(I(h_1), \ldots, I(h_n)),$$

where $h_1, \ldots, h_n \in L^2([0,T])$, $I(h_i) := \int_0^T h_i(t)dB_t$ *and* $\varphi : \mathbb{R}^n \to \mathbb{R}$ *is a* $C^\infty(\mathbb{R}^n)$ *function having all its partial derivatives and its growth at infinity is at most polynomial.*

The family of these smooth Brownian functionals are denoted by $\mathcal{M}$*.*

We will see that the space $\mathcal{M}$ is a toy space for us to prove some properties for the Brownian functionals, because it turns out that you can generalize all the properties you have in this space to larger spaces like $\mathbb{L}^p(\Omega)$ since $\mathcal{M} \subset \mathbb{L}^p(\Omega)$ for any $p \geq 1$ using theorem A.6.3 that will be introduced later in this section. Lastly note that the space $\mathcal{M}$ is closed under multiplication and addition.

Considering $t \in [0,T]$ and $h \in L^2([0,T])$ the following random variables are examples of smooth Brownian functionals.

1. $I(h) \Rightarrow \varphi(x) = \mathbb{I}(x)$ where $\mathbb{I}(x) := x$ is defined as the identity function.
2. $B_t^2 \Rightarrow \varphi(x) = x^2$ and $h := \mathbb{1}_{[0,t]}$.
3. $\sin(I(h))B_T \Rightarrow \varphi(x_1, x_2) = sin(x_1)x_2$, moreover $h_1(x) = h$ and $h_2(x) = \mathbb{1}_{[0,T]}$.

However note that the Brownian functionals

$$|B_t| \quad \textit{and} \quad e^{B_t} \tag{A.6.1}$$

are not *smooth* Brownian functionals.

Theorem A.6.3. *Let* $p \geq 1$*. If* F *is a Brownian functional in* $\mathbb{L}^p(\Omega)$*, then* $\exists$ *a sequence* $\{F_n\}_{n\geq 1}$ *in space* $\mathcal{M}$ *such that:*

$$F_n \to F \quad \text{in } \mathbb{L}^p(\Omega).$$

So by theorem A.6.3, we can generalize the findings regarding space $\mathcal{M}$ to the more general one $\mathbb{L}^p(\Omega)$. For example the 2 previous examples in expression (A.6.1) are elements in $\mathbb{L}^p(\Omega)$, then due to theorem A.6.3 there must be sequences for which will converge to them. Indeed they are:

$$\left(B_t^2 - \frac{1}{n}\right)^{1/2} \xrightarrow{\mathbb{L}^p(\Omega)} |B_t|$$
$$\left(1 + \frac{B_t}{n}\right)^n \xrightarrow{\mathbb{L}^p(\Omega)} e^{B_t}$$

as $n \to \infty$. As one can see the objects on the LHS are all elements in $\mathcal{M}$ $\forall n \geq 1$.

A.6.2 The Malliavin Derivative for Smooth Brownian Functionals

The main aim in defining a derivative is to see how function depends on its variables. In order to see how a Brownian functional depends based on the Brownian path, one thing that can be done is to use variational calculus and perturb the Brownian path a little and then to check how does the function behave. One example will be given below in this section.

Let $F := \varphi(I(h_1), \ldots, I(h_n)) \in \mathcal{M}$ then, for $h \in L^2([0,T])$ and $\epsilon > 0$ we consider the following perturbation to the Brownian path:

$$\left\{\tilde{B}_t\right\}_{t\in[0,T]} \to \left\{B_t + \epsilon \int_0^t h(s)ds\right\}_{t\in[0,T]}.$$

Now we will see how does the Brownian functional of our interest F will change according to this perturbation to the path. Note that the differential $d\tilde{B}_t$ can easily be found using Itô formula (A.3.6). In the light of all that, we note that, under this perturbation:

$$\begin{aligned} I(h_i) = \int_0^T h_i(t)d\tilde{B}_t &\to \int_0^T h_i(t)(dB_t + \epsilon h(t)dt) \\ &= \int_0^T h_i(t)dB_t + \epsilon \int_0^T h_i(t)h(t)dt \\ &= I(h_i) + \epsilon\langle h_i, h\rangle_{L^2([0,T])}, \end{aligned}$$

where $\langle h_i, h\rangle_{L^2([0,T])}$ denotes the inner product of $h_i(t)$ and $h(t)$ functions and for the sake of simplicity from now on it will be denoted by $\langle h_i, h\rangle$. So from the above expression we see how a perturbation to the Brownian path affects the related Itô integral. Using this fact we see how the Brownian function F is affected:

$$F := \varphi(I(h_1), \ldots, I(h_n)) \to \varphi(I(h_1) + \epsilon\langle h_1, h\rangle, \ldots, I(h_n) + \epsilon\langle h_n, h\rangle) := F_\epsilon.$$

