The stability of numerical simulations of complex stochastic differential equations

Author(s): Perret, Christian
Publication Date: 2010
Permanent Link: https://doi.org/10.3929/ethz-a-006026507

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The Stability of Numerical Simulations of Complex Stochastic Differential Equations

A dissertation submitted to
ETH Zürich

for the degree of
Doctor of Sciences

presented by
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2010
Aknowledgements

First of all, my thanks go to Prof. Wesley P. Petersen for his support, his cheerfulness, his general straightforward way and for always keeping his door open for me. I appreciated that you let me go my way while always ready to give me some advice. It really has been a pleasure to work with you.

I also want to express my gratitude to Prof. Rolf Jeltsch for giving me the opportunity to start a doctorate at SAM and for accepting to be my co-examiner. The discussion we had almost 5 years ago after I handed in my diploma thesis started me on this road.

An honorable mention goes to Philippe Corboz and Roman Andreev for proof-reading my thesis willingly. A remarkable feat.

My thanks also go to my lovely wife Edith for the support over the years (in particular during the last few weeks), despite being herself under heavy pressure for her own doctorate. I’ll write more in a place where you will read it more than once.

Of course, my family and friends deserve to be thanked too. I have trouble finding words that do not sound cheesy, but the intention is there.

Special thanks to my (former) office-mates for their time, patience, availability and pleasant company. Among them are Sibylle Arnold, Imran Biswas, Alexey Chernov, Carlos Jerez Hanckes, Patrick Meury, Andrea Moiola, Manuel Naumann, Lukas Wampfler and Christoph Winter.

Thanks to the SAM staff in general, be it fellow assistants, professors or secretaries for the general good atmosphere at the institute and the time spent both at the ETH and outside. These four (ok, four and a half) years here have been great overall. The guys from the IT support also deserve a clap for their helpfulness.
Abstract

Many methods exist for solving stochastic differential equations (SDEs) numerically, yet there are SDEs for which simply applying a time-stepping algorithm on will lead to the divergence of the solution in finite time. Indeed, in the nonlinear case, where the drift and diffusion coefficients of an SDE might not satisfy a Lipschitz and a linear growth condition, various types of instability can be expected, if not always encountered. The existence of an exact solution which exists only for a random duration is one of the problems one is up against.

One important example is the complex-valued $\alpha, \beta$-SDE representation obtained for the one-mode Bose-Einstein condensate (BEC) anharmonic oscillator. The aim of this thesis is the development of new numerical methods for solving and controlling unstable SDEs, where the SDE for the one-mode BEC and several related complex SDEs are used as a testing ground for the designed methods. A wide range of numerical schemes are presented and tested on these SDEs.

Among the methods derived in this thesis, three stand out as the most promising. The *split-step method* combines an ODE solver with a modified stochastic scheme, making use of existing robust ODE routines to perform the drift calculations with a higher degree of precision than usually done in the numerical approximation of SDEs. Another advantages of this is the flexibility offered in the choice of the ODE and SDE methods used and the easy access to stiff solvers and features such as already implemented adaptive time-stepping. Although all split-step combinations tested on the $\alpha, \beta$-SDE fail to prevent the divergence of the numerical solution, the method yields reasonable results for less unstable SDEs.

One technique which worked very well when applied on the $\alpha, \beta$-SDE is the use of *artificial boundary conditions* to gently guide the sample paths that are straying towards areas of instability of the complex plane back into more hospitable regions (each complex variable should stay within a bounded annulus to avoid sudden divergence). It is shown that combining the annulus boundary condition with a semi-implicit solver yields simulations where the numerical solution is a reliable approximation of the exact solution for a *twice as long* duration as any other method.

The *Wick rotation* uses a complex change of time to solve a rotated SDE more stable than the original SDE (but which has of course a completely different solution), before converting the gathered numerical data into an approximation corresponding to the original setting. The conversion of the numerical data from one SDE to the other presents some challenges, but is shown that it can be overcome. The approach is not
free of suspicion from a theoretical point of view yet, as the link between the solution of the original and rotated SDE is not clear in the nonlinear case. Results for the complex linear scalar SDE are good, while some extra information has still to be used to make the procedure work for the $\alpha, \beta$-SDE, hence the need for some more research effort in that area. In particular in the case of the latter SDE, the stability improvement is potentially tremendous and a great spur to resolve the remaining challenges.
Zusammenfassung

Viele numerische Verfahren existieren zur Lösung von stochastischen Differentialgleichungen (SDEs). Jedoch divergiert die numerische Lösung bei gewissen SDEs falls nur ein einfaches Zeitschrittverfahren benützt wird. Instabilität kann besonders dann zu einem Problem werden, wenn die SDEs nichtlinear sind und weder Lipschitz- noch lineare Wachstumsbedingungen erfüllen. In diesem fall kann es passieren, dass eine exakte Lösung existiert, aber nur für eine zufällige Dauer.

Ein wichtiges Beispiel ist die komplexe $\alpha, \beta$-SDE, die den harmonischen Oszillator des Bose-Einstein-Kondensats modelliert. Das Ziel dieser Dissertation ist die Entwicklung von numerischen Verfahren für instabile SDEs, wobei die $\alpha, \beta$-SDE und weitere ähnlichen komplexen SDEs als Testprobleme benützt werden. Eine breite Palette von Verfahren werden vorgestellt und getestet.

Zu den drei meistversprechenden Verfahren dieser Dissertation gehört das *split-step Verfahren*. Die Idee ist dabei ein Verfahren für gewöhnliche Differentialgleichungen (ODEs) mit einem Verfahren für SDEs zu kombinieren. Das ODE Verfahren kann eine beliebige (idealerweise bereits implementierte) Routine sein, was den Vorteil mit sich bringt, dass adaptive Schrittwartensteuerung ohne grossen Programmieraufwand möglich ist. Das split-step Verfahren kann zwar die Divergenz der numerischen Lösung der $\alpha, \beta$-SDE nicht vermeiden, aber es liefert gute Ergebnisse für stabilere SDEs.

