

Stochastic Schrödinger Equations for Markovian and non-Markovian Cases

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(Received: September 20, 2013; Accepted: November 7, 2013; Published: February 28, 2014)

1. Introduction

Typically, an open quantum system is a system interacting with an external environment which experimentalists cannot control [1, 2, 3]. It is well known that the dynamics of an open quantum system can be described in one of the

following ways: local and non-local master equations for the density matrix [4, 5, 6], Feynman's path integrals [7], stochastic Schrödinger equations (SSE) [3, 8–11] and quantum trajectories [3, 10].

In this review we give a description of the technique based on the SSE, which can be used for the description of Markovian and non-Markovian dynamics of open quantum systems. Moreover, we shall illustrate the Markovian and non-Markovian theory by giving some simulations. In the non-Markovian case we also use the stochastic simulations to check the validity of an analytic approximation for the mean state.

The stochastic representation of quantum Markovian processes already appeared in the fundamental work by Davies [1, 12] and it was applied to the derivation of a photocounting formula. While the theory was originally formulated in terms of a stochastic process for the reduced density matrix, it was recognised by Barchielli and Belavkin [10], Dalibard, Castin and Mølmer [13] and by Dum, Zoller and Ritsch [14] that it can also be formulated as a stochastic process for the state vector in the reduced system Hilbert space and that it leads to efficient numerical simulation algorithms. At the same time, there has been considerable interest in the unravelling of master equations for density operators into quantum trajectories which are the realisations of the underlying stochastic process [3]. Just as different ensembles of state vectors may be represented by one density operator, one master equation may be decomposed in many different ways into SSEs.

The SSE is a differential equation for a wave-function process $\psi(t)$ which contains a stochastic term to describe the relaxation dynamics of an open quantum system. The link with the traditional master equation is given by the average property $\mathbb{E}[|\psi(t)\rangle\langle\psi(t)|] = \eta(t)$, where \mathbb{E} denotes the ensemble average over the realisations of process $\psi(t)$ and $\eta(t)$ is the statistical operator satisfying the master equation. To find the SSE providing a given master equation by averaging is called *unravelling* [15].

Also, in special situations, the SSE can be interpreted in terms of quantum measurements. In these cases, the solution $\psi(t)$ is called a *quantum trajectory* [16] and describes the evolution of an open system undergoing indirect continuous measurement. This interpretation is important for understanding quantum optics experiments such as direct photo-detection, spectral photo-detection, homodyning and heterodyning [17–20].

In the regime of the validity of the Markov approximation (no memory effects) [21] it is known how to construct an appropriate unravelling in terms of a SSE. It is always possible to derive a linear SSE for a non-normalised vector $\phi(t)$, such that $\psi(t) = \|\phi(t)\|^{-1} \phi(t)$. Moreover, the linear and non-linear versions of the SSE are related by a change of probability measure, and it is this link that allows for a measurement interpretation [20]. Also, these stochastic differential equations can be deduced from purely quantum evolution equations for the measured system coupled with a quantum envi-

ronment, combined with a continuous monitoring of the environment itself [22, 23, 24].

In the non-Markovian case [25, 26, 27], to find relevant SSEs describing both non-Markovian quantum evolutions and continuous monitoring is a complex task. Other than in the Markovian case, no general theory has been developed. Nevertheless, it is possible to follow a general strategy. This strategy is first to generalise directly the Markovian SSE, second to show if it provides an unravelling of a corresponding master equation, and third to check if it has a measurement interpretation [15, 28–31]. To work at the Hilbert space level guarantees automatically the complete positivity of the evolution of the statistical operator. It seems possible to adapt the Markovian approach by replacing white noises with more general noises and by allowing for random coefficients in the equation. We will show how to introduce memory effects in the SSE with the help of coloured noise. Specifically, we will illustrate the approach by replacing the Wiener process with the Ornstein–Uhlenbeck process. Such approaches are efficient for simulating corresponding non-Markovian evolutions. Also, the non-Markovian SSE is formulated in a way that allows for an interpretation in terms of measurements in continuous time.

This paper introduces the general theory of the SSE as well as the corresponding simulation techniques and is structured as follows. Section 2 describes the general theory of the SSEs in the Markovian case. It presents the general mathematical framework of the linear and non-linear SSE. We consider a linear stochastic equation with “multiplicative noise” for the wave function $\phi(t)$ in the purely diffusive case. Then, we discuss how to get the physical probabilities and we derive the non-linear SSE for the conditional states $\psi(t)$. In Sect. 3 we describe the simulation techniques for SSEs and we show the simulations for two Markovian processes, the damped harmonic oscillator and a two-level atom with homodyne photodetection. Section 4 is devoted to the introduction of coloured noise in the SSEs; we limit the presentation of this part of the theory to a restricted, but significant, class of SSEs with memory and with measurement interpretation. The simulation of such non-Markovian processes is also proposed and applied as a test of other approximation techniques. In Sect. 5 we briefly summarise the main results and indicate some directions of future work. Basic concepts from the theory of stochastic processes are summarized in Appendix A.

2. Stochastic Schrödinger Equations

In this paper we will show the approach to the theory of open quantum systems based on stochastic differential equations (SDEs), with particular emphasis on continuous measurements. In this theory there are four kinds of SDEs: the linear stochastic Schrödinger equation (LSSE), a linear SDE for

non-normalised vectors in the Hilbert space of the system (7), the SSE, a non-linear SDE for normalised vectors in the Hilbert space (18), the linear stochastic master equation [20, Sects. 3.1.2 and 3.4.1], a linear SDE for positive trace-class operators, and the stochastic master equation [20, Sects. 3.5 and 5.1], a non-linear SDE for density matrices. Two kinds of noises may appear in the SSEs and characterise the jump and the diffusive cases. Here we will focus on the diffusive case. For SSEs and SMEs of the diffusive type, a Wiener process B appears in the linear equations and a Wiener process W in the non-linear equations; B and W are connected by the Girsanov transformation (15).

To have some hints on what we will construct, let us consider an instantaneous and pure state preserving measurement of some quantity X with discrete values $\{x_k\}$.

In the Hilbert space formulation of quantum mechanics, such an observation is represented by a collection of positive operators $\{E_k\}$ such that $\sum_k E_k^\dagger E_k = \mathbb{1}$; these operators acts on \mathcal{H} , the Hilbert space of the system. The map $x_k \mapsto E_k^\dagger E_k$ is a (discrete) positive-operator valued measure, the modern generalisation of quantum observable. Let $\varphi \in \mathcal{H}$, $\|\varphi\| = 1$,

be the pre-measurement state and set $\phi_k = E_k \varphi$. Then, $\|\phi_k\|^2 \equiv \langle \varphi | E_k^\dagger E_k \varphi \rangle$ is interpreted as the probability of the result $\{X = x_k\}$ in the measurement and $\psi_k = \phi_k / \|\phi_k\|$ as the state of the system after the measurement given the result $\{X = x_k\}$. The conditional state ψ_k is often called the *a posteriori state* [20]. For the case of measurement in continuous time the output is not discrete, but it is a whole trajectory of some observed quantity; this brings into play the stochastic processes. Apart from this complication, the LSSE is an evolution equation for the analog of the non-normalised vectors ϕ_k , while the SSE is the evolution equation for the analog of the post-measurement states ψ_k . Note that the map $\varphi \mapsto \phi_k = E_k \varphi$ is linear, while the map $\phi \mapsto \psi_k$ is non-linear due to the normalisation; the same difference will characterize the passage from the LSSE to the SSE.

2.1. THE LINEAR STOCHASTIC SCHRÖDINGER EQUATION

The SDEs we consider are driven by white noise. Some notions on Wiener process and stochastic calculus are given in Appendix A, but for a full description see [32, 33] and for a summary, see [20].

First of all we work in a reference probability space $(\Omega, \mathcal{F}, \mathbb{Q})$, where Ω is the sample space, \mathcal{F} the σ -algebra of events, and \mathbb{Q} a reference probability. A

filtration is a family $(\mathcal{F}_t)_{t \geq 0}$ of increasing sub- σ -algebras of \mathcal{F} , i.e. $\mathcal{F}_s \subset \mathcal{F}_t \subset \mathcal{F}$ for $0 \leq s < t < +\infty$. Sometimes, $(\Omega, \mathcal{F}, (\mathcal{F}_t), \mathbb{Q})$ is said to be a stochastic basis. Typically, a filtration describes the accumulation of information during time: each \mathcal{F}_t is the collection of all the events which we can decide whether they have been verified or not by observations up to time t . In the basis $(\Omega, \mathcal{F}, (\mathcal{F}_t), \mathbb{Q})$ a continuous, adapted d -dimensional Wiener process

$B = \{B_j(t) : t \geq 0, j = 1, \dots, d\}$ is defined (see Appendix A.1).

Let us start from a generic homogeneous linear SDE with “multiplicative” noise for the process $\phi(t)$ [20]:

$$d\phi(t) = K(t)\phi(t) dt + \sum_{j=1}^d R_j(t)\phi(t) dB_j(t), \quad (1)$$

where $\phi(0) = \psi_0$, $\psi_0 \in \mathcal{H}$, the coefficients $R_j(t)$, $K(t)$ are (non-random) linear operators on \mathcal{H} . The SDE (1) is to be intended in integral sense and the solution ϕ is the continuous, adapted Itô process satisfying

$$\phi(t) = \psi_0 + \int_0^t K(s)\phi(s) ds + \sum_{j=1}^d \int_0^t R_j(s)\phi(s) dB_j(s).$$

The last term in the above equation is a stochastic Itô integral (see Appendix A.3).