Now in order to see the change in F as a result of this perturbation, we differentiate F_ϵ with respect to ϵ and let $\epsilon = 0$ since we don't actually care about F_ϵ but rather see the dependence of the original F.

$$\begin{aligned} \frac{dF_\epsilon}{d\epsilon}\bigg|_{\epsilon=0} &= \frac{d}{d\epsilon}\varphi\big(I(h_1) + \epsilon\langle h_1, h\rangle, \ldots, I(h_n) + \epsilon\langle h_n, h\rangle\big)\bigg|_{\epsilon=0} \\ &= \sum_{i=1}^n \partial_{x_i}\varphi\big(I(h_1), \ldots, I(h_n)\big)\langle h_i, h\rangle \\ &= \int_0^T \left(\sum_{i=1}^n \partial_{x_i}\varphi\big(I(h_1), \ldots, I(h_n)\big)h_i(t)\right) h(t)dt \\ &= \Big\langle \sum_{i=1}^n \partial_{x_i}\varphi\big(I(h_1), \ldots, I(h_n)\big)h_i(t), h\Big\rangle. \end{aligned} \tag{A.6.2}$$

where the last two lines can also be interpreted as the directional derivative of the Brownian functional along the function $h(t)$. In line with this define the *Malliavin derivative* of a smooth Brownian functional.

Definition A.6.4. *The* Malliavin derivative *of a smooth Brownian functional in the form*

$$F := \varphi\big(I(h_1), \ldots, I(h_n)\big),$$

is the stochastic process denoted as $\{D_t F\}_{t\in[0,T]}$ *and it is defined as:*

$$D_t F := \sum_{i=1}^{n} \partial_{x_i}\varphi\big(I(h_1), \ldots, I(h_n)\big) h_i(t), \quad t \in [0, T].$$

Similarly, the directional derivative of F *along the function* $h(t)$ *is defined as the projection of* $D_t F$ *along* $h(t)$ *as:*

$$D_h F := \langle D_t F, h\rangle.$$

Lemma A.6.5. *For* $F \in \mathcal{M}$ *and* $h \in L^2([0, T])$ *one can say that:*

$$\mathbb{E}[\langle DF, h\rangle] = \mathbb{E}[F I(h)]$$

.

Proof. Due to the expression (A.6.2), we know that

$$\frac{dF_\epsilon}{d\epsilon}\bigg|_{\epsilon=0} = \langle DF, h\rangle.$$

So it can be said that:

$$\mathbb{E}[\langle DF, h\rangle] = \mathbb{E}\left[\frac{dF_\epsilon}{d\epsilon}\bigg|_{\epsilon=0}\right] = \lim_{\epsilon\to 0} \frac{\mathbb{E}[F_\epsilon] - \mathbb{E}[F]}{\epsilon}.$$

By the celebrated Girsanov theorem, the one can say that there exists a measure $\mathbb{Q}$, such that in this measure, the process $\left\{B_t + \epsilon\int_0^t h(s)ds\right\}_{t\in[0,T]}$ is translated to $\{B_t\}_{t\in[0,T]}$. The explicit relation is given below:

$$\frac{d\mathbb{Q}}{d\mathbb{P}} = \exp\left\{\epsilon I(h) - \frac{\epsilon^2}{2}||h||^2\right\}.$$

where the symbol $||h||^2 := \left(\int_0^T h^2(t)dt\right)^{1/2}$. So now we can use this fact to transfer the expectation of F_ϵ in measure $\mathbb{P}$ to an expectation of F in measure $\mathbb{Q}$.

$$\mathbb{E}_{\mathbb{P}}[F_\epsilon] = \mathbb{E}_{\mathbb{Q}}[F] = \mathbb{E}_{\mathbb{P}}\left[F \cdot \frac{d\mathbb{Q}}{d\mathbb{P}}\right],$$

so now we drop the subscript $\mathbb{P}$ under the expectations since we understand them with respect to measure $\mathbb{P}$.

$$\mathbb{E}[F_\epsilon] = \mathbb{E}\left[F \exp\left\{\epsilon I(h) - \frac{\epsilon^2}{2}||h||^2\right\}\right].$$

Substituting this identity to the expression before:

$$\begin{aligned}
\mathbb{E}[\langle DF, h\rangle] &= \lim_{\epsilon\to 0} \frac{\mathbb{E}[F_\epsilon] - \mathbb{E}[F]}{\epsilon} \\
&= \lim_{\epsilon\to 0} \frac{\mathbb{E}\left[F \exp\left\{\epsilon I(h) - \frac{\epsilon^2}{2}||h||^2\right\}\right] - \mathbb{E}[F]}{\epsilon} \\
&= \mathbb{E}\left[F \lim_{\epsilon\to 0} \frac{\exp\left\{\epsilon I(h) - \frac{\epsilon^2}{2}||h||^2\right\} - 1}{\epsilon}\right] \\
&= \mathbb{E}[FI(h)].
\end{aligned} \tag{A.6.3}$$