Ein sehr erfolgreicher Ansatz bei der Simulation der $\alpha, \beta$-SDE sind sogennante *künstlichen Randbedingungen*. Da ein Pfad die Tendenz hat zu divergieren, wenn er zu klein oder zu gross ist, zwingt man die $\alpha$- und $\beta$-Pfäsde in einem komplexen Kreisring zu bleiben. Wenn man diese Randbedingungen mit einem semi-impliziten Verfahren verbindet, bleibt die numerische Lösung der $\alpha, \beta$-SDE begrenzt und ist eine gute Approximation der exakten Lösung für eine doppelt so lange Zeit wie bei anderen Methoden.

Die Wick-Rotation benützt eine komplexe Zeitänderung, um anstatt die ursprüngliche SDE eine stabilere SDE zu lösen (die natürlich nicht die gleiche Lösung hat). Dann wird diese numerische Lösung zu einer Approximation der exakten Lösung der ursprünglichen SDE konvertiert. Dies kann Schwierigkeiten mit sich bringen, ist aber machbar. Das Verfahren wird jedoch auf der theoretischen Seite noch nicht ganz verstanden, da z.B. der Zusammenhang zwischen den Lösungen von beiden SDEs im nichtlinearen Fall unklar ist. Im Fall der linearen skalaren SDE sind die Ergebnisse zufriedenstellend, jedoch wird noch zusätzliche Information gebraucht für die $\alpha, \beta$-SDE. Das Verfahren sollte also weiter untersucht werden. Insbesondere könnte der potenzielle Stabilitätsgewinn für die $\alpha, \beta$-SDE sehr gross sein.
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<tr>
<td>( \mathbb{C} )</td>
<td>the set of all complex numbers</td>
</tr>
<tr>
<td>( \mathbb{R} )</td>
<td>the set of all real numbers</td>
</tr>
<tr>
<td>( \mathbb{Q} )</td>
<td>the set of all rational numbers</td>
</tr>
<tr>
<td>( \mathbb{Z} )</td>
<td>the set of all integers</td>
</tr>
<tr>
<td>( \mathbb{N} )</td>
<td>the set of the natural numbers (including zero)</td>
</tr>
<tr>
<td>( \mathbb{C}^d, \mathbb{R}^d, \mathbb{Q}^d, \mathbb{Z}^d, \mathbb{N}^d )</td>
<td>their multidimensional counterparts</td>
</tr>
<tr>
<td>( \mathbb{R}^{m \times n}, \mathbb{C}^{m \times n} )</td>
<td>the sets of ( m )-by-( n ) matrices with coefficients in ( \mathbb{R} ), respectively ( \mathbb{C} )</td>
</tr>
<tr>
<td>( \mathbb{R}_+ )</td>
<td>the set ( { x \in \mathbb{R}; x \geq 0 } )</td>
</tr>
<tr>
<td>( i )</td>
<td>the imaginary unit ( (i = \sqrt{-1}) )</td>
</tr>
<tr>
<td>( z = z_r + i z_i )</td>
<td>the decomposition of ( z \in \mathbb{C} ) into its real and imaginary parts</td>
</tr>
<tr>
<td>( \text{Re } z, \text{Im } z )</td>
<td>an alternative notation for ( z_r ) and ( z_i )</td>
</tr>
<tr>
<td>(</td>
<td>z</td>
</tr>
<tr>
<td>( i \mathbb{R} )</td>
<td>the set ( { z \in \mathbb{C}; \text{Re } z = 0 } ) of the purely imaginary numbers</td>
</tr>
<tr>
<td>( A \cup \mathbb{B} )</td>
<td>the union of the sets ( A ) and ( B )</td>
</tr>
<tr>
<td>( A \cap \mathbb{B} )</td>
<td>the intersection of the sets ( A ) and ( B )</td>
</tr>
<tr>
<td>( A \setminus \mathbb{B} )</td>
<td>the set of elements of ( A ) that are not in ( B )</td>
</tr>
<tr>
<td>( I_m )</td>
<td>the ( m )-by-( m ) identity matrix</td>
</tr>
<tr>
<td>( (a, b) ) or ( ]a, b[ )</td>
<td>the open real interval ( a &lt; x &lt; b )</td>
</tr>
<tr>
<td>( [a, b] )</td>
<td>the closed real interval ( a \leq x \leq b )</td>
</tr>
<tr>
<td>:=</td>
<td>defined as or denoted by</td>
</tr>
<tr>
<td>( \equiv )</td>
<td>identically equal to</td>
</tr>
<tr>
<td>( \approx )</td>
<td>approximately equal to</td>
</tr>
<tr>
<td>( \sim )</td>
<td>distributed as</td>
</tr>
<tr>
<td>( X \sim \mathcal{N}(\mu, \sigma^2) )</td>
<td>the random variable ( X ) has a normal distribution with mean ( \mu ) and variance ( \sigma^2 )</td>
</tr>
<tr>
<td>i.i.d.</td>
<td>independent and identically distributed</td>
</tr>
<tr>
<td>( x_j ) or ( x^j )</td>
<td>the ( j )th element of a vector ( x ) (or the ( j )th element of ( X ))</td>
</tr>
<tr>
<td>( f', f'', f^{(k)} )</td>
<td>the first, second and ( k )th derivative of the function ( f )</td>
</tr>
<tr>
<td>( \partial_{x_j} f, \frac{\partial f}{\partial x_j} ) or ( \partial_j f )</td>
<td>the partial derivative of ( f ) with respect to ( x_j )</td>
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<td>( \partial_{x_j}^k f, \frac{\partial^k f}{\partial x_j^k} ) or ( \partial_j^k f )</td>
<td>the ( k )th order partial derivative of ( f ) with respect to ( x_j )</td>
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<tr>
<td>( \mathbb{E}[X] ) or ( \mathbb{E}X )</td>
<td>the expectation of the random variable ( X )</td>
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<td>( \langle X^j \rangle_j )</td>
<td>mean value of the samples ( X^j )</td>
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List of Notation