The physical probability

To develop the theory, we need $\|\phi(t)\|^2$ to be a probability density, cf. the hints at the beginning of Sect. 2. Precisely, let us define

$$\mathbb{P}_{\psi_0}^t(F) := \int_F \|\phi(t, \omega)\|^2 \mathbb{Q}(d\omega) = \mathbb{E}_{\mathbb{Q}}[\|\phi(t)\|^2 1_F], \quad \forall F \in \mathcal{F}_t, \quad (2)$$

where 1_F is the indicator function of the set F . To guarantee that (2) defines a probability measure, we have to ask only the normalisation:

$$\mathbb{E}_{\mathbb{Q}}[\|\phi(t)\|^2] = 1, \quad \forall t \geq 0. \quad (3)$$

Since observations in the future cannot change the probabilities of past events, we need to ensure that a consistency property holds:

$$\mathbb{P}_{\psi_0}^t(F) = \mathbb{P}_{\psi_0}^s(F), \quad \forall F \in \mathcal{F}_s, \quad \forall t, s \quad t \geq s \geq 0. \quad (4)$$

This is equivalent to asking $\|\phi(t)\|^2$ to be a \mathbb{Q} -martingale (Appendix A.2). Then, its mean is a constant and the normalisation for every time reduces to the normalisation of the initial state ψ_0 .

Using Itô’s lemma (Appendix A.4) for $d\|\phi(t)\|^2$ we can derive as in [20, Sect. 2.2.3]:

$$\begin{aligned} \|\phi(t)\|^2 &= \|\psi_0\|^2 + \int_0^t \langle \phi(s) | (K(s) + K(s)^\dagger + \sum_j R_j(s)^\dagger R_j(s)) \phi(s) \rangle ds \\ &\quad + \sum_{j=1}^d \int_0^t \langle \phi(s) | (R_j(s) + R_j(s)^\dagger) \phi(s) \rangle dB_j(s). \end{aligned} \quad (5)$$

In order to reduce $\|\phi(t)\|^2$ to a martingale, we need the integrand in the time integral in (5) to vanish for every initial condition, i.e.

$$K(t) + K(t)^\dagger + \sum_j R_j(t)^\dagger R_j(t) = 0.$$

Then, the operator $K(t)$ has the structure

$$K(t) = -iH(t) - \frac{1}{2} \sum_{j=1}^d R_j(t)^\dagger R_j(t), \quad (6)$$

where $H(t)$ is a self-adjoint operator on \mathcal{H} , called the *effective Hamiltonian* of the system.

The LSSE

Finally, the *linear stochastic Schrödinger equation* (diffusive type) is given by

$$d\phi(t) = \left(-iH(t) - \frac{1}{2} \sum_{j=1}^d R_j(t)^\dagger R_j(t) \right) \phi(t) dt + \sum_{j=1}^d R_j(t) \phi(t) dB_j(t), \quad (7)$$

$$\phi(0) = \psi_0, \quad \psi_0 \in \mathcal{H}, \quad \|\psi_0\| = 1, \quad H(t) = H(t)^\dagger. \quad (8)$$

The linear stochastic Schrödinger equation (7) reduces to an ordinary Schrödinger equation $d\phi(t)/dt = -iH(t)\phi(t)$ when we switch off the measurement and the interactions with the environment ($R_j(t) \equiv 0$).

2.2. THE A POSTERIORI STATES, THE OUTPUT AND THE MASTER EQUATION

Let us consider now a finite time interval $[0, T]$; the current time t will always be inside this interval. We also introduce the normalised version $\psi(t)$ of the vector $\phi(t)$:

$$\psi(t) = \frac{\phi(t)}{\|\phi(t)\|}. \quad (9)$$

Then, the interpretation of the theory is similar to the hints given at the beginning of Sect. 2 and it is given below.

1. The physical probability of the events occurring up to time T is $\mathbb{P}_{\psi_0}^T$. By the consistency property (4) the choice of T is immaterial.
2. The cumulated output of the continuous measurement is the d -dimensional process B and its distribution is given by the physical probability,

so that it is no more a Wiener process. More precisely the output in any time interval $[s, t]$ is $B(t) - B(s)$, so that the instantaneous output is the formal time derivative $\dot{B}(t)$. The structure of the output under the physical probability is given in (16).

3. The normalised vector $\psi(t)$ (9) is the *a posteriori state*, i.e. the conditional state of the system at time t given the observed output up to time t . The evolution of $\psi(t)$ is given by the SSE (18).

Let us introduce now the average state

$$\eta(t) = \mathbb{E}_{\mathbb{P}_{\psi_0}^T} [|\psi(t)\rangle\langle\psi(t)|] \equiv \int_{\Omega} |\psi(t, \omega)\rangle\langle\psi(t, \omega)| \mathbb{P}_{\psi_0}^T(d\omega), \quad T \geq t \geq 0. \quad (10)$$

Note that, by construction, $\eta(t)$ is a positive operator and that, by the normalisation of $\psi(t)$, one has $\text{Tr}\{\eta(t)\} = 1$, so that $\eta(t)$ is a statistical operator.

4. The statistical operator $\eta(t)$ is the state we attribute to the system at time t , when the output is not known; it is called the *a priori state* and satisfies the master equation (12).

By the consistency property (4) we can take $T = t$. Then, by the fact that $\mathbb{P}_{\psi_0}^T(d\omega) = \|\phi(t, \omega)\|^2 \mathbb{Q}(d\omega)$ and

$$\|\phi(t, \omega)\|^2 |\psi(t, \omega)\rangle\langle\psi(t, \omega)| = |\phi(t, \omega)\rangle\langle\phi(t, \omega)|,$$

we get the equivalent expression

$$\eta(t) = \mathbb{E}_{\mathbb{Q}}[|\phi(t)\rangle\langle\phi(t)|] \equiv \int_{\Omega} |\phi(t, \omega)\rangle\langle\phi(t, \omega)| \mathbb{Q}(d\omega). \quad (11)$$

By computing the stochastic differential of $|\phi(t)\rangle\langle\phi(t)|$ and by taking the \mathbb{Q} -mean of the resulting equation one gets the *master equation*

$$\dot{\eta}(t) = \mathcal{L}(t)[\eta(t)], \quad (12a)$$

$$\mathcal{L}(t)[\varrho] = -i[H(t), \varrho] + \sum_{j=1}^d \left(R_j(t) \varrho R_j(t)^\dagger - \frac{1}{2} \left\{ R_j(t)^\dagger R_j(t), \varrho \right\} \right). \quad (12b)$$

Note that the Liouville operator $\mathcal{L}(t)$ turns out to be in the usual Lindblad form.

From (5) with condition (6) and the normalization of ψ_0 , we get [20, Sect. 2.3.1], by the rules of stochastic calculus,

$$\|\phi(t)\|^2 = \exp \left\{ \sum_j \int_0^t m_j(s) dB_j(s) - \frac{1}{2} \int_0^t m_j(s)^2 ds \right\}, \quad (13)$$

$$m_j(t) = 2\text{Re}\langle\psi(t)|R_j(t)\psi(t)\rangle. \quad (14)$$

Then, Girsanov theorem gives that under the probability $\mathbb{P}_{\psi_0}^T$ the process

$$W_j(t) = B_j(t) - \int_0^t m_j(s) ds, \quad j = 1, \dots, d, \quad t \in [0, T], \quad (15)$$

is a d -dimensional Wiener process [20, Sects 2.3.2 and A.5.4]. Clearly we can write

$$B_j(t) = W_j(t) + \int_0^t m_j(s) ds. \quad (16)$$

We can say that the instantaneous output $\dot{B}_j(t)$ is the sum of the white noise $\dot{W}_j(t)$ and the regular process $m_j(t)$ (the signal). However, let us stress that white noise and signal are not in general independent under the physical probability.

The theory of continuous measurements gives also all the correlations of the output process [20, Sect. 4.3]. In particular, by taking the mean of both sides in (16) and taking into account (10) and (14), we obtain the mean of the output

$$\mathbb{E}_{\mathbb{P}_{\psi_0}^T} [B_j(t)] = \text{Tr}\{(R_j(t) + R_j(t)^\dagger)\eta(t)\}. \quad (17)$$

This equation suggests to interpret the j -th output as a continuous indirect monitoring of the system quantum observable $R_j(t) + R_j(t)^\dagger$. However, the final interpretation depends on the specific model. The output B_j could also represent the photocurrent in homodyne or heterodyne detection; in this case the system operator $R_j(t)$ depends on the interaction with the electromagnetic field and on the local oscillator wave. The channel j could also represent a pure dissipative effect due to the environment; in this case $B_j(t)$ is not observed and the role of this channel is only for introducing a dissipative contribution into the Liouville operator (12b).

2.3. THE NON-LINEAR STOCHASTIC SCHRÖDINGER EQUATION

By using the rules of Itô calculus and the LSSE, it is possible to compute the stochastic differential of the *a posteriori state* $\psi(t) = \|\phi(t)\|^{-1} \phi(t)$. By expressing the result in terms of the new Wiener process (15), the final result is the SSE

$$\begin{aligned} d\psi(t) &= \sum_j \left[R_j(t) - \frac{1}{2} m_j(t) \right] \psi(t) dW_j(t) \\ &+ \left[-iH(t) - \frac{1}{2} \sum_j R_j(t)^\dagger R_j(t) + \frac{1}{2} \sum_j m_j(t) R_j(t) - \frac{1}{8} \sum_j m_j(t)^2 \right] \psi(t) dt. \end{aligned} \quad (18)$$

As $m_j(t)$ (14) is a bilinear function of $\psi(t)$, the SSE (18) turns out to be a closed SDE for the process $\psi(t)$ under the probability $\mathbb{P}_{\psi_0}^T$ [20, Sect. 2.5.1].

Let us note that the master equation (12) is invariant under the transformation $R_j(t) \rightarrow e^{i\theta_j} R_j(t)$. However, this is not true for the LSSE (7), the SSE (18) and the output (16). Indeed, $m_j(t)$ (14) and its mean (17) are sensible to the phase of $R_j(t)$. So, the *a posteriori* states and the output depend on a phase shift in the operators of the dissipative part, while the mean dynamics is independent from such phases.