☐

Lemma A.6.5 can be used to prove a more general and important result, that is:

Proposition A.6.6. *Let $F, G \in \mathcal{M}$ and $h \in L^2([0,T])$, then:*

$$\mathbb{E}[\langle DF, h\rangle G] = -\mathbb{E}[F\langle DG, h\rangle] + \mathbb{E}[FGI(h)].$$

Proof. The proof is essentially the same of Lemma A.6.5 once you notice

$$\frac{d}{d\epsilon} F_\epsilon G_\epsilon \Big|_{\epsilon=0} = G_\epsilon \frac{dF_\epsilon}{d\epsilon}\Big|_{\epsilon=0} + F_\epsilon \frac{dG_\epsilon}{d\epsilon}\Big|_{\epsilon=0}.$$

☐

A.6.3 Malliavin Derivative of a More General Set of Functions

The next proposition will state the closability of the Malliavin operator D.

Proposition A.6.7. *Let $p \geq 1$. If we have a sequence $\{F_n\}_{n\geq 1}$ such that $F_n \in \mathcal{M}\, \forall n \geq 1$, which is a sequence converging to 0 in $\mathbb{L}^p(\Omega)$ and the sequence $\{DF_n\}_{n\geq 1}$ converges to a random variable η in $\mathbb{L}^p(\Omega; L^2([0,T]))$, then $\eta = 0$, $\mathbb{P} \times dt$-almost surely. In other words it is said that the operator D is closable from $\mathbb{L}^p(\Omega)$ to $\mathbb{L}(\Omega; L^2([0,T]))$, for all $p \geq 1$.*

Proof. The statement in the proposition, $\{DF_n\}_{n\geq 1}$ converges to η in $\mathbb{L}(\Omega; L^2([0,T]))$ means that:

$$\lim_{n\to\infty} \mathbb{E}(||DF_n - \eta||^p) = 0.$$

This implies that $\langle DF_n, h\rangle \to \langle \eta, h\rangle$ in $\mathbb{L}^p(\Omega; L^2([0,T]))$. Similarly:

$$\lim_{n\to\infty} \mathbb{E}[\langle DF_n, h\rangle G] = \mathbb{E}[\langle \eta, h\rangle G],$$

for all G in a dense set of $\mathbb{L}^q(\Omega)$ such that $\frac{1}{p}+\frac{1}{q}=1$.

Define $\mathcal{M}_b := \{G \in \mathcal{M} : G$ and $GI(h)$ are bounded for all $h \in L^2([0,T])\}$ and note that $\mathcal{M}_b$ is dense in $\mathbb{L}^q(\Omega)$ for all $q \in [1,\infty]$. Now use the Proposition A.6.6 to show that:

$$\begin{aligned}\mathbb{E}[\langle \eta, h\rangle G] &= \lim_{n\to\infty} \mathbb{E}[\langle DF_n, h\rangle G] \\ &= \lim_{n\to\infty} \big(-\mathbb{E}[F_n\langle DG, h\rangle] + \mathbb{E}[F_n G I(h)]\big) = 0.\end{aligned}$$

Due to the fact that F_n converges to 0. Now, because $G \in \mathcal{M}_b$ which is a dense subset of $\mathbb{L}^q(\Omega)$ for all $q \in [1,\infty]$, having $\mathbb{E}[\langle \eta, h\rangle G] = 0$ for all $G \in \mathcal{M}_b$ implies $\langle \eta, h\rangle = 0$ $\mathbb{P}$-a.s. (recall to prove $\mathbb{P}(F=0)=1$ for $F \in \mathbb{L}^p$, one can just show $\mathbb{E}[FG]=0$ for all G in a dense subset of $\mathbb{L}^q$ with $\frac{1}{p}+\frac{1}{q}=1$). Moreover since $\langle \eta, h\rangle = 0$ for all $h \in L^2([0,T])$, similarly this implies $\eta = 0$ dt-a.s. In total this means $\eta = 0$, $\mathbb{P}\times dt$-a.s. □

Now the space of Malliavin differentiable Brownian functionals will be defined.

Definition A.6.8. *For $p \geq 1$, a Brownian functional F belongs to the space $\mathbb{D}^{1,p}$, if it satisfies 2 conditions: if ∃ a sequence $\{F_n\}_{n\geq 1}$ of smooth Brownian functionals such that*

1. $F_n \xrightarrow{\mathbb{L}^p(\Omega)} F$.
2. $\{DF_n\}_{n\geq 1}$ *converges to a limit in* $\mathbb{L}^p(\Omega; L^2([0,T]))$.

In this case we call

$$DF := \lim_{n\to\infty} DF_n \quad in\, \mathbb{L}^p(\Omega; L^2([0,T])),$$

where DF is called the Malliavin derivative of F. Also note that $F \in \mathbb{D}^{1,p}$ satisfies that:

$$||F||_{1,p} := \big(\mathbb{E}[|F|^p] + \mathbb{E}[||DF||^p]\big)^{1/p} < \infty$$

.