$C^0(V, W)$  the space of continuous functions from $V$ to $W$
$C^\ell(V, W)$  the space of $\ell$ times continuously differentiable functions from $V$ to $W$
$O(h^p)$  the expression divided by $h^p$ remains bounded as $h \to 0$
$o(h^p)$  the expression divided by $h^p$ converges to 0 as $h \to 0$
$\hat{a}^\dagger$  the creation operator of the boson field
$\hat{a}$  the annihilation operator of the boson field
$z^\dagger$  the Hermitian conjugate of the expression $z$
$[A, B]$  the commutator of $A$ and $B$, i.e. $[A, B] = AB - BA$
$\delta_{kj}$  the Kronecker delta symbol
$\kappa_2(A)$  the condition number of the matrix $A$ w.r.t. the 2-norm
$log(x)$  the natural logarithm of $x$
w.p.1  with probability 1
BC  boundary condition
BEC  Bose-Einstein condensation
FPE  Fokker-Planck equation
ODE  ordinary differential equation
PDE  partial differential equation
SDE  stochastic differential equation

Curly and square brackets are used in various formulas in the same way as round brackets to improve readability.
Indices might be written both as subscripts and superscripts (depending on the context, readability might be given the priority over consistency). As an example: $\text{Re} \alpha = \alpha_r$, but $\text{Re} \, X_0 =: X_0^r$. 
Introduction

Stochastic differential equations (SDEs) arise in various fields, be it in finance, biology, quantum statistics, seismology and many more. They are, loosely speaking, a generalization of ordinary differential equations (ODEs) obtained by adding some random noise to an ODE. The solution to an SDE, if there is one, is a stochastic process. Several methods exist to solve SDEs numerically, but the stochastic term introduces statistical variability which makes it hard to compute the paths (the aim of strong solvers) or even the moments (using weak solvers) accurately. However, the statistical sampling problem is not the only problem, as it will be demonstrated that the stochastic perturbation might make a stable ODE with exact bounded solution into an extremely volatile process. As will be seen, even linear SDEs are not always easy to control. Complex SDEs have not been investigated as extensively as their real counterparts. A reason for this might be that any complex SDE can be rewritten as a real system. However, the corresponding system can display some peculiar dynamics, particularly when the driving Brownian motion is complex also.

The background for this thesis is the following. Quantum simulations of mesoscopic dynamical systems have long been considered to be intractable without making some simplifying model assumptions due to the gargantuan size of the corresponding Hilbert spaces. One way to get around this problem is the use of the positive $P$-representation as presented in [37], which allows bulk properties to be described by the solution of SDEs of a manageable size. However, the difficulties to solve the SDEs numerically increases with the nonlinearity of the drift, as the representation will often only be valid until the solution can be expected to have unbounded sample paths (see [44]).

One important example is the SDE representation of the one-mode Bose-Einstein condensate (BEC) as described in [31]. Despite the fact that all the moments of its solution process can be derived exactly and are bounded over any finite time interval, its numerical solution diverges in finite time for conventional SDE schemes. The motivation is to use this SDE as a testing ground for developing new numerical methods for solving and controlling (numerically) unstable SDEs. For this purpose, several related SDEs are derived to gain some insight into the causes of the instability and a wide range of numerical schemes are designed and tested on these SDEs.

In this thesis, stability considerations are based mostly on computational aspects. Is a numerical SDE integration scheme able to return approximations that are relevant statistically when solving a specific SDE? Can the solution diverge (numerically) in finite time despite the fact that moments of the exact solution are bounded? More elaborated
definitions of stability as seen in \cite{5,10,12,47,49,89} are not delved into, since the focus here is not to decide whether a given SDE is unstable or not, but to find new techniques to solve problems that are unstable numerically.

In Chapter 1 a short overview of the theory about SDEs and coherent states needed for the next chapters is given. In Chapter 2 the focus is mainly on deriving the SDEs used throughout the thesis, discussing their stability properties and deriving some metrics with which one can measure the accuracy of the numerical solution. In Chapter 3 a selection of the methods used to solve the various SDEs will be introduced and their performances will be discussed. Chapter 4 will summarise the most important results of the thesis and will hint at what there is left to do.
1. Preliminaries

In this chapter, a summary of the theory needed for the next chapters will be given briefly. For a much more complete theory about probability and stochastic processes than given in Section 1.1, see for example [81]. Section 1.2 will assume some degree of familiarity with SDEs and how to solve them. An extensive overview of the theoretical background and numerical treatment of SDEs can be found among others in [57], [61], [64] and [69]. In Section 1.3, the quantum mechanical framework needed for the derivation of the SDEs presented in Chapter 2 and the computation of related metrics will be introduced shortly.

The material presented in Section 1.3 is to be seen mainly as the set of mathematical tools needed for the purposes stated above. The SDEs from Chapter 2 will be used purely as toy problems: their physical interpretation is irrelevant for the purpose of this thesis. Interested readers wishing to learn more about coherent states and the concepts mentioned in Section 1.3 are invited to looking into [41], [55], [56] and [75].

1.1. Stochastic processes

Definition 1.1.1. A stochastic process $X = \{X_t\}_{t \geq t_0}$ is a collection of random variables $X_t$ on the probability space $(\Omega, A, P)$. For $\omega \in \Omega$, $(X_t(\omega))_{t \geq t_0}$ is a realization, a trajectory or a sample path of the stochastic process.