It is also possible to start from the SSE (18). In this case W is a Wiener process under a probability \mathbb{P} , which is directly the physical probability. Then, the output is defined by (16) and (14) and a LSSE can be introduced by a change of normalisation and of probability [20, Sect. 2.5.4]. A characteristic feature of the non-linear SSEs is to preserve the normalisation of the state $\psi(t)$.

2.4. THE CASE OF A RANDOM UNITARY EVOLUTION

A very particular case is when all the operators $R_j(t)$ are anti-selfadjoint:

$$R_j(t) = -iV_j(t), \quad V_j(t)^\dagger = V_j(t). \quad (19)$$

Then, (2), (9), (13), (14), (16) give $m_j(t) = 0$, $\|\phi(t)\|^2 = 1$, $\psi(t) = \phi(t)$, $\mathbb{P}_{\psi_0}^T = \mathbb{Q}$, $W_j(t) = B_j(t)$. This means that the B_j are pure noises and there is no true measurement on the system. Moreover, the LSSE and the non-linear one coincide and give a random unitary evolution:

$$d\psi(t) = -i\left[H(t)dt + \sum_j V_j(t) dW_j(t)\right]\psi(t) - \frac{1}{2} \sum_j V_j(t)^2 \psi(t) dt. \quad (20)$$

Formally, $H(t) + \sum_j V_j(t) \dot{W}_j(t)$ is the random Hamiltonian which generates the unitary evolution. The last term is the Itô correction due to the presence of the white noise $\dot{W}_j(t)$ in the formal Hamiltonian. This class of SSEs was introduced as a model of dissipative evolution, without observation. In this case, all the physical quantities are obtained as a mean with respect to W [34].

3. Simulating SSEs for the Markovian Case

The idea of unravelling has been a real breakthrough for simulating master equations; it is at the root of the Monte-Carlo wave function method [2, 25, 35, 36]. The basic idea of these methods is to generate independent realisations of the underlying stochastic process by a numerical algorithm and to estimate, with the help of statistical means, all desired expectation values from a sample

of such realisations. A stochastic simulation thus amounts to perform an experiment on a computer. It yields the outcomes of single runs with their correct probabilities and provides, in addition to the mean values, estimates for the statistical errors of the quantities of interest.

Let us consider the SSE (18) for the *a posteriori states* $\psi(t)$, with a standard Wiener process W in a stochastic basis $(\Omega, \mathcal{F}, (\mathcal{F}_t), \mathbb{P})$.

A stochastic simulation algorithm serves to generate a sample of independent realisations of the stochastic process $\psi(t)$ for the conditional wave function. Let us denote these realisations by $\psi^r(t)$, $r = 1, 2, \dots, R$, where R is the number of realisations in the sample. A quantity of interest can be thought as a real functional $F[\psi, t]$ of the *a posteriori states* $\psi(s)$, $s \in [0, t]$; then, let

$$M_t = \mathbb{E}_{\mathbb{P}}[F[\psi, t]] \quad (21)$$

be its mean value. An *unbiased and consistent estimator* for the expectation value M_t is provided by the *sample mean*

$$\widehat{M}_t = \frac{1}{R} \sum_{r=1}^R F[\psi^r, t], \quad (22)$$

where a hat is used to indicate an estimator. It is clear that the estimate is subjected to statistical errors. A natural measure of the goodness of an estimator is its *mean square error*, which coincides with its variance in the case of an unbiased estimator. By the independence of the realisations we have

$$\text{MSE}_{\widehat{M}_t} = \text{Var}_{\mathbb{P}}[\widehat{M}_t] = \frac{\text{Var}_{\mathbb{P}}[F[\psi, t]]}{R}, \quad (23)$$

$$\text{Var}_{\mathbb{P}}[F[\psi, t]] = \mathbb{E}_{\mathbb{P}} \left[(F[\psi, t] - M_t)^2 \right] = \mathbb{E}_{\mathbb{P}} [F[\psi, t]^2] - M_t^2. \quad (24)$$

Clearly, $\text{Var}_{\mathbb{P}}[F[\psi, t]]$ is a theoretical quantity and needs to be estimated; its natural unbiased estimator is the *sample variance*. At the end, the natural unbiased estimator of the mean square error is

$$\begin{aligned} \widehat{\sigma}_t^2 &= \widehat{\text{MSE}}_{\widehat{M}_t} = \frac{1}{R(R-1)} \sum_{r=1}^R \left(F[\psi^r, t] - \widehat{M}_t \right)^2 \\ &= \frac{1}{R-1} \left(\frac{1}{R} \sum_r F[\psi^r, t]^2 - \widehat{M}_t^2 \right). \end{aligned}$$

The quantity $\widehat{\sigma}_t$ is known as the *sample standard error* of the estimate of the mean value M_t . If the realisations in the sample are statistically independent, as we have assumed, and $\text{Var}_{\mathbb{P}}[F[\psi, t]]$ is finite, the standard error $\widehat{\sigma}_t$ decreases

with the square root of the sample size R :

$$\widehat{\sigma}_t \sim \frac{1}{\sqrt{R}}. \quad (25)$$

Of particular interest are the *a posteriori* quantum expectation values of some selfadjoint operator C : $F[\psi, t] = \langle \psi(t) | C \psi(t) \rangle$. Note that to have these quantities for any C in a basis in the space of the bounded selfadjoint operators is equivalent to give all the matrix elements of the *a posteriori state* $\rho(t) = |\psi(t)\rangle\langle\psi(t)|$. By (10) and (21) we get

$$M_t = \mathbb{E}_{\mathbb{P}}[\langle \psi(t) | C \psi(t) \rangle] = \text{Tr} \{ C \eta(t) \}. \quad (26)$$

Now the estimator of M_t takes the form

$$\widehat{M}_t = \frac{1}{R} \sum_{r=1}^R \langle \psi^r(t) | C \psi^r(t) \rangle, \quad (27)$$

and the estimator of its mean square error becomes

$$\widehat{\sigma}_t^2 = \frac{1}{R(R-1)} \sum_{r=1}^R \left(\langle \psi^r(t) | C \psi^r(t) \rangle - \widehat{M}_t \right)^2. \quad (28)$$

Let us stress that the sample standard error $\widehat{\sigma}_t$ is a measure of the statistical fluctuations, not of the numerical errors in the simulations, such that the ones due to approximations or to the discretisation of the time in solving the evolution equation.

3.1. HOMODYNE PHOTODETECTION

Let us consider as a first example the stochastic Schrödinger equation corresponding to homodyne photodetection [2] of the light emitted by a two-level atom stimulated by a perfectly coherent laser in resonance with the atomic frequency [20, Sects. 8.1.3.2 and 9.2]. We consider the ideal case in which all the emitted light is detected and no other dissipative contribution is present, apart from the emission of light.

Let $|1\rangle$ ($|0\rangle$) be the excited (ground) state and let $\sigma_x, \sigma_y, \sigma_z$ be the usual Pauli matrices and σ_- and σ_+ be the lowering and rising operators; then, $\sigma_+ + \sigma_- = \sigma_x$, $i(\sigma_- - \sigma_+) = \sigma_y$ and $\sigma_+\sigma_-$ is the projection on the excited state.

The model we are considering is determined by the SSE (18), (14) with $d = 1$,

$$H(t) = \frac{\omega_0}{2} \sigma_z - \frac{\Omega_R}{2} (e^{i\omega_0 t} \sigma_- + e^{-i\omega_0 t} \sigma_+), \quad \omega_0 > 0, \quad \Omega_R \geq 0, \quad (29a)$$

$$R(t) = \sqrt{\gamma} e^{i(\omega_0 t + \theta)} \sigma_-, \quad \gamma > 0. \quad (29b)$$

In this model the frequencies of the atom, of the stimulating laser and of the local oscillator are equal and given by ω_0 ; Ω_R is the *Rabi frequency* (Ω_R^2 is proportional to the laser intensity), γ is the *natural linewidth* of the atom ($1/\gamma$ is the relaxation time) and θ is the phase shift of the local oscillator with respect to the emitted light. Homodyne detection is sensitive to θ , as discussed in Sect. 2.3. Here, we take $\theta = \pi/2$.

The explicit time dependencies can be eliminated by a unitary transformation:

$$\check{\psi}(t) := \exp\left\{\frac{i}{2}\omega_0\sigma_z t\right\}\psi(t). \quad (30)$$

Then, by (14), (18), (29) we get the SSE in the rotating frame:

$$\begin{aligned} d\check{\psi}(t) &= -iH_L\check{\psi}(t)dt + \frac{\gamma}{2}\left(m_y(t)i\sigma_- - \sigma_+\sigma_- - \frac{1}{4}m_y(t)^2\right)\check{\psi}(t)dt \\ &\quad + \sqrt{\gamma}\left(i\sigma_- - \frac{1}{2}m_y(t)\right)\check{\psi}(t)dW(t), \end{aligned} \quad (31)$$

$$H_L = -\frac{\Omega_R}{2}\sigma_x, \quad m_y(t) = \langle\check{\psi}(t)|\sigma_y\check{\psi}(t)\rangle. \quad (32)$$

Moreover, by (16) and (14), the cumulated output (the integrated *homodyne photocurrent*) is given by

$$B(t) = W(t) + \sqrt{\gamma}\int_0^t m_y(s)ds. \quad (33)$$

The master equation corresponding to the SSE (31) is

$$\frac{d\check{\eta}(t)}{dt} = \check{\mathcal{L}}[\check{\eta}(t)], \quad \check{\mathcal{L}}[\varrho] = \frac{i\Omega_R}{2}[\sigma_x, \varrho] + \gamma\sigma_-\varrho\sigma_+ - \frac{\gamma}{2}\{\sigma_+\sigma_-, \varrho\}. \quad (34)$$