One example would be the following:

Example A.6.9. *Note that $F := |B_t|$ and $G := e^B_t$ belongs to $\mathbb{D}^{1,p}$ for any $p \geq 1$. It should be apparent that $F; G \notin \mathcal{M}$ and that for any $p \geq 1$ we have*

$$\mathcal{M} \ni F_n = \left(\frac{1}{n} + B_t^2\right)^{1/2} \xrightarrow{\mathbb{L}^p(\Omega)} F,$$

and

$$S \ni G_n := \left(1 + \frac{B_t}{n}\right)^n \xrightarrow{\mathbb{L}^p(\Omega)} G.$$

Then we can carry on the Malliavin derivatives of smooth Brownian functionals:

$$DF_n := \frac{B_t \mathbb{1}_{[0,t]}}{\sqrt{\frac{1}{n} + B_t^2}} \xrightarrow{\mathbb{L}^p(\Omega;L^2([0,T]))} \operatorname{sgn}(B_t)\mathbb{1}_{[0,t]},$$

and

$$DG_n := \left(1 + \frac{B_t}{n}\right)^{n-1} \mathbb{1}_{[0,t]} \xrightarrow{\mathbb{L}^p(\Omega;L^2([0,T]))} e^{B_t}\mathbb{1}_{[0,t]}.$$

This way in the light of Definition A.6.8, it can be said that the Malliavin derivative of ***non****-smooth Brownian functionals F and G are defined as:*

$$DF := D|B_t| = \operatorname{sgn}(B_t)\mathbb{1}_{[0,t]}, \qquad DG := De^{B_t} = e^{B_t}\mathbb{1}_{[0,t]}.$$

Due to this relation we see explicitly one can generalize it as in Proposition A.6.10 below.

Proposition A.6.10. *Let $\psi : \mathbb{R}^m \to \mathbb{R}$ is a continuously differentiable function with bounded partial derivatives and $F = (F_1, \ldots, F_m)$ is a random vector with components in $\mathbb{D}^{1,p}$, then $\psi(F) \in \mathbb{D}^{1,p}$ and*

$$D(\psi(F)) = \sum_{i=1}^{m} (\partial_{x_i}\psi)(F) DF_i.$$

Where this definition of Malliavin derivative makes it more apparent why it is called a *derivative*.

One can also define higher order Malliavin derivatives.

Definition A.6.11. *Let $p \geq 1$ and $k \in \mathbb{N}$; a Brownian functional F belongs to the space $\mathbb{D}^{k,p}$ is there exists a sequence $\{F_n\}_{n\geq 1}$ of smooth Brownian functionals such that:*

1. $F_n \xrightarrow{\mathbb{L}^p(\Omega)} F$.
2. $\{D^j F_n\}_{n\geq 1}$ *converges to a limit in* $\mathbb{L}^p(\Omega; L^2([0,T]^j))$*, for all* $j \in \{1, \ldots, k\}$.

If so, for $j \in \{1, \ldots, k\}$ we define

$$D^j F := \lim_{n\to\infty} D^j F_n \quad \text{in } \mathbb{L}^p(\Omega; L^2([0,T])),$$

and the term $D^j F$ is called the j'th order Malliavin derivative of F. The random variables belonging to the space $\mathbb{D}^{k,p}$ satisfy the condition:

$$||F||_{k,p} := \left(\mathbb{E}[|F|^p] + \sum_{j=1}^{k} \mathbb{E}\left[||D^j F||^p_{L^2([0,T]^j)}\right]\right)^{1/p} < \infty,$$

where due to convention we set $\mathbb{D}^{0,p} := \mathbb{L}^p(\Omega)$ which results in the identity $||F||_{0,p} := \mathbb{E}[|F|^p]^{1/p}$.

The technical definition of $\mathbb{D}^{k,p}$ is the closure of $\mathcal{M}$ with respect to the norm $||\cdot||_{k,p}$. From the definition above the following inclusions can be deducted:

$$\mathbb{D}^{l,q} \subseteq \mathbb{D}^{k,p} \subseteq \mathbb{L}^{p}(\Omega) \quad \text{for } q \geq p \text{ and } l \geq k.$$

A.7 The Divergence Operator

In this section we're going to represent the adjoint operator of the Malliavin derivative operator D.

Definition A.7.1. *We plan to define the adjoint operator of D using the virtue of the inner product. For this purpose, let $\mathrm{Dom}(\delta)$ be the collection of stochastic processes $u \in \mathbb{L}(\Omega; L^2([0,T]))$ such that*

$$\mid E[\langle DG, u\rangle] \mid \leq C_u ||G||_2 \quad for\ all\ G \in \mathbb{D}^{1,2},$$

where C_u is a positive constant depending on u. If $u \in \mathrm{Dom}(\delta)$, we define $\delta(u)$ to be the unique element in $\mathbb{L}^2(\Omega)$ characterized by the identity

$$\mathbb{E}[G\delta(u)] = \mathbb{E}[\langle DG, u\rangle], \quad for\ all\ G \in \mathbb{D}^{1,2}. \tag{A.7.1}$$

The random variable $\delta(u)$ is called divergence of u and $\mathrm{Dom}(\delta)$ is the domain of the divergence operator δ.