Definition 1.1.2. A stochastic process $\{X_t\}_{t \geq t_0}$ has independent increments if for every $n \in \mathbb{N}$, $t_0 < t_1 < \cdots < t_n$, the increments $X_{t_0}, X_{t_1} - X_{t_0}, \ldots, X_{t_n} - X_{t_{n-1}}$ are independent.

Definition 1.1.3. A Brownian motion in $\mathbb{R}$ (or Wiener process, or real Brownian motion) is a continuous stochastic process $W$ (where $W_t \in \mathbb{R}, \forall t \geq 0$) with independent increments satisfying $W_0 = 0$ w.p.1 (with probability one) and $W_t - W_s \sim N(0, t-s), \forall 0 \leq s < t$.

Definition 1.1.4. A Brownian motion in $\mathbb{R}^m$ is a stochastic process $W = (W^1, \ldots, W^m)^\top$, where the $W^j$ are pairwise independent Brownian motions in $\mathbb{R}$, $j = 1, \ldots, m$. This means that for $t, s \geq 0$, any $j, k = 1, \ldots, m$ with $j \neq k$ and any Borel sets $B_1, B_2 \in \mathcal{B}(\mathbb{R})$ (the Borel $\sigma$-algebra), $P(W^j_t \in B_1, W^k_s \in B_2) = P(W^j_t \in B_1) P(W^k_s \in B_2)$. In particular, it follows that $E[W^j_t W^k_s] = E[W^j_t]E[W^k_s] = 0$ for $j \neq k, t, s \geq 0$. 

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**Definition 1.1.5.** A complex Brownian motion is a stochastic process of the type $W = W^r + iW^i$, where $W^r, W^i$ are pairwise independent Brownian motions in $\mathbb{R}$. A Brownian motion in $\mathbb{C}^m$ is a stochastic process $W = (W^1, \ldots, W^m)^\top$, where the $W^j$ are independent complex Brownian motions, $j = 1, \ldots, m$, in the sense that $W^1, W^1, \ldots, W^m, W^m$ are pairwise independent real Brownian motions.

**Remark 1.1.6.** Note that the moments of a complex Brownian motion differ significantly from its real counterpart. Let $W = W^r + iW^i$, where $W^r, W^i$ are i.i.d. Brownian motions in $\mathbb{R}$. Namely, by considering $M_W(\lambda) := \mathbb{E}[e^{\lambda W}]$, the moment-generating function of $W$, one obtains

$$M_W(t) = \mathbb{E}[e^{\lambda W^r}] \mathbb{E}[e^{i\lambda W^i}] = e^{\lambda^2 t} e^{-\lambda^2 t} = 1, \forall t \geq 0.$$  

(1.1)

From (1.1) follows that

$$\mathbb{E}[W_k t] = \frac{\partial^k}{\partial \lambda^k} \mathbb{E}[e^{\lambda W}] \bigg|_{\lambda = 0} \equiv 0, \forall k \in \mathbb{N}, \forall t \geq 0.$$  

(1.2)

This is an interesting result and should serve as a warning against generalizing results from the real to the complex case without care. The expectation of the magnitude of $W$ is not zero, however, since

$$\mathbb{E}[|W|^2] = \mathbb{E}[(W^r)^2] + \mathbb{E}[(W^i)^2] = 2t.$$  

In the computation of (1.1), the following important Lemma was used:

**Lemma 1.1.7.** For $\sigma \in \mathbb{C}$ constant, $t_1 > t_0 \geq 0$ and a real Brownian motion $W \in \mathbb{R}$, it holds

$$\mathbb{E}[e^{\sigma(W_{t_1} - W_{t_0})}] = e^{\frac{\sigma^2}{2}(t_1 - t_0)}.$$  

(1.3)

This result is of course widely known for $\sigma \in \mathbb{R}$, but not so for $\sigma \in \mathbb{C}$. In order to prove it, one first needs another

**Lemma 1.1.8.** For any $\mu \in \mathbb{C}$, $t \in \mathbb{R}$, the following holds true:

$$\int_{-\infty}^{\infty} e^{-\frac{(x-\mu)^2}{2}} \, dx = \sqrt{2\pi t}.$$  

(1.4)

Proof of Lemma 1.1.7: Remembering that $W_{t_1} - W_{t_0} \sim N(0, t_1 - t_0)$ and setting $\Delta t = t_1 - t_0$, it holds

$$\mathbb{E}[e^{\sigma(W_{t_1} - W_{t_0})}] = \frac{1}{\sqrt{2\pi \Delta t}} \int_{-\infty}^{\infty} e^{\sigma w} e^{-\frac{w^2}{2\Delta t}} \, dw = \frac{1}{\sqrt{2\pi \Delta t}} e^{\frac{\sigma^2 \Delta t}{2}} \int_{-\infty}^{\infty} e^{-\frac{(w-\sigma \Delta t)^2}{2\Delta t}} \, dw$$  

(1.4)

$$= e^{\frac{\sigma^2 \Delta t}{2}} = e^{\frac{\sigma^2}{2}(t_1 - t_0)}.$$  

Before proving Lemma 1.1.8, however, one needs to recall a few facts from complex analysis.
1.1. Stochastic processes

Definition 1.1.9. For \( a, b \in \mathbb{R} \) let \( \gamma : [a, b] \to \mathbb{C} \) be a continuously differentiable curve and \( f : \gamma([a, b]) \to \mathbb{C} \) a continuous function. The complex line integral (or contour integral) \( \int_{\gamma} f(z) \, dz \) is then defined as the integral

\[
\int_{\gamma} f(z) \, dz := \int_{a}^{b} f(\gamma(s))\gamma'(s) \, ds. \tag{1.5}
\]

One says that \( \gamma \) is a closed curve if \( \gamma(a) = \gamma(b) \).