This equation can be easily solved [2] and we get, with the initial condition $\eta(0) = |0\rangle\langle 0|$ and $\Omega_R^2 > \gamma^2/16$, [20, Sect. 8.2.2.2]

$$\eta(t)_{11} = \langle 1|\eta(t)|1\rangle = v_+e^{-a+t} + v_-e^{-a-t} + \frac{\Omega_R^2}{2\Omega_R^2 + \gamma^2}, \quad (35)$$

$$\text{Tr}\{\sigma_y\eta(t)\} = u_+e^{-a+t} + u_-e^{-a-t} - \frac{\Omega_R\gamma}{\Omega_R^2 + \gamma^2/2}, \quad \text{Tr}\{\sigma_x\eta(t)\} = 0, \quad (36)$$

$$u_{\pm} = \frac{\Omega_R\left[\gamma\sqrt{\Omega_R^2 - \gamma^2/16} \mp i(\Omega_R^2 - \gamma^2/4)\right]}{\sqrt{\Omega_R^2 - \gamma^2/16}(2\Omega_R^2 + \gamma^2)},$$

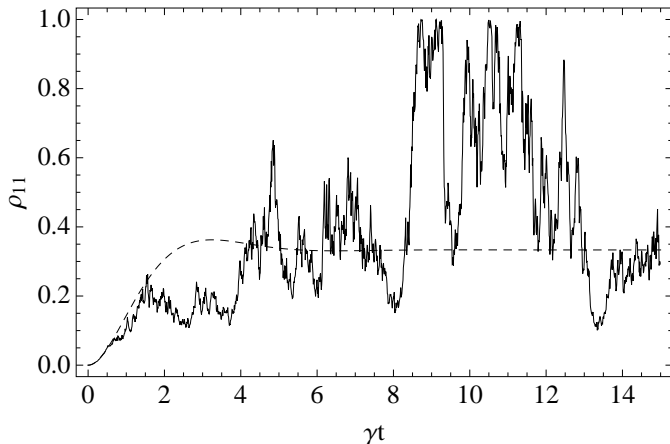


Fig. 1: A single realisation of the occupation of the excited state $\rho_{11} = |\langle 1|\check{\psi}(t)\rangle|^2$ computed from (38) for the parameters: $\Omega_R = 1$, $\gamma = 1$, $\Delta t = 0.01$. The dashed line is the plot of the component $\eta(t)_{11}$ of the exact solution (35).

$$v_{\pm} = \frac{\Omega_R^2 \left(\mp 3i\gamma/4 - \sqrt{\Omega_R^2 - \gamma^2/16} \right)}{2\sqrt{\Omega_R^2 - \gamma^2/16} (2\Omega_R^2 + \gamma^2)},$$

$$a_{\pm} = \frac{3}{4}\gamma \pm i\sqrt{\Omega_R^2 - \frac{\gamma^2}{16}}.$$

Note that

$$\mathbb{E}_{\mathbb{P}}[B(t)] = \sqrt{\gamma} \int_0^t \text{Tr}\{\sigma_y \eta(s)\} ds. \quad (37)$$

To simulate this model we use the Euler algorithm to get an approximation for the state vector $\check{\psi}$, with a correction to maintain the normalisation. We discretise the time and set $t_n = n\Delta t$; then, the algorithm takes the form

$$\psi_{n+1} = \check{\psi}_n + A_1(\check{\psi}_n)\Delta t + A_2(\check{\psi}_n)\Delta W_n, \quad (38a)$$

$$\check{\psi}_{n+1} = \frac{\psi_{n+1}}{\|\psi_{n+1}\|}, \quad (38b)$$

where $\Delta W_n = W(t_{n+1}) - W(t_n) = Z_n\sqrt{\Delta t}$, Z_0, \dots, Z_n, \dots is a sequence of independent random variables with standard normal distribution, and the functions A_1, A_2 are given by

$$A_1(\psi) = -iH_L\psi + \frac{\gamma}{2} \left(\langle \psi | \sigma_y \psi \rangle i\sigma_- - \sigma_+ \sigma_- - \frac{1}{4} \langle \psi | \sigma_y \psi \rangle^2 \right) \psi, \quad (38c)$$

$$A_2(\psi) = \sqrt{\gamma} \left(i\sigma_- - \frac{1}{2} \langle \psi | \sigma_y \psi \rangle \right) \psi. \quad (38d)$$

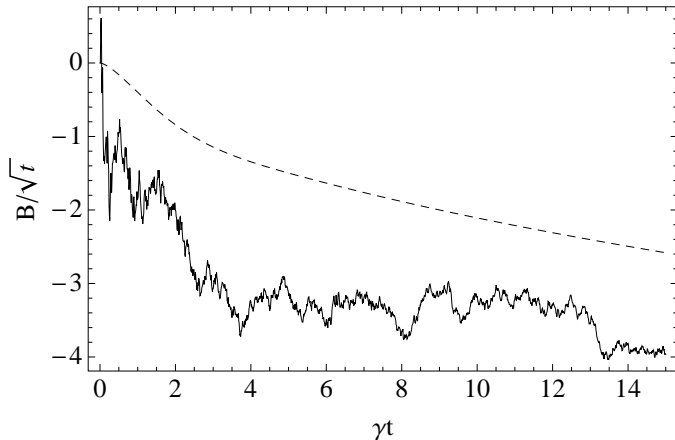


Fig. 2: A single realisation of the output $B(t)/\sqrt{t}$ computed from (39) and the plot of the mean output from (37) and (36) for the parameters: $\Omega_R = 1$, $\gamma = 1$, $\Delta t = 0.01$.

As initial condition we take the ground state

$$\check{\psi}_0 = \psi_0 = |0\rangle. \quad (38e)$$

By construction, ψ_n is an approximation of $\check{\psi}(t_n)$, so that

$$\psi(t_n) \simeq \exp\left\{-\frac{i}{2}\omega_0 t_n \sigma_z\right\}\psi_n.$$

Correspondingly, by (33), the approximation of the integrated homodyne current is

$$B(t_n) \simeq B_n = \sum_{k=0}^{n-1} (\Delta W_k + \sqrt{\gamma}\langle\psi_k|\sigma_y\psi_k\rangle\Delta t). \quad (39)$$

Let us note that, by the properties of the Wiener process, $\Delta W_n/\sqrt{\Delta t}$, $n = 1, 2, \dots$, is a sequence of independent and identically distributed random variables with standard normal distribution.

The results of the simulation are shown in Figs. 1–3. A single realisation is shown in Fig. 1 for the occupation of the excited state. In Fig. 2 we plot a single realisation of the output and, for comparison, its mean. Finally, in Fig. 3 we analyse the dependence of the simulation algorithm on the time step size. It is clearly seen that the quality of the simulation with the help of Euler algorithm decreases with increasing time step. In principle, extrapolation techniques can correct the results. However, it is more efficient to use the higher order scheme such as the Platen scheme as we shall demonstrate in the next section.

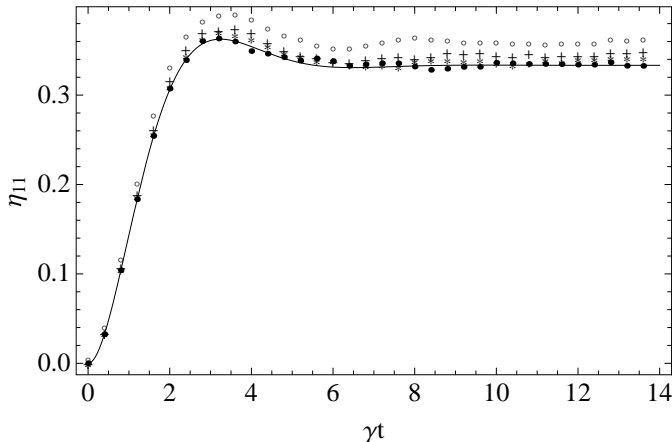


Fig. 3: The average over 10^4 realisations of the homodyne photodetection (31) for the driven two-level atom. The realisations are computed with the Euler algorithm for the parameters $\Omega = 1$, $\gamma = 1$. The dots show η_{11} computed from the average over the realisations for the different sizes of time steps $\Delta t_1 = 0.01$ (dots), $\Delta t_2 = 0.05$ (stars), $\Delta t_3 = 0.1$ (pluses) and $\Delta t_4 = 0.2$ (circles). The solid line represents the analytical solution for η_{11} according to (35). The statistical errors have the same size as the graphic symbols used in the figure.

3.2. DAMPED HARMONIC OSCILLATOR

Another typical example of an open system in the Markovian regime is the stochastic Schrödinger equation (18) for the damped harmonic oscillator [2, Sect. 7.3.1.2]:

$$\begin{aligned}
 d\psi(t) &= \frac{\gamma}{2} \left(\langle a + a^\dagger \rangle_{\psi(t)} a - a^\dagger a - \frac{1}{4} \langle a + a^\dagger \rangle_{\psi(t)}^2 \right) \psi(t) dt \\
 &\quad + \sqrt{\gamma} \left(a - \frac{1}{2} \langle a + a^\dagger \rangle_{\psi(t)} \right) \psi(t) dW(t), \quad (40) \\
 \langle a + a^\dagger \rangle_\psi &= \langle \psi | (a + a^\dagger) \psi \rangle.
 \end{aligned}$$

The SSE (40) could be obtained as (31) by considering a harmonic oscillator with homodyning and by performing a unitary transformation. However, here the interest in this model is mainly to use it for introducing a higher order numerical scheme.