First it should be noted that the expression (A.7.1) is the generalziation of the Lemma A.6.5 from smooth Brownian functionals to $\mathbb{D}^{1,2}$. Because this relation will be useful in the proofs of first two properties in A.7.2.

Proposition A.7.2. *Now we list properties of the divergence operator:*

1. *$L^2([0,T]) \subset \mathrm{Dom}(\delta)$ and $\delta(h) = I(h)$, for all $h \in L^2([0,T])$;*
2. *If $F \in \mathcal{M}$ and $h \in L^2([0,T])$, then $Fh \in \mathrm{Dom}(\delta)$ and*
$$\delta(Fh) = F\delta(h) - \langle DF, h\rangle. \tag{A.7.2}$$
3. *For $u, v \in \mathrm{Dom}(\delta)$ and $\alpha, \beta \in \mathbb{R}$, then $\alpha u + \beta v \in \mathrm{Dom}(\delta)$ and*
$$\delta(\alpha u + \beta v) = \alpha\delta(u) + \beta\delta(v)$$
4. *If $u \in \mathrm{Dom}(\delta)$, then $\mathbb{E}[\delta(u)] = 0$.*
5. *δ is a closed operator. Namely if $\{u_n\}_{n\geq 1} \subseteq \mathrm{Dom}(\delta)$ such that $u_n \xrightarrow{\mathbb{L}^2(\Omega;L^2([0,T]))} u$ and $\delta(u_n) \xrightarrow{\mathbb{L}(\Omega} U$, then we can say that $u \in \mathrm{Dom}(\delta)$ and $\delta(u) = U$.*

Proof. Here the proofs will be provided of the Proposition A.7.2.

1. The proof is the same with the integration by parts formula in (A.6.6).
2. First, it should be verified that $Fh \in \mathrm{Dom}(\delta)$ and then the rest will be proven. Let $G \in \mathbb{D}^{1,2}$, then the equation (A.6.6) gives

$$\begin{aligned}\mathbb{E}[\langle DG, Fh\rangle] &= \mathbb{E}[\langle DG, h\rangle F] \\ &= -\mathbb{E}[G\langle DF, h\rangle] + \mathbb{E}[GF\delta(h)] \\ &= \mathbb{E}[G\big(F\delta(h) - \langle DF, h\rangle\big)] \\ &\leq ||G||_2\, ||F\delta(h) - \langle DF, h\rangle||_2.\end{aligned} \tag{A.7.3}$$

   Which in turn, yields:

$$|\ \mathbb{E}[\langle DG, Fh\rangle]\ |\leq C_{Fh}||G||_2, \quad \text{for all } G \in \mathbb{D}^{1,2},$$

   It can be seen this inequality proves that $Fh \in \mathrm{Dom}(\delta)$. In addition to this, another consequence of expression (A.7.3), can be used to directly verify:

$$\begin{aligned}\mathbb{E}[\langle DG, Fh\rangle] = \mathbb{E}[\langle G, \delta(Fh)\rangle] &= \mathbb{E}[G\big(F\delta(h) - \langle DF, h\rangle\big)], \quad \forall\, G \in \mathbb{D}^{1,2} \\ \Rightarrow \delta(Fh) &= F\delta(h) - \langle DF, h\rangle\end{aligned}$$

3. If $u, v \in \mathrm{Dom}(\delta)$, then for all $G \in \mathbb{D}^{1,2}$, it is true that

$$|\ \mathbb{E}[\langle DG, u\rangle]\ |\leq C_u||G||_2 \quad \text{and} \quad |\ \mathbb{E}[\langle DG, v\rangle]\ |\leq C_v||G||_2.$$

   Thus,

$$\begin{aligned}|\ \mathbb{E}[\langle DG, \alpha u + \beta v\rangle]\ | &\leq |\alpha|\ |\ \mathbb{E}[\langle DG, u\rangle]\ | + |\beta|\ |\ \mathbb{E}[\langle DG, v\rangle]\ | \\ &\leq \big(|\alpha|C_u + |\beta|C_v\big)||G||_2\end{aligned}$$

   proving that $\alpha u + \beta v \in \mathrm{Dom}(\delta)$. Moreover,

$$\begin{aligned}\mathbb{E}[DG, \delta(\alpha u + \beta v)] = \mathbb{E}[\langle DG, \alpha u + \beta v\rangle] &= \alpha\mathbb{E}[\langle DG, u\rangle] + \beta\mathbb{E}[\langle DG, v\rangle] \\ &= \alpha\mathbb{E}[G\delta(u)] + \beta\mathbb{E}[G\delta(v)] = \mathbb{E}[G\big(\alpha\delta(u) + \beta\delta(v)\big)],\end{aligned}$$

   for any $G \in \mathbb{D}^{1,2}$. This gives $\delta(\alpha u + \beta v) = \alpha\delta(u) + \beta\delta(u)$.
4. The property is proven once $G = 1$ in expression (A.7.1).
5. By assumption

$$\mathbb{E}[\langle DG, u^n\rangle] = \mathbb{E}[G\delta(u^n)], \qquad \text{for all } G \in \mathbb{D}^{1,2}.$$