Definition 1.1.10. Let \( f : U \subseteq \mathbb{C} \to \mathbb{C} \) be a function of \( z = x + iy \). Define \( u, v : \mathbb{R}^2 \to \mathbb{R} \) by

\[
f(z) = u(x, y) + iv(x, y). \]

If \( u, v \) are both in \( C^1(\mathbb{R}^2, \mathbb{R}) \) and satisfy the Cauchy-Riemann equations

\[
\frac{\partial u}{\partial x} = \frac{\partial v}{\partial y}, \quad \frac{\partial u}{\partial y} = -\frac{\partial v}{\partial x}, \tag{1.6}
\]

then \( f \) is called holomorphic.

Remark 1.1.11. If \( \gamma : [a, b] \to U \subset \mathbb{C} \) is a closed curve, where \( U \) is an open simply connected set and \( f : U \to \mathbb{C} \) is holomorphic, then as a consequence of Cauchy’s integral theorem,

\[
\oint_{\gamma} f(z) \, dz = 0. \tag{1.7}
\]

Proof of Lemma 1.1.8 Write \( \mu = \mu_r + i\mu_i \). Consider the following differentiable curves

\[
\begin{align*}
\gamma_0(s) &= s - i\mu_i, \quad \text{for } s \in [-R, R], \tag{1.8} \\
\gamma_1(s) &= R + i\mu_i(s - 1), \quad \text{for } s \in [0, 1], \tag{1.9} \\
\gamma_2(s) &= -s, \quad \text{for } s \in [-R, R], \tag{1.10} \\
\gamma_3(s) &= -R - i\mu_is, \quad \text{for } s \in [0, 1], \tag{1.11}
\end{align*}
\]

which are shown in Figure 1.1. It holds

\[
\int_{-\infty}^{\infty} e^{-\frac{(x-\mu)^2}{2\sigma}} \, dx = e^{-\frac{(y-\mu_i)^2}{2\sigma}} \int_{-\infty}^{\infty} e^{-\frac{(y-\mu_i)^2}{2\sigma}} \, dy = \lim_{R \to \infty} \int_{\gamma_0}^{\gamma} e^{-\frac{z^2}{2\sigma}} \, dz.
\]

The path \( \gamma := \bigcup_{j=0}^{3} \gamma_j \) is closed. Thus, using Remark 1.1.11 and the fact that \( \exp(-\frac{z^2}{2\sigma}) \) is holomorphic in \( z \),

\[
\int_{\gamma} e^{-\frac{z^2}{2\sigma}} \, dz = \sum_{j=0}^{3} \int_{\gamma_j} e^{-\frac{z^2}{2\sigma}} \, dz = 0. \tag{1.12}
\]

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Figure 1.1.: Differentiable curves $\gamma_0, \ldots, \gamma_3$.

Now estimate the complex line integrals

$$\left| \int_{\gamma_1} e^{-z^2/2t} \, dz \right| = \left| \int_0^1 e^{-\frac{(R+\mu i(s-1))^2}{2t}} \, ds \right| = e^{-\frac{R^2}{2t}} |\mu_i| \left| \int_0^1 e^{\frac{\mu_i^2(s-1)^2}{2t}} e^{-\frac{\mu_i R s}{t}} \, ds \right| \leq e^{-\frac{R^2}{2t}} |\mu_i| e^{\frac{\mu_i^2}{2t}} R \to \infty \to 0,$$

$$\int_{\gamma_2} e^{-z^2/2t} \, dz = \int_{-R}^R e^{-z^2/2t} \cdot (-1) \, ds \to -\sqrt{2\pi}t, \text{ (Gaussian distribution)}$$

$$\int_{\gamma_3} e^{-z^2/2t} \, dz = e^{-\frac{R^2}{2t}} |\mu_i| \left| \int_0^1 e^{\frac{\mu_i^2 s^2}{2t}} e^{-\frac{\mu_i R s}{t}} \, ds \right| \leq e^{-\frac{R^2}{2t}} |\mu_i| e^{\frac{\mu_i^2}{2t}} R \to \infty \to 0.$$ 

It follows that

$$\int_{-\infty}^{\infty} e^{-\frac{(x-\mu)^2}{2t}} \, dx = \lim_{R \to \infty} \int_{x_0}^x e^{-\frac{z^2}{2t}} \, dz \quad \text{1.12} \quad - \lim_{R \to \infty} \sum_{j=1}^3 \int_{\gamma_j} e^{-\frac{z^2}{2t}} \, dz = \sqrt{2\pi}t.$$
1.2. Stochastic differential equations

In this thesis, the SDEs will be written mainly in their differential Itô form

\[ dX_t = a(t, X_t) \, dt + b(t, X_t) \, dW_t, \]  

(1.13)

with (possibly random) initial condition \( X_{t_0} \) at the time \( t_0 \), where \( t_0 \) is mostly zero, \( a(t, X_t) \in \mathbb{R}^d \) (or \( \mathbb{C}^d \)) is the drift vector, \( b(t, X_t) \in \mathbb{R}^{d \times m} \) (or \( \mathbb{C}^{d \times m} \)) is the diffusion matrix and \( W \) is a Brownian motion in \( \mathbb{R}^m \) (or \( \mathbb{C}^m \)). An Itô SDE written in its differential form (1.13) it to be interpreted as

\[ X_t = X_{t_0} + \int_{t_0}^t a(s, X_s) \, ds + \int_{t_0}^t b(s, X_s) \, dW_s, \]  

(1.14)

where the second integral is an Itô stochastic integral as defined in [57]. An important property of Itô stochastic integrals is that they are martingales.

If \( X_t \) is always real (i.e. if \( a, b \) and \( W \) are all real), one will denote the SDE (1.13) as being a real SDE. If \( X_t \) is allowed to have complex values, one says that (1.13) is a complex SDE. In the rest of this thesis, SDEs will mostly be given without any explicit mention of their corresponding initial condition.