As an example, the initial state is taken to be $\psi_0 = |n_0 = 9\rangle$ (a pure Fock state with 9 photons) and the Hilbert space has been truncated at $n_{\max} = 12$ which means that the simulation was performed in a subspace of dimension $N = 13$. The size of the time steps is $\Delta t = 0.02$. To simulate this model we

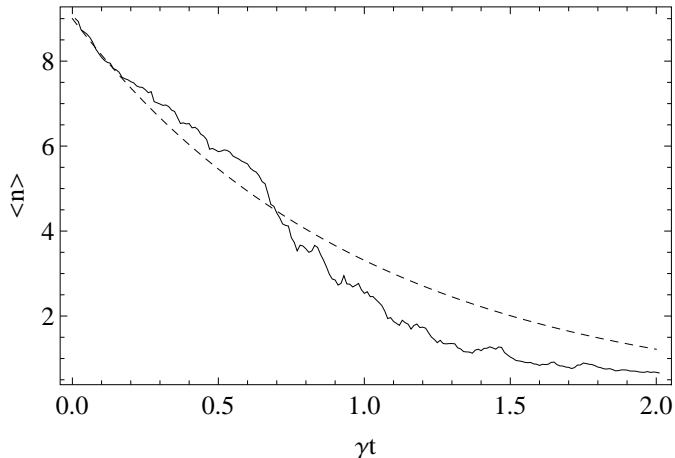


Fig. 4: A single realisation of the damped harmonic oscillator for the a posteriori expectation of $n = a^\dagger a$ computed from (40) with parameters: $\gamma = 1$ and $\Delta t = 0.01$. The initial condition is $|n_0 = 9\rangle$. The dashed line shows the exact solution for the master equation associated to the SSE (40) according to [2].

use the second-order weak scheme of Platen [2]. This algorithm has the form

$$\begin{aligned} \psi_{n+1} &= \psi_n + \frac{1}{2} \left(D_1(\tilde{\psi}_n) + D_1(\psi_n) \right) \Delta t \\ &\quad + \frac{1}{4} \left(D_2(\psi_n^+) + D_2(\psi_n^-) + 2D_2(\psi_n) \right) \Delta W_n \\ &\quad + \frac{1}{4} \left(D_2(\psi_n^+) - D_2(\psi_n^-) \right) \{ (\Delta W_n)^2 - \Delta t \} \Delta t^{-1/2}, \end{aligned}$$

where

$$\begin{aligned} \tilde{\psi}_n &= \psi_n + D_1(\psi_n) \Delta t + D_2(\psi_n) \Delta W_n, \\ \psi_n^\pm &= \psi_n + D_1(\psi_n) \Delta t \pm D_2(\psi_n) \sqrt{\Delta t}. \end{aligned}$$

For the model under consideration the functions D_1 and D_2 are

$$\begin{aligned} D_1(\psi) &= \frac{\gamma}{2} \left(\langle a + a^\dagger \rangle_\psi a - a^\dagger a - \frac{1}{4} \langle a + a^\dagger \rangle_\psi^2 \right) \psi, \\ D_2(\psi) &= \sqrt{\gamma} \left(a - \frac{1}{2} \langle a + a^\dagger \rangle_\psi \right) \psi. \end{aligned}$$

A single realisation for the damped harmonic oscillator is shown in Fig. 4. The number of photons, computed from the average of 1000 realisations is shown in Fig. 5.

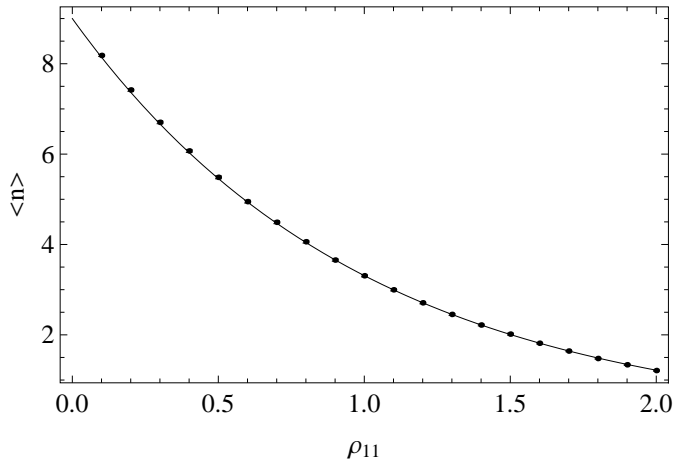


Fig. 5: The average over 1000 realisations of the damped harmonic oscillator by (40). The dots show $\langle n \rangle$ (the mean number of photons) computed from the average over the realisations. The continuous line represents the analytical solution for $\langle n \rangle$ according to [2]. The simulation was performed for the following parameters: $\gamma = 1$ and $\Delta t = 0.01$ with the initial condition $|n_0 = 9\rangle$. The statistical errors have the same size as the dots.

4. SSEs with Memory Effects

One of the methods for the introduction of memory effects in the system is to start from the LSSE (7), but with random coefficients $H(t)$, $R_j(t)$ and with the white noise replaced by some coloured noise. In this way we get memory in the dynamical equations, while complete positivity of the dynamical maps and the continuous measurement interpretation are preserved [15, 29, 30].

In this section we limit our presentation to a very particular case of non-Markovian SSE: we start with a LSSE driven by a coloured noise with coefficients depending on this noise at most linearly. The noise is chosen to be the Ornstein-Uhlenbeck (O-U) process. The big difference is that the *a priori* state does not satisfy a usual master equation as (12), but a generalised one which can be obtained by the Nakajima-Zwanzig projection method.

After the presentation of the theory, we use this model to illustrate two methods of numerical approximations: the simulation of the SSE and an approximation derived in [30] based on the Nakajima-Zwanzig projection method.

4.1. THE SSE WITH COLOURED NOISE

Let us consider a one-dimensional driving noise $X(t)$ and three non-random operators C , D and R on \mathcal{H} . The starting point is the basic linear stochastic

Schrödinger equation

$$d\phi(t) = (C + DX(t))\phi(t) dt + R\phi(t) dX(t). \quad (41)$$

For $X(t)$ we take the stationary O-U process. Such a process is defined by

$$X(t) = e^{-kt} \frac{Z}{\sqrt{2k}} + \int_0^t e^{-k(t-s)} dB(s), \quad k > 0, \quad (42)$$

where $B(t)$ is a one-dimensional Wiener process, defined on the stochastic basis $(\Omega, \mathcal{F}, (\mathcal{F}_t), \mathbb{Q})$, and Z is a standard normal random variable (mean 0 and variance 1); Z is \mathcal{F}_0 -measurable, which means that it is independent of the Wiener process. The O-U process $X(t)$ is a Gaussian process with zero mean and correlation function

$$\mathbb{E}_{\mathbb{P}}[X(t)X(s)] = \frac{e^{-k|t-s|}}{2k}. \quad (43)$$

It satisfies the stochastic differential equation

$$dX(t) = -kX(t) dt + dB(t), \quad X(0) = Z/\sqrt{2k}. \quad (44)$$

The formal derivative of the O-U process, which we shall take as driving noise for the new SSE, has a two-time correlation which is no more a δ -function, as in the case of white noise, but it has the expression

$$\mathbb{E}_{\mathbb{P}}[\dot{X}(t)\dot{X}(s)] = \delta(t-s) - \frac{k}{2} e^{-k|t-s|}.$$

Note that the white noise is recovered in the limit $k \downarrow 0$.

It is then straightforward that (41) can be rewritten in the form

$$d\phi(t) = (C + X(t)D - kX(t)R)\phi(t) dt + R\phi(t)dB(t), \quad (45)$$

the initial condition is a wave function $\psi_0 \in \mathcal{H}$, such that $\|\psi_0\|^2 = 1$.

As discussed in Sect. 2.1 for the Markovian case, to construct consistent probabilities we need the process $\|\phi(t)\|^2$ to be a martingale. By Itô calculus rules (see Appendix A.4), the stochastic differential of $\|\phi(t)\|^2$ turns out to be

$$\begin{aligned} d\langle\phi(t)|\phi(t)\rangle &= \langle d\phi(t)|\psi(t)\rangle + \langle d\phi(t)|d\phi(t)\rangle + \langle\phi(t)|d\phi(t)\rangle \\ &= \langle\phi(t)|\left[C^\dagger + C + X(t)(D^\dagger + D - kR - kR^\dagger) + R^\dagger R\right]\psi(t)\rangle dt \\ &\quad + \langle\phi(t)|(R^\dagger + R)\phi(t)\rangle dB(t). \end{aligned} \quad (46)$$

Then, the process $\|\phi(t)\|^2$ can be a martingale only if the term in front of dt is equal to zero. For it we must have for all t

$$C^\dagger + C + R^\dagger R = X(t)(kR^\dagger + kR - D^\dagger - D),$$

which implies $D^\dagger + D = kR^\dagger + kR$ and $C^\dagger + C + R^\dagger R = 0$. These conditions impose that there are two self-adjoint operators K and H_0 such that

$$D = -iK + \frac{k}{2}(R + R^\dagger), \quad C = -iH_0 - \frac{1}{2}R^\dagger R. \quad (47)$$

As a consequence the initial equation (41) becomes

$$d\phi(t) = \left(-iH(t) - \frac{1}{2}R^\dagger R \right) \phi(t) dt + R\phi(t) dB(t), \quad (48a)$$

$$H(t) := H_0 + X(t)L, \quad L := K + \frac{ik}{2}(R^\dagger - R). \quad (48b)$$

We are in the same situation of the LSSE (7), however, there is now some extra randomness introduced by the term with $X(t)$.

Let us stress that the class of models presented in this section is very peculiar. The process $(X(t), \psi(t))_{t \geq 0}$ satisfies the couple of SDEs (44) and (48), whose coefficients depend only on the process of time t ; then, this composed process is Markovian.