   The left hand side converges, as n tends to infinity, to $\mathbb{E}[\langle DG, u^n\rangle]$ and the right hand side converges to $\mathbb{E}[GU]$. Therefore,

$$\mathbb{E}[\langle DG, u\rangle] = \mathbb{E}[GU], \qquad \text{for all } G \in \mathbb{D}^{1,2},$$

   which gives $u \in \mathrm{Dom}(\delta)$ and $\delta(u) = U$.

□

Remark A.7.3. *It is worth to mention that, the divergence operator is a* generalization *of the Itô integral to non adapted processes. This means all Itô integrable stochastic processes is included in Dom*(δ)*.*

Namely if v_t *is an Itô integrable process, then:*

$$\delta(v) := \int_0^T v_t dB_t,$$

where the right hand side is the Itô integral of v_t*, interpreted as in Chapter A.2.2.*

However if a stochastic process u *is not adapted, we utilize the symbol*

$$\delta(u) = \int_0^T u_t \delta B_t.$$

The divergence operator δ *coincides with an extension of the Itô integral to non adapted stochastic processes introduced by Skorohod in 1975. This is why the divergence operator* δ *is also called* Skorohod integral.

This result is something intuitive since the adjoint operator of the Malliavin *derivative* was expected to be in some form of *integral.*

Proposition A.7.4. *Define* u_t *be a stochastic process in the form*

$$u_t := \sum_{j=1}^{n} F_j h_j(t), \quad t \in [0,T], \tag{A.7.4}$$

where $F_j \in \mathcal{M}$ *and* $h_j \in L^2([0,T])$*, for all* $j \in \{1,\ldots,n\}$*. Then,*

$$D_t\delta(u) = u_t + \delta(D_t u), \quad t \in [0,T]. \tag{A.7.5}$$

Proof. By using the expression (A.7.2) one gets:

$$\begin{aligned}\delta(u) = \delta\left(\sum_{j=1}^{n} F_j h_j\right) &= \sum_{j=1}^{n} \delta(F_j h_j) \\ &= \sum_{j=1}^{n} F_j \delta(h_j) - \sum_{j=1}^{n} \langle DF_j, h_j\rangle.\end{aligned}$$

In addition to that, note the expression:

$$D_t u_s = \sum_{j=1}^{n} D_t F_j h_j(s),$$

is also in the form of expression (A.7.4), since $D_tF \in \mathcal{M}$. Therefore:

$$\begin{aligned}
D_t\delta(u) &= D_t\left(\sum_{j=1}^{n} F_j\delta(h_j) - \sum_{j=1}^{n}\langle DF_j, h_j\rangle\right)\\
&= \sum_{j=1}^{n} D_tF_j\delta(h_j) + \sum_{j=1}^{n} F_jh_j - \sum_{j=1}^{n}\langle D_tDF_j, h_j\rangle\\
&= \sum_{j=1}^{n} F_jh_j(t) + \sum_{j=1}^{n} D_tF_j\delta(h_j) - \sum_{j=1}^{n}\langle DD_tF_j, h_j\rangle\\
&= u_t + \sum_{j=1}^{n} D_tF_j\delta(h_j) - \sum_{j=1}^{n}\Big(\delta(D_tF_jh_j) + D_tF_j\delta(h_j)\Big) \quad \text{by (A.7.2)}\\
&= u_t + \delta(D_tu).
\end{aligned}$$

□

Remark A.7.5. *The formula (A.7.5) can be extended to a wider class of processes while the identity is preserved. Essentally, when u is an Itô integrable process, formula (A.7.5) shows how to Malliavin-differentiate an Itô integral:*

$$\begin{aligned}
D_t\int_0^T u_s dB_s = D_t\delta(u) = u_t + \delta(D_tu)\\
= u_t + \int_0^T D_tu_s dB_s = u_t + \int_t^T D_tu_s dB_s.
\end{aligned}$$

due to Itô integrable processes being adapted to $\mathcal{F}_t^B$.

Where this remark is basically showing us how to take the Malliavin derivative of an Itô integral analogous to the Leibniz rule of regular calculus. So with the help of this final remark we report all the necessary tools of stochastic calculus which are required in the thesis.