As in the ODEs case, it is always possible to rewrite (1.13) in autonomous form

\[ dY_t = a(Y_t) \, dt + b(Y_t) \, dW_t, \]  

(1.15)

by picking \( Y_t^j = X_t^j, \ j = 1, \ldots, d, \ Y_t^{d+1} = t, \) and defining \( a^{d+1} = 1, \ b^{d+1,k} = 0, \) \( k = 1, \ldots, m. \)

**Remark 1.2.1.** Note that the components of \( a, b \) and \( W \) in (1.13) or (1.15) need not all be real or all complex. An example of this is for instance the SDE (2.1)-(2.3), where the Brownian motions and \( \tilde{\theta} \) (as well as its corresponding drift and diffusion coefficients) are real, while \( \phi, \psi \) and their corresponding drift and diffusion coefficients are complex.

**Remark 1.2.2.** If the diffusion coefficient \( b \) of (1.15) is linear in \( Y \), the SDE is said to have multiplicative noise. If \( b \) is constant, the SDE (1.15) has additive noise.

**Remark 1.2.3.** The time index might be dropped later in \( dX_t \) and/or \( dW_t \), as will often be the case in Chapter 2.

There exists many methods to solve SDEs numerically. The general principle is the same as for ODEs: the more terms of the (stochastic) Taylor series expansion of the exact solution (assuming there is one) are approximated by the Taylor series of a given method, the higher the order of the method w.r.t. the time step (and in principle the better). Naturally, increasing the order of the method means the more complex it becomes, as more terms must be included. Note that due to the stochastic terms, the order can have as value any \( \frac{p}{2} \), where \( p \in \mathbb{N} \setminus \{0\} \).
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In the SDE setting, several other considerations come into play. One is that one must decide whether one wants to approximate only the moments (the aim of weak solvers) of the solution $Y_t$ of (1.15) or if the precision of the individual paths matters (in which case one uses strong solvers). Another is that, as the order of the methods grows, the number of terms involved grows non-linearly with the order, most of them containing stochastic integrals of increasing complexity. Add the Monte-Carlo nature of the approximation of the stochastic integrals (halving the sampling error needs simulating four times as many paths) and the fact that most methods in use are of relatively low order, mostly only up to order 2.0 (strong or weak). See [57] for details about stochastic Taylor series and SDEs methods.

**Example 1.2.4 (the Euler-Maruyama method).** For the SDE (1.15), starting at $Y_0$ at time $t_0$, one step of the (explicit) Euler(-Maruyama) method computes the approximation of the exact solution $Y_t$ as

$$Y_1 = Y_0 + a(Y_0)h + b(Y_0)ξ,$$

where $ξ$ is an approximation of the $m$-dimensional (Itô) stochastic integral $∫_{t_0}^{t_1} dW_s$, e.g. distributing the $ξ_1,...,ξ_m$ as i.i.d. $N(0, t_1 - t_0)$ (pseudo)random variables.

1.2.1. The Itô formula

Consider a process $Y$ satisfying the autonomous $d$-dimensional real SDE (1.15) (in particular, $Y_t ∈ ℝ^d$, $W_t ∈ ℝ^m$) and the function $U : [0, T] × ℝ^d → ℝ^N$ with continuous partial derivatives $∂U^ℓ/∂t$, $∂U^ℓ/∂y^i$, $∂^2U^ℓ/∂y^i∂y^k$, $ℓ = 1,...,N$, $i,k = 1,...,d$. Define the process $\{Z_t\}_{t ∈ [0,T]}$ by $Z_t = U(t,Y_t)$. Then the SDE for $Z_t$ is

$$dZ_t^ℓ = \left\{ \frac{∂U^ℓ}{∂t} + \sum_{k=1}^{d} a^k(Y_t) \frac{∂U^ℓ}{∂y^k} + \frac{1}{2} \sum_{j=1}^{m} \sum_{i,k=1}^{d} b^{j,i}(Y_t)b^{k,j}(Y_t) \frac{∂^2U^ℓ}{∂y^i∂y^k} \right\} dt$$

$$+ \sum_{j=1}^{m} \sum_{k=1}^{d} b^{k,j}(Y_t) \frac{∂U^ℓ}{∂y^k} dW_t^j, \; ℓ = 1,\ldots,N.$$ (1.17)

This is called the Itô formula. The proof for the case $Y ∈ ℝ^d$, $U : [0, T] × ℝ^d → ℝ^N$, as well as more details and applications can be found in [57]. Complex variants of the Itô rule (1.17) also exist, see Remark 1.2.5 Theorem 1.2.6 and Theorem 1.2.9.

**Remark 1.2.5.** By the linearity of the differentiation, it is obvious that (1.17) also holds when $U : [0, T] × ℝ^d → ℂ^N$.

**Theorem 1.2.6** (Itô formula for complex SDEs driven by real Brownian motions). Let $Y = (Y^1,\ldots,Y^d)^\top ∈ ℂ^d$ be a stochastic process satisfying the complex SDE

$$dY_t = a(Y_t) dt + b(Y_t) dW_t$$

(1.18)
with drift vector \( a(Y_t) \in \mathbb{C}^d \), diffusion matrix \( b(Y_t) \in \mathbb{C}^{d \times m} \) and \textit{real} Brownian motion \( W_t \in \mathbb{R}^m \). Write \( Y^k = x^k + iy^k \), with \( x^k, y^k \in \mathbb{R} \) for \( k = 1, \ldots, d \). Consider further the function \( U : [0, T] \times \mathbb{C}^d \rightarrow \mathbb{C}^N \) and use the notation \( U = (U^1, \ldots, U^N)^T \in \mathbb{C}^N \), where \( U^\ell(t, Y)^T(t, x^1, y^1, \ldots, x^d, y^d) + iU^\ell(t, x^1, y^1, \ldots, x^d, y^d), \) i.e. \( U^\ell, U^\ell : [0, T] \times \mathbb{R}^d \rightarrow \mathbb{R}, \ell = 1, \ldots, N \). If \( U \) is componentwise holomorphic, i.e. if \( U \)