Now we can go on in developing the theory as in the Markovian case. The physical probability $\mathbb{P}_{\psi_0}^t$ is defined by (2) and the *a posteriori state* $\psi(t)$ by (9). The *a priori state* is given by the average (10) or by (11):

$$\eta(t) = \mathbb{E}_{\mathbb{P}_{\psi_0}^T} [\langle \psi(t) | \psi(t) \rangle] = \mathbb{E}_{\mathbb{Q}} [\langle \phi(t) | \phi(t) \rangle], \quad 0 \leq t \leq T. \quad (49)$$

By the same steps giving (13)–(18), we obtain that the probability density $\|\phi(t)\|^2$ has the expression (13), with a single value for the index j , and

$$m(t) = 2\text{Re}\langle \psi(t) | R\psi(t) \rangle. \quad (50)$$

Then, under the probability $\mathbb{P}_{\psi_0}^T$ the process

$$W(t) = B(t) - \int_0^t m(s) ds, \quad t \in [0, T], \quad (51)$$

is a Wiener process.

Now the output is $X(t)$, which can be rewritten as

$$X(t) = e^{-kt} \frac{Z}{\sqrt{2k}} + \int_0^t e^{-k(t-s)} (dW(s) + m(s) dt). \quad (52)$$

By differentiation we get the SDE

$$dX(t) = (m(t) - kX(t))dt + dW(t). \quad (53)$$

Moreover, by (49), (50), (52) we get the mean of the output under the physical probability:

$$\mathbb{E}_{\mathbb{P}_{\psi_0}^T} [X(t)] = \text{Tr}\{(R + R^\dagger)\eta(t)\}. \quad (54)$$

Finally, similarly to (18), we get the SDE satisfied by the *a posteriori* state $\psi(t) = \|\phi(t)\|^{-1}\phi(t)$. By expressing the result in terms of the new Wiener process (15), we get the non-linear SSE

$$\begin{aligned} d\psi(t) &= \left[R - \frac{1}{2} m(t) \right] \psi(t) dW(t) \\ &\quad - \left[iH(t) + \frac{1}{2} R^\dagger R - \frac{1}{2} m(t) R + \frac{1}{8} m(t)^2 \right] \psi(t) dt. \end{aligned} \quad (55)$$

Seemingly, up to now the only difference from the Markovian case is that the Hamiltonian $H(t)$ is a random operator. However, this changes extensively the structure of the theory, as we can see, for instance, in the evolution equation of the *a priori* state $\eta(t)$, studied in the following section.

4.2. PROJECTION TECHNIQUES AND CLOSED MASTER EQUATIONS WITH MEMORY

The *a priori* state is introduced as in the Markovian case by the average (49). However, to get a closed equation for $\eta(t)$ is not a trivial task [30]. The final result is a generalised master equation with memory. The important point is that the complete positivity of the map $\eta(0) \mapsto \eta(t)$ is guaranteed by the stochastic representation (49). We illustrate these techniques on the model of Sect. 4.1.

Let us define the process

$$\sigma(t) = |\phi(t)\rangle\langle\phi(t)|. \quad (56)$$

By (48a) and Itô rules, we can compute the stochastic differential of $\sigma(t)$; the result is the linear stochastic master equation

$$d\sigma(t) = \mathcal{L}(t)[\sigma(t)] dt + \mathcal{R}[\sigma(t)] dB(t), \quad \mathcal{R}[\sigma] = R\sigma + \sigma R^\dagger, \quad (57)$$

$$\mathcal{L}(t)[\sigma] = \mathcal{L}_0[\sigma] - iX(t)[L, \sigma],$$

$$\mathcal{L}_0[\sigma] = -i[H_0, \sigma] + R\sigma R^\dagger - \frac{1}{2}\{R^\dagger R, \sigma\}. \quad (58)$$

By using (44) and (48b), (57) can be rewritten in such a way that only the process $X(t)$ appears:

$$\begin{aligned} d\sigma(t) &= \mathcal{L}_0[\sigma(t)] dt + X(t) \left(-i[K, \sigma(t)] + \frac{k}{2} \{R + R^\dagger, \sigma(t)\} \right) dt \\ &\quad + \mathcal{R}[\sigma(t)] dX(t). \end{aligned} \quad (59)$$

By taking the \mathbb{Q} -mean of (57) and by recalling that B has mean zero and increments independent from the past we get

$$\dot{\eta}(t) = \mathcal{L}_0[\eta(t)] - i[L, \mathbb{E}_{\mathbb{Q}}[X(t)\sigma(t)]], \quad (60)$$

which is a kind of master equation with non-Markovian effects introduced by the last term. However, this master equation is not closed, because the $X(t)$ and $\sigma(t)$ are random and not independent.

A closed equation can be obtained by using the Nakajima-Zwanzig method and the generalised master equation one obtains in this way can be the starting point for some approximations [30]. Indeed, the operation of taking the mean is a projection in the space of random trace class operators. We can think of $\eta(t)$ as the *relevant* part of $\sigma(t)$, while $\sigma_{\perp}(t) = \sigma(t) - \eta(t)$ is the *non-relevant* part. As we took a non-random initial state, we have $\sigma(0) = \eta(0)$, $\sigma_{\perp}(0) = 0$. By taking the stochastic differential of $\sigma_{\perp}(t)$ and by using (57) and (60), we get the system of equations

$$\dot{\eta}(t) = \mathcal{L}_0[\eta(t)] - i[L, \mathbb{E}_{\mathbb{Q}}[X(t)\sigma_{\perp}(t)]], \quad (61a)$$

$$\begin{aligned} d\sigma_{\perp}(t) &= \mathcal{L}_0[\sigma_{\perp}(t)] dt - i[L, X(t)(\eta(t) + \sigma_{\perp}(t)) - \mathbb{E}_{\mathbb{Q}}[X(t)\sigma_{\perp}(t)]] dt \\ &\quad + \mathcal{R}[\eta(t) + \sigma_{\perp}(t)] dB(t). \end{aligned} \quad (61b)$$

Let us introduce now the propagator of the homogeneous part of Eq. (61b), which is defined by the SDE

$$\mathcal{V}(t, s) = \mathbb{1} + \int_s^t (\mathcal{L}_0 + \mathcal{K} \circ \mathcal{X}(r)) \circ \mathcal{V}(r, s) dr + \int_s^t \mathcal{R} \circ \mathcal{V}(r, s) dB(r), \quad (62)$$

where \circ denotes the composition of maps, $\mathcal{X}(t)$ is the map $\sigma \mapsto X(t)\sigma - \mathbb{E}_{\mathbb{Q}}[X(t)\sigma]$ and \mathcal{K} the map $\sigma \mapsto -i[L, \sigma]$. Then, the formal solution of (61b) with $\sigma_{\perp}(0) = 0$ can be written as

$$\sigma_{\perp}(t) = \int_0^t \mathcal{V}(t, s) \circ \mathcal{K}[X(s)\eta(s)] ds + \mathcal{V}(t, 0) \circ \int_0^t \mathcal{V}(s, 0)^{-1} \circ \mathcal{R}[\eta(s)] dB(s). \quad (63)$$

In the last term we used $\mathcal{V}(t, 0) \circ \mathcal{V}(s, 0)^{-1}$ instead of $\mathcal{V}(t, s)$ in order to have an adapted integrand in the stochastic integral, as required by the Itô formulation. By inserting the expression (63) into (61a) we get the *generalised master equation* for the *a priori* states

$$\begin{aligned} \dot{\eta}(t) &= \mathcal{L}_0[\eta(t)] + \int_0^t \mathcal{K} \circ \mathbb{E}_{\mathbb{Q}}[X(t)X(s)\mathcal{V}(t, s)] \circ \mathcal{K}[\eta(s)] ds \\ &\quad + \mathbb{E}_{\mathbb{Q}} \left[X(t) \mathcal{K} \circ \mathcal{V}(t, 0) \circ \int_0^t \mathcal{V}(s, 0)^{-1} \circ \mathcal{R}[\eta(s)] dB(s) \right]. \end{aligned} \quad (64)$$

Equations (62) and (64) are very complicated, but they are useful as a starting point to find approximations. In [30] it is suggested to take the non-random approximation of the propagator (62): $\mathcal{V}(t, s) \simeq e^{\mathcal{L}_0(t-s)}$. Then, the mean values in (64) can be computed and the generalised master equation takes the form

$$\dot{\eta}(t) \simeq \mathcal{L}_0[\eta(t)] - \int_0^t \left[L, e^{(\mathcal{L}_0 - k)(t-s)} \left(\frac{1}{2k} [K, \eta(s)] + iJ\eta(s) + i\eta(s)J^\dagger \right) \right] ds, \quad (65)$$

where we have introduced the operator

$$J := \frac{3}{4}R - \frac{1}{4}R^\dagger.$$

4.3. A RANDOM UNITARY EVOLUTION

An interesting particular case is when the LSSE (41) is driven by the coloured noise, but the coefficients are not random. In this way the memory is encoded in the driving noise of the LSSE, not in the coefficients. As we shall see, in this case, the new LSSE will be norm-preserving, as in Sect. 2.4, and will represent a quantum system evolving under a random Hamiltonian dynamics, while the Hamiltonian is very singular and produces dissipation.

So we take $D = 0$ in (41), which gives also $K = 0$. Moreover, the conditions (47) become

$$R = -iV, \quad V^\dagger = V, \quad C = -iH_0 - \frac{1}{2}V^2.$$

Then, we get

$$\begin{aligned} L &= -kV, & J &= -\frac{i}{2}V, & H(t) &= H_0 - kX(t)V, \\ \mathcal{R}[\sigma] &= -i[V, \sigma], & \mathcal{K} &= -k\mathcal{R}, & m(t) &= 0, \end{aligned}$$

$$d\phi(t) = -i[(H_0 - kX(t)V)dt + V dB(t)]\phi(t) - \frac{1}{2}V^2\phi(t) dt. \quad (66)$$

Apart from the further randomness introduced by the term with $X(t)$, the linear SSE has the same structure of (20) and it preserves the norm of $\phi(t)$. The evolution of the quantum system is then completely determined by the time-dependent, random Hamiltonian

$$H(t) = H_0 + (\dot{B}(t) - kX(t))V. \quad (67)$$

Let us stress that it is a formal expression, due to the presence of the white noise $\dot{B}(t)$.