A.8 Malliavin Derivative and Divergence Operator of Iterated Itô Integrals

First we mention the two notable dense subsets of $\mathbb{L}^2(\Omega)$:

$$\mathtt{F} := \left\{\sum_{n=0}^{M} I_n(h_n),\ \text{for some } M \in \mathbb{N}\cup\{0\},\ h_0 \in \mathbb{R} \text{ and } h_n \in L_s^2([0,1]^n),\ n = 1, ..., M\right\},$$

where the term $I_n(h_n)$ is the n-iterated Itô integral of function h_n, as defined in Chapter A.4. This set collects the random variables with a finite order chaos expansion, and

$$\mathtt{E} := \left\{\mathcal{E}(f) := \sum_{n\geq 0} I_n\left(\frac{f^{\otimes n}}{n!}\right),\ \text{for some } f \in L^2([0,1])\right\}, \tag{A.8.1}$$

which is the family of the so-called *stochastic exponentials*. We saw in the previous section that the Malliavin derivative acts analogously to Itô integrals as regular derivatives act to regular integrals. In this section we're going to explain how they will affect the multiple Itô integrals. The *Malliavin derivative* of $\Phi = \sum_{n=0}^{M} I_n(h_n) \in \mathtt{F}$, denoted $\{D_x\Phi\}_{x\in[0,1]}$, is the element of $L^2([0,1];\mathtt{F})$ defined by

$$D_x\Phi := \sum_{n=0}^{M-1}(n+1)I_n(h_{n+1}(\cdot,x)), \quad x \in [0,1].$$

For $l \in L^2([0,1])$ and $\Phi = \sum_{n=0}^{M} I_n(h_n) \in \mathtt{F}$, we also write

$$\begin{aligned} D_l\Phi := \langle D\Phi, l\rangle_{L^2([0,1])} &= \sum_{n=0}^{M-1}(n+1)I_n\left(\int_0^1 h_{n+1}(\cdot,y)l(y)dy\right) \\ &= \sum_{n=0}^{M-1}(n+1)I_n\left(h_{n+1}\otimes_1 l\right) \end{aligned}$$

for the *directional Malliavin derivative* of Φ along l. Here, we denote the *r-th order contraction* of h_n and h_m by $h_n \otimes_r h_m$, i.e.

$$\begin{aligned} &(h_n \otimes_r h_m)(x_1, ..., x_{n+m-2r}) \\ &:= \int_{[0,1]^r} h_n(x_1,...,x_{n-r},y_1,...,y_r)h_m(y_1,...,y_r,x_{n-r+1},...,x_{n+m-2r})dy_1\cdots dy_r. \end{aligned}$$

We have:

$$D_x\mathcal{E}(f) = f(x)\mathcal{E}(f), x\in[0,1] \qquad \text{and} \qquad D_l\mathcal{E}(f) = \langle f,l\rangle_{L^2([0,1])}\mathcal{E}(f).$$

where $\mathcal{E}(f)$ is the stochastic exponential of function f as introduced in expression (A.8.1). If we now take $l \in L^2([0,1])$, $\Phi = \sum_{n=0}^{M} I_n(h_n) \in \mathtt{F}$ and $\Psi = \sum_{n=0}^{K} I_n(g_n) \in \mathtt{F}$, we can write

$$\mathbb{E}[D_l\Phi \cdot \Psi] = \mathbb{E}[\Phi \cdot D_l^\star\Psi],$$

where

$$D_l^\star\Psi := \sum_{n=1}^{K+1} I_n(l\hat{\otimes}g_{n-1})$$

is the adjoint operator of Malliavin derivative, which we called the divergence operator in Chapter A.7. Moreover

$$(l\hat{\otimes}g_{n-1})(x_1,...,x_n) := \frac{1}{n}\sum_{i=1}^{n} f(x_i)g_{n-1}(x_1,...,x_{i-1},x_{i+1},...,x_n).$$

The following identity holds:

$$D_l^\star \Psi + D_l \Psi = \Psi \cdot I_1(l)$$

which is essentially a direct result of the expression (A.7.2) given that l is a deterministic function. Carrying on, we also introduce the act of the adjoint of D_x, denoted δ on $\Phi(\cdot)$:

$$\delta(\Phi(\cdot)) := \sum_{n=0}^{M} I_{n+1}(\tilde{h}_n) \in \mathtt{F},$$

where $\tilde{h}_n$ stands for the symmetrization of h_n with respect to the $n+1$ variables $x_1, ..., x_n, x$. It is also worth to mention that $D_l^\star \Psi$ it is sometimes written as $\Phi \diamond \delta(l)$.