1. has continuous partial derivatives \( \frac{\partial U^\ell}{\partial t}, \frac{\partial U^\ell}{\partial x^k}, \frac{\partial U^\ell}{\partial y^k}, \frac{\partial^2 U^\ell}{\partial x^k \partial y^k}, \frac{\partial^2 U^\ell}{\partial x^k \partial x^\ell}, \frac{\partial^2 U^\ell}{\partial y^k \partial y^\ell}, \forall \ell = 1, \ldots, N, i, k = 1, \ldots, d, \)

2. satisfies

\[
\frac{\partial U^\ell}{\partial y^k} = \frac{\partial U^\ell}{\partial x^k} \quad \text{and} \quad \frac{\partial U^\ell}{\partial y^k} = -\frac{\partial U^\ell}{\partial x^k}, \forall k = 1, \ldots, d, \ell = 1, \ldots, N, \tag{1.19}
\]

then the complex stochastic process \( Z = (Z^1 + iZ^1, \ldots, Z^N + iZ^N) \in \mathbb{C}^N \) defined by \( Z_t = U(t, Y_t) \) satisfies the following complex SDE

\[
dZ^\ell_t = \left\{ \frac{\partial U^\ell}{\partial t} + \sum_{k=1}^d a^k(Y_t) \frac{\partial U^\ell}{\partial y^k} + \frac{1}{2} \sum_{j=1}^m \sum_{i,k=1}^d b^{i,j}(Y_t) b^{k,j}(Y_t) \frac{\partial^2 U^\ell}{\partial y^i \partial y^k} \right\} dt \]

\[
+ \sum_{j=1}^d b^{k,j}(Y_t) \frac{\partial U^\ell}{\partial y^k} dW^j_t, \quad \ell = 1, \ldots, N. \tag{1.20}
\]

where \( \frac{\partial}{\partial y^\ell} \) is understood as the complex derivative \( \frac{\partial}{\partial y^\ell} = \frac{1}{2} (\frac{\partial}{\partial y^\ell} - i \frac{\partial}{\partial y^\ell}) \).

Idea of proof: by decomposing each equation in \(1.20\) in its real and imaginary part, one obtains the following real equations

\[
dZ^\ell_r = \left\{ \frac{\partial U^\ell}{\partial t} + \sum_{k=1}^d \text{Re} \left[ a^k(Y_t) \frac{\partial U^\ell}{\partial y^k} \right] + \frac{1}{2} \sum_{j=1}^m \sum_{i,k=1}^d \text{Re} \left[ b^{i,j}(Y_t) b^{k,j}(Y_t) \frac{\partial^2 U^\ell}{\partial y^i \partial y^k} \right] \right\} dt \]

\[
+ \sum_{j=1}^d \text{Re} \left[ b^{k,j}(Y_t) \frac{\partial U^\ell}{\partial y^k} \right] dW^j_t, \quad \ell = 1, \ldots, N, \tag{1.21}
\]

\[
dZ^\ell_i = \left\{ \frac{\partial U^\ell}{\partial t} + \sum_{k=1}^d \text{Im} \left[ a^k(Y_t) \frac{\partial U^\ell}{\partial y^k} \right] + \frac{1}{2} \sum_{j=1}^m \sum_{i,k=1}^d \text{Im} \left[ b^{i,j}(Y_t) b^{k,j}(Y_t) \frac{\partial^2 U^\ell}{\partial y^i \partial y^k} \right] \right\} dt \]

\[
+ \sum_{j=1}^d \text{Im} \left[ b^{k,j}(Y_t) \frac{\partial U^\ell}{\partial y^k} \right] dW^j_t, \quad \ell = 1, \ldots, N. \tag{1.22}
\]

With some straightforward yet lengthy algebra, it is easy to check that as long as \(1.19\) holds, the \(2N\) SDEs given by \(1.21\)-\(1.22\) match their counterparts obtained for \(Z^\ell_r, Z^\ell_i\) with the real Itô formula \(1.17\). ⊗
1. Preliminaries

Remark 1.2.7. Note that considering real Brownian motions in Theorem 1.2.6 is by no means restrictive, since any SDE of the type
\[ dY_t = a(Y_t) \, dt + b(Y_t) \, dW_t \] (1.23)
with \( a(Y_t) \in \mathbb{C}^d \), \( b(Y_t) \in \mathbb{C}^{d \times m} \) and \( W_t \in \mathbb{C}^m \) can be rewritten as
\[ dY_t = a(Y_t) \, dt + \hat{b}(Y_t) \, d\hat{W}_t, \]
where \( \hat{b}(Y_t) \in \mathbb{C}^{d \times 2m} \), \( \hat{W}_t \in \mathbb{R}^{2m} \).

Remark 1.2.8. Since complex SDEs of the form (1.18) can always be rewritten as real SDEs, it is of course possible (and in some cases necessary, see Section 1.2.2) to stick to the original real Itô rule (1.17) for most purposes (e.g. controlling the validity of an assumed solution of an SDE, see [57]), limiting thus the use of (1.20). However, Theorem 1.2.6 shows that although a trivial extension of the Itô formula from the real to the complex case is possible, caution is necessary in the complex case because of the required componentwise holomorphicity of \( U \).