By the normalisation of the initial condition we have $\|\phi(t)\| = 1$; moreover, $m(t) = 0$, which follows from (50) and R anti-selfadjoint. This implies that the probabilities and Wiener processes do not change and that there is no need of normalisation to get the *a posteriori states*:

$$\mathbb{P}_{\psi_0}^T = \mathbb{Q}, \quad W(t) = B(t), \quad \psi(t) = \phi(t). \quad (68)$$

Finally, the evolution equations for the *a priori* states also simplifies slightly. The SDE for the propagator $\mathcal{V}(t, s)$ (62) and the generalised master equation for the *a priori* states (64) become

$$\begin{aligned} \mathcal{V}(t, s) &= \mathbb{1} + \int_s^t (\mathcal{L}_0 - k\mathcal{R} \circ \mathcal{X}(r)) \circ \mathcal{V}(r, s) dr + \int_s^t \mathcal{R} \circ \mathcal{V}(r, s) dB(r), \quad (69) \\ \dot{\eta}_t &= \mathcal{L}_0[\eta(t)] + k^2 \int_0^t \mathcal{R} \circ \mathbb{E}_{\mathbb{P}}[X(t)X(s)\mathcal{V}(t, s)] \circ \mathcal{R}[\eta(s)] ds \\ &\quad - k\mathbb{E}_{\mathbb{P}}\left[X(t)\mathcal{R} \circ \mathcal{V}(t, 0) \circ \int_0^t \mathcal{V}(s, 0)^{-1} \circ \mathcal{R}[\eta(s)] dW(s)\right], \quad (70) \end{aligned}$$

while the approximation (65) reduces to

$$\dot{\eta}(t) \simeq \mathcal{L}_0[\eta(t)] + \frac{k}{2} \int_0^t \left[V, e^{(\mathcal{L}_0 - k)(t-s)} [V, \eta(s)] \right] ds. \quad (71)$$

As the case in Sect. 2.4, the model we have constructed represents a dissipative evolution, now with memory, but without observation of the quantum system. There is no change of probability, \mathbb{Q} is also the physical probability, $\|\phi(t)\| = 1, \forall t$, and the output $X(t)$ remains an O-U process and does not carry any information on the quantum system.

4.4. A NON-MARKOVIAN MODEL: A DISSIPATIVE QUBIT

In this section we introduce a very simple example based on a qubit with dissipation in order to have a toy model with a non-Markovian dynamics for which we can do stochastic simulations and test the approximation (71).

Let us take a two-level system as in Sect. 3.1 and consider the stochastic dynamics (66) with

$$H_0 = \frac{\omega_0}{2} \sigma_z, \quad \omega_0 > 0, \quad V = \sqrt{\frac{\gamma}{2}} \sigma_y, \quad \gamma > 0. \quad (72)$$

Then, the SSE (66) becomes

$$d\phi_1(t) = -\frac{1}{2} \left(\frac{\gamma}{2} + i\omega_0 \right) \phi_1(t) dt - \sqrt{\frac{\gamma}{2}} \phi_2(t) dX(t), \quad (73a)$$

$$d\phi_2(t) = -\frac{1}{2} \left(\frac{\gamma}{2} - i\omega_0 \right) \phi_2(t) dt + \sqrt{\frac{\gamma}{2}} \phi_1(t) dX(t). \quad (73b)$$

The O-U process $X(t)$ is given by (42) and its stochastic differential by (44). For this model we have

$$\mathcal{L}_0[\sigma] = -\frac{i\omega_0}{2} [\sigma_z, \sigma] - \frac{\gamma}{4} [\sigma_y, [\sigma_y, \sigma]]. \quad (74)$$

By representing the states in the Bloch sphere, the master equation $\dot{\xi}(t) = \mathcal{L}_0[\xi(t)]$ can be explicitly solved and the right-hand side of (71) can be given an explicit expression. Indeed, by writing

$$\eta(t) = \frac{1}{2} (\mathbb{1} + \vec{x}(t) \cdot \vec{\sigma}), \quad (75)$$

from (71) we get

$$\begin{cases} \dot{x}(t) = -\omega_0 y(t) - \gamma x(t) + k\gamma \int_0^t e^{-(k+\gamma)(t-s)} x(s) ds, \\ \dot{y}(t) = \omega_0 x(t), \\ \dot{z}(t) = -\gamma z(t) \\ \quad + k\gamma \int_0^t e^{-(k+\gamma/2)(t-s)} \left(\cos \nu(t-s) - \frac{\gamma}{2\nu} \sin \nu(t-s) \right) z(s) ds. \end{cases} \quad (76)$$

We assume to have $\omega_0 > \gamma/2$ and set $\nu = \sqrt{\omega_0^2 - \gamma^2/4}$. Recall that (75) and (76) give an approximation of the *a priori* states.

Equations (76) can be solved by Laplace transform techniques or, equivalently, by increasing the degrees of freedom. Let us set

$$\xi(t) = \gamma \int_0^t e^{-(k+\gamma/2)(t-s)} \cos(\nu(t-s)) z(s) ds, \quad (77a)$$

$$\epsilon(t) = -\frac{\gamma^2}{2\nu} \int_0^t e^{-(k+\gamma/2)(t-s)} \sin(\nu(t-s)) z(s) ds, \quad (77b)$$

$$\zeta(t) = \gamma \int_0^t e^{-(k+\gamma)(t-s)} x(s) ds. \quad (77c)$$

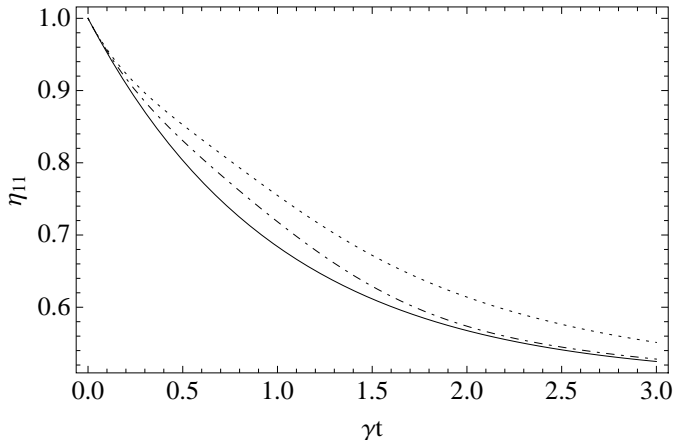


Fig. 6: Plot of the mean occupation of the excited state η_{11} computed from (78b) for the parameters: $\gamma = 1$, $\nu = 3$ and $k = 0$ (solid line), $k = 1$ (dot-dashed line), $k = 2$ (dotted line).

Then, (76) reduce to the two decoupled systems of linear equations with constant coefficients

$$\begin{cases} \dot{x}(t) = -\omega_0 y(t) - \gamma x(t) + k \zeta(t), \\ \dot{y}(t) = \omega_0 x(t), \\ \dot{\zeta}(t) = -(k + \gamma) \zeta(t) + \gamma x(t), \end{cases} \quad (78a)$$

$$\begin{cases} \dot{\xi}(t) = -\left(k + \frac{\gamma}{2}\right) \xi(t) + \frac{2\nu^2}{\gamma} \epsilon(t) + \gamma z(t), \\ \dot{\epsilon}(t) = -\left(k + \frac{\gamma}{2}\right) \epsilon(t) - \frac{\gamma}{2} \xi(t), \\ \dot{z}(t) = -\gamma z + k(\xi(t) + \epsilon(t)). \end{cases} \quad (78b)$$

To get the mean state $\eta(t)$ we can now use stochastic simulations or the analytical approximation of (75), (78). We concentrate on the study of the occupation of the excited state $\eta(t)_{11} = \frac{1}{2} [1 + z(t)]$. Let us stress that it is easy to prove that $\lim_{t \rightarrow +\infty} \eta(t)_{11} = 0.5$.

In Fig. 6 we plot $\eta(t)_{11}$ obtained by solving system (78b) by using the internal function of Mathematica ‘DSolve’. The choice of parameters is $\gamma = 1$, $\omega_0 = \sqrt{37}/2$ (which gives $\nu = 3$) and $k = 0, 1, 2$; recall that $k = 0$ is the Markovian case. The initial state is

$$\eta(0) = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}.$$

We can say that in this model the effect of memory (increasing k) is to modify and to slow down the decay.

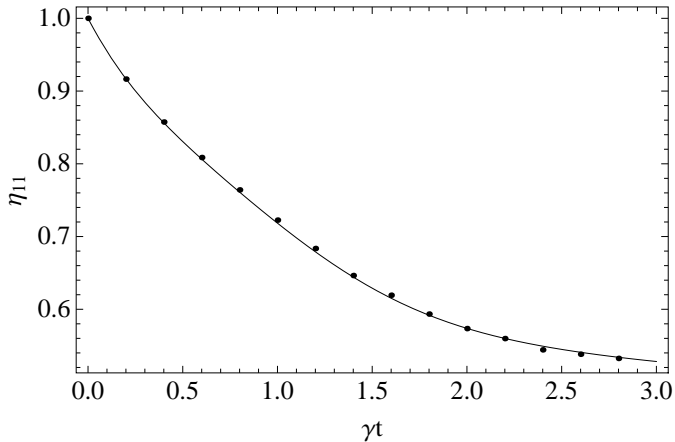


Fig. 7: Plot of the mean occupation number of the excited state for the parameters $\gamma = 1$, $\omega_0 = \sqrt{37}/2$, $k = 1$, $\Delta t = 0.01$. The solid line represents the analytical approximation, while the dots represent the stochastic simulations.