A.8.1 Second Quantization Operators

Let $A : L^2([0,1]) \to L^2([0,1])$ be a bounded linear operator; for $\Phi = \sum_{n=0}^{M} I_n(h_n) \in \mathtt{F}$ we define the *second quantization operator* of A as

$$\Gamma(A)\Phi := \sum_{n=0}^{M} I_n\left(A^{\otimes n} h_n\right),$$

and the *differential second quantization operator* of A as

$$d\Gamma(A)\Phi := \sum_{n=1}^{M} I_n\left(\sum_{i=1}^{n} A_i h_n\right),$$

where A_i stands for the operator A acting on the i-th variable of h_n. Notice in addition that for A being the identity, we recover from $d\Gamma(A)$ the well known *number operator*:

$$\mathtt{N}\Phi = \sum_{n=1}^{M} n I_n\left(h_n\right).$$

The following identities hold true:

$$\begin{aligned}
&\mathbb{E}[\Gamma(A)\Phi] = \mathbb{E}[\Phi]; \quad \mathbb{E}[d\Gamma(A)\Phi] = 0;\\
&\mathbb{E}[\Gamma(A)\Phi \cdot \Psi] = \mathbb{E}[\Phi \cdot \Gamma(A^\star)\Psi]; \quad \mathbb{E}[d\Gamma(A)\Phi \cdot \Psi] = \mathbb{E}[\Phi \cdot d\Gamma(A^\star)\Psi];\\
&\Gamma(A)\mathcal{E}(f) = \mathcal{E}(Af); \quad d\Gamma(A)\mathcal{E}(f) = D_{Af}^\star \mathcal{E}(f); \quad d\Gamma(A)\Phi = \delta\left(AD.\Phi\right).
\end{aligned}$$

A.9 A Space of Generalized Random Variables

Let

$$\mathtt{F}^\star := \left\{ \sum_{n \geq 0} I_n(h_n), \text{ for some } h_0 \in \mathbb{R} \text{ and } h_n \in L_s^2([0,1]^n),\, n \geq 1 \right\}$$

be a family of *generalized* random variables. The action of $T = \sum_{n\geq 0} I_n(h_n) \in \mathtt{F}^\star$ on $\varphi = \sum_{n=0}^{M} I_n(g_n) \in \mathtt{F}$ is defined as

$$\langle\langle T, \varphi \rangle\rangle := \sum_{n=0}^{M} n! \langle h_n, g_n \rangle_{L^2([0,1]^n)}.$$

By construction, we have the inclusions

$$\mathtt{F} \subset \mathbb{L}^2(\Omega) \subset \mathtt{F}^\star$$

with

$$\langle\langle T, \varphi \rangle\rangle = \mathbb{E}[T\varphi],$$

whenever $T \in \mathbb{L}^2(\Omega)$. We will say that $T = U$ in $\mathtt{F}^\star$ if

$$\langle\langle T, \varphi \rangle\rangle = \langle\langle U, \varphi \rangle\rangle, \quad \text{for all } \varphi \in \mathtt{F}.$$

Let

$$\mathtt{F}^\star := \left\{ \sum_{n\geq 0} I_n(h_n), \text{ for some } h_0 \in \mathbb{R} \text{ and } h_n \in L_s^2([0,1]^n),\ n \geq 1 \right\}$$

be a family of *generalized* random variables. The action of $T = \sum_{n\geq 0} I_n(h_n) \in \mathtt{F}^\star$ on $\varphi = \sum_{n=0}^{M} I_n(g_n) \in \mathtt{F}$ is defined as

$$\langle\langle T, \varphi \rangle\rangle := \sum_{n=0}^{M} n! \langle h_n, g_n \rangle_{L^2([0,1]^n)}.$$

By construction, we have the inclusions

$$\mathtt{F} \subset \mathbb{L}^2(\Omega) \subset \mathtt{F}^\star$$

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$$\langle\langle T, \varphi \rangle\rangle = \mathbb{E}[T\varphi],$$

whenever $T \in \mathbb{L}^2(\Omega)$. We will say that $T = U$ in $\mathtt{F}^\star$ if

$$\langle\langle T, \varphi \rangle\rangle = \langle\langle U, \varphi \rangle\rangle, \quad \text{for all } \varphi \in \mathtt{F}.$$

Wick Product Property for Generalized Random Variables

Given two generalized random variables X and Y, their Wick product is defined to be the unique element $X \diamond Y$ such that

$$\langle\langle X \diamond Y, \mathcal{E}(f) \rangle\rangle = \langle\langle X, \mathcal{E}(f) \rangle\rangle \langle\langle Y, \mathcal{E}(f) \rangle\rangle, \quad \text{for all } f \in C_0^\infty(\mathbb{R}).$$

Where $\mathcal{E}(f)$ is the stochastic exponential as defined in expression (A.8.1).

Stroock-Taylor Formula

Lastly, we recall a generalized version of the so-called Stroock-Taylor formula: if $T = \sum_{n\geq 0} I_n(h_n) \in \mathtt{F}^\star$, then

$$h_n(x_1, ..., x_n) = \frac{1}{n!}\mathbb{E}[D_{x_1}...D_{x_n}T], \quad (x_1, ..., x_n) \in [0,1]^n. \tag{A.9.1}$$

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