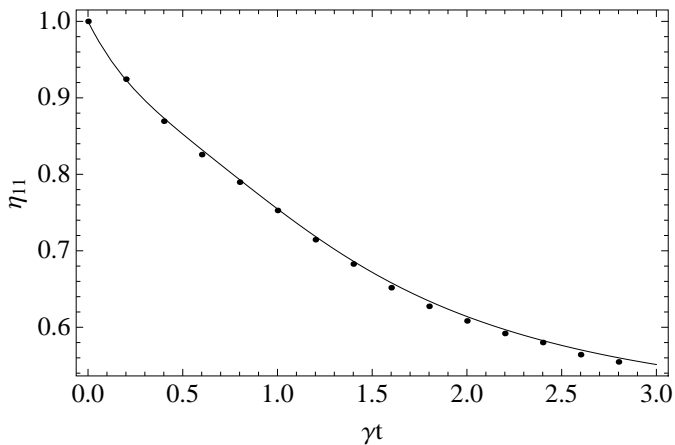


Fig. 8: Plot of the mean occupation number of the excited state for the parameters $\gamma = 1$, $\omega_0 = \sqrt{37}/2$, $k = 2$, $\Delta t = 1/200$.

The solid line represents the analytical approximation, while the dots represent the stochastic simulations.

However, (78b) are approximated, but we can compare this solution with the simulations based on the exact equations (73), (44). We use the Euler algorithm applied to the Markov process $(X(t), \phi_1(t), \phi_2(t))_{t \geq 0}$ with normalisation of $\phi(t)$ at every step as in Sect. 3.1 (10^4 realisations). In Figs. 7 and 8 the dots represent the simulations and the solid line represents the analytical approximation; we see an extremely good agreement of simulations and approximated analytical solution.

5. Conclusions

The theory of linear and non-linear SSEs has been presented in the Markovian diffusive case. Moreover we have discussed their links with the dissipative dynamics of open systems and with measurements in continuous time. Two simple cases have been used to show how to make stochastic simulations based on the SSE. A two-level atom with homodyne detection has been used to show the Euler algorithm, while the Platen algorithm was illustrated in the case of a damped harmonic oscillator.

We have also shown how to use coloured noise in order to construct non-Markovian models. Now the average state does not satisfy the usual Markovian quantum master equation. However, by adapting the Nakajima-Zwanzig projection method, it is possible to arrive at a generalised master equation and we have shown how to get an approximate solution for this equation. On the other hand, the original SDEs can be simulated and the exact solution can be obtained up to numerical errors and statistical fluctuations.

In a concrete model of a dissipative qubit we have compared the analytical approximation with the stochastic simulation of the exact equation. Such a comparison gives a strong support to the proposed approximation. This gives confidence in the possibility of studying more elaborated Markovian models, for which the two computational ways of treating them are open: analytic approximations and stochastic simulations. In the proposed model we see also some effects of the non-Markovianity: there is a slowdown of the decay and a modification of its functional form.

Acknowledgement

This work is based upon research supported by the South African Research Chair Initiative of the Department of Science and Technology and national Research Foundation.

A. Some Theory of Random Processes

A.1. THE WIENER PROCESS

A *standard Wiener process* $\{W(t)\}_{t \geq 0}$ is a continuous Gaussian process starting from 0, with independent and stationary increments, with mean zero and variance proportional to t ; in particular, $\mathbb{E}[W(t)] = 0$ and $\text{Cov}[W(t)W(s)] = \mathbb{E}[W(t)W(s)] = \min(t, s)$.

Due to the Gaussianity and the independence of the increments, if we take a sequence of times $0 \leq t_0 < t_1 < \dots < t_n$ and set

$$Z_k = \frac{W(t_k) - W(t_{k-1})}{\sqrt{t_k - t_{k-1}}},$$

then the random variables Z_1, Z_2, \dots, Z_n are independent and identically distributed, each with standard normal distribution. This fact is used for the simulation of Wiener processes and SDEs.

Finally, a d -dimensional Wiener process is a collection of d independent one-dimensional Wiener processes.

A.2. MARTINGALES AND CHANGE OF MEASURE

Let $(\Omega, \mathcal{F}, (\mathcal{F}_t), \mathbb{P})$ be a stochastic basis as defined at the beginning of Sect. 2.1.

An *adapted process* $\{X(t)\}_{t \geq 0}$ is a stochastic process in the probability space $(\Omega, \mathcal{F}, \mathbb{P})$, such that $X(t)$ is \mathcal{F}_t -measurable, $\forall t \geq 0$.

A stochastic process $\{X(t)\}_{t \geq 0}$ is said to be a *martingale* if (a) it is adapted, (b) $\mathbb{E}[|X(t)|] < +\infty, \forall t \geq 0$, (c) $\mathbb{E}[X(t)|\mathcal{F}_s] = X(s), \forall t \geq s \geq 0$.

An adapted Wiener process is a martingale.

Let $Z = \{Z(t), t \geq 0\}$ be a non-negative martingale with $\mathbb{E}[Z(t)] = 1$. For every fixed $t \geq 0$, the random variable $Z(t)$ can be used as a density to define a new probability measure \mathbb{Q}_t on (Ω, \mathcal{F}_t) :

$$\forall F \in \mathcal{F}_t \quad \mathbb{Q}_t(F) := \int_F Z(t, \omega) \mathbb{P}(d\omega) \equiv \mathbb{E}[Z(t)1_F].$$

Being Z a martingale, all the probabilities $\mathbb{Q}_t, t \geq 0$, are consistent, in the sense that

$$\mathbb{Q}_t(F) = \mathbb{Q}_s(F), \quad \forall t \geq s \geq 0, \quad \forall F \in \mathcal{F}_s.$$

Indeed, 1_F is \mathcal{F}_s -measurable and, by the properties of conditional expectations, one has

$$\begin{aligned} \mathbb{Q}_t(F) &= \mathbb{E}[Z(t)1_F] = \mathbb{E}[\mathbb{E}[Z(t)1_F|\mathcal{F}_s]] = \mathbb{E}[\mathbb{E}[Z(t)|\mathcal{F}_s]1_F] \\ &= \mathbb{E}[Z(s)1_F] = \mathbb{Q}_s(F). \end{aligned}$$

A.3. STOCHASTIC INTEGRALS

Let $(\Omega, \mathcal{F}, (\mathcal{F}_t), \mathbb{P})$ be a stochastic basis, W an adapted Wiener process and F a continuous, adapted, stochastic process with $\mathbb{E}[|F(t)|^2] < +\infty, \forall t \in [0, T]$. Then, it is possible to define the *Itô integral*

$$Y(T) = \int_0^T F(t) dW(t) \tag{A.1}$$

as the mean square limit for $\Delta t \downarrow 0$ of

$$Y_{\Delta t}(T) = \sum_{k=1}^{n-1} F(t_k)(W(t_{k+1}) - W(t_k)), \tag{A.2}$$

where $0 = t_0 < t_1 < \dots < t_n = T$ is a partition of $[0, T]$ and $\Delta t = \max_k \{t_{k+1} - t_k\}$. This means

$$\lim_{\Delta t \downarrow 0} \mathbb{E} \left[\left| Y_{\Delta t}(T) - Y(T) \right|^2 \right] = 0. \quad (\text{A.3})$$

By approximation techniques, the definition of the stochastic integral can be generalised to an integrand $F(t)$ such that it is adapted and

$$\int_0^T \mathbb{E} \left[|F(t)|^2 \right] dt < +\infty.$$

Let us consider the stochastic integral as a process $Y = \{Y(t) : t \in [0, T]\}$. The main properties of *the integral process* are that it is a *martingale with vanishing mean*, $\mathbb{E}[Y(t)] = 0$, and that *the Itô isometry holds*:

$$\mathbb{E}[|Y(t)|^2] = \int_0^t \mathbb{E}[|F(s)|^2] ds. \quad (\text{A.4})$$

These properties are easily proved on the discrete approximation (A.2) and then it is possible to show that they survive to the limiting procedure.

The definition of stochastic integral can be extended to a larger class of integrands (now limits in probability have to be used), but it is no more guaranteed that the main properties hold; we can only say that the integral process is a *local martingale*.

Other definitions of stochastic integral are possible, in particular the Stratonovich integral, whose definition starts from the discrete approximation

$$\sum_{k=1}^{n-1} F((t_k + t_{k+1})/2)(W(t_{k+1}) - W(t_k)).$$

While the rules of the stochastic calculus based on the Stratonovich definition are simpler than the ones based on Itô integral, the important properties above are lost.

A.4. ITÔ CALCULUS

Now let W be a d -dimensional Wiener process defined in the stochastic basis $(\Omega, \mathcal{F}, (\mathcal{F}_t), \mathbb{P})$. An *Itô process* X is a continuous, adapted process such that $X(0)$ is \mathcal{F}_0 -measurable and

$$X(t) = X(0) + \int_0^t F(s) ds + \sum_{j=1}^d \int_0^t G_j(s) dW_j(s),$$

for some adapted process, F Lebesgue integrable and G_j stochastically integrable. It is usual to say that X admits the *stochastic differential*

$$dX(t) = F(t) dt + \sum_{j=1}^d G_j(t) dW_t(t). \quad (\text{A.5})$$

Now take another Itô process with stochastic differential

$$dY(t) = M(t) dt + \sum_{j=1}^d N_j(t) dW_t(t). \quad (\text{A.6})$$

The *Itô lemma* says that the product $X(t)Y(t)$ of two Itô processes is an Itô process with initial value $X(0)Y(0)$ and stochastic differential

$$d(X(t)Y(t)) = X(t) dY(t) + Y(t) dX(t) + (dX(t))(dY(t)),$$

where $dX(t)$, $dY(t)$ have the expressions (A.5), (A.6), and the *Itô correction* $(dX(t))(dY(t))$ must be computed from the product of the two differentials by using the *Itô table*

$$(dt)^2 = 0, \quad dt dW_j(t) = 0, \quad dW_j(t) dW_i(t) = \delta_{ij} dt.$$

This result can be generalised to polynomials in W and then to smooth functions of W ; this is the Itô formula [32, 33], [20, Sects. A.3.3 and A.3.4].

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