It is possible to extend the Itô rule further to complex SDEs driven by complex Brownian motions. As will be seen, the corresponding transformation rule displays some interesting properties:

Theorem 1.2.9 (Itô formula for complex SDEs driven by complex Brownian motions). Let \( Y = (Y^1, \ldots, Y^d)^T \in \mathbb{C}^d \) be a stochastic process satisfying the complex SDE (1.23) with drift vector \( a(Y_t) \in \mathbb{C}^d \), diffusion matrix \( b(Y_t) \in \mathbb{C}^{d \times m} \) and complex Brownian motion \( W_t = W^r_t + i W^i_t \in \mathbb{C}^m \). Let further \( U : [0, T] \times \mathbb{C}^d \to \mathbb{C}^N \) be componentwise holomorphic, as defined in Theorem 1.2.6. Then the complex stochastic process \( Z_t := U(t, X_t) \) satisfies the following complex SDEs:
\[ dZ^\ell_t = \left\{ \frac{\partial U^\ell}{\partial t} + \sum_{k=1}^d a^k(Y_t) \frac{\partial U^\ell}{\partial Y^k} \right\} \, dt + \sum_{j=1}^m \sum_{k=1}^d b^{j-k}(Y_t) \frac{\partial U^\ell}{\partial Y^k} \, dW^j_t, \quad \ell = 1, \ldots, N. \] (1.24)

Proof: define
\[ \hat{W} := \begin{pmatrix} W^r \\ W^i \end{pmatrix} \in \mathbb{R}^{2m} \text{ and } \sigma \in \mathbb{C}^{d \times 2m} \text{ where } \sigma^{kj} = \begin{cases} b^{kj}, & j \leq m, \\ i b^{k\ell}, & j = m + \ell. \end{cases} \]
Since \( \sigma \, d\hat{W}_t = b \, dW_t \), one can rewrite (1.18) in the form (1.18):
\[ dY_t = a(Y_t) \, dt + \sigma(Y_t) \, d\hat{W}_t, \]
which allows the use of Theorem 1.2.6 since \( U \) is componentwise holomorphic. It follows for \( \ell = 1, \ldots, N \):
\[ dZ^\ell_t = \left\{ \frac{\partial U^\ell}{\partial t} + \sum_{k=1}^d a^k \frac{\partial U^\ell}{\partial Y^k} + \frac{1}{2} \sum_{j=1}^{2m} \sum_{i,k=1}^d \sigma^{ij} \sigma^{kj} \frac{\partial^2 U^\ell}{\partial Y^i \partial Y^k} \right\} \, dt \]
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\[ + \sum_{j=1}^{2m} \sum_{k=1}^d \sigma^{k,j} \frac{\partial U^\ell}{\partial Y_k} d\tilde{W}^j_t \]

\[ = \left\{ \frac{\partial U^\ell}{\partial t} + \sum_{k=1}^d a^k \frac{\partial U^\ell}{\partial Y_k} + \frac{1}{2} \sum_{j=1}^m \sum_{i,k=1}^d \left( b^{i,j} b^{k,j} + i^2 b^{i,j} b^{k,j} \right) \frac{\partial^2 U^\ell}{\partial Y_i \partial Y_k} \right\} dt \]

\[ + \sum_{j=1}^{m} \sum_{k=1}^d \frac{\partial U^\ell}{\partial Y_k} \left( b^{k,j} dW^j_t + i b^{k,j} dW^j_t \right) \]

\[ = \left\{ \frac{\partial U^\ell}{\partial t} + \sum_{k=1}^d a^k (Y_t) \frac{\partial U^\ell}{\partial Y_k} \right\} dt + \sum_{j=1}^{m} \sum_{k=1}^d b^{k,j} (Y_t) \frac{\partial U^\ell}{\partial Y_k} dW^j_t. \]

1.2.2. Linear SDEs

Linear SDEs have the advantage of having a unique known solution (at least in the scalar or real case), meaning they can be used as a testing ground for various methods. A short summary of some of their properties will therefore be presented here. Consider first the complex geometric Brownian motion \( X_t \), described by the scalar complex linear SDE with multiplicative real noise

\[ dX_t = bX_t dt + \sigma X_t dW_t, \quad (1.25) \]

where \( b, \sigma \in \mathbb{C} \) are constants and \( W \) is a Brownian motion in \( \mathbb{R} \). As in the real case (see [57]), it is easy to show that the exact solution to (1.25) is

\[ X_t = e^{(b - \frac{\sigma^2}{2})t + \sigma W_t} X_0. \quad (1.26) \]

In order to see this, rewrite (1.25) as an SDE in \( \mathbb{R}^2 \) and compare its coefficients with those of the SDEs obtained when using the real Itô rule on

\[ U_1(t, W_t) = \text{Re} \left[ e^{(b - \frac{\sigma^2}{2})t + \sigma W_t} X_0 \right], \]

\[ U_2(t, W_t) = \text{Im} \left[ e^{(b - \frac{\sigma^2}{2})t + \sigma W_t} X_0 \right]. \]

**Remark 1.2.10.** Note that one cannot use (1.20) directly to check the validity of (1.26), since the obvious choice \( X_t = U(t, W_t) \) is not holomorphic in \( W_t \).

The moments of \( X_t \) are easy to compute using Lemma [1.1.7]

\[ \mathbb{E}[X_t] = \mathbb{E}\left[ e^{(b - \frac{\sigma^2}{2})t + \sigma W_t} X_0 \right] = e^{(b - \frac{\sigma^2}{2})t} \mathbb{E} \left[ e^{\sigma W_t} \right] X_0 = e^{bt} X_0, \quad (1.27) \]
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\[ \mathbb{E}[X_t^2] = \mathbb{E}[e^{(2b - \sigma^2)t + 2\sigma W_t} X_0^2] = e^{(2b - \sigma^2)t + 2\sigma^2 t} X_0^2, \quad (1.28) \]

\[ \mathbb{E}[|X_t|] = \mathbb{E} \left[ e^{(b - \frac{1}{2} \text{Re} \sigma^2)t + \sigma W_t} |X_0| \right] = e^{\left( b - \frac{\sigma^2}{2} \right) t} |X_0|, \quad (1.29) \]

\[ \mathbb{E}[|X_t|^2] = \mathbb{E} \left[ e^{(2b - \sigma^2)t + 2\sigma W_t} |X_0|^2 \right] = e^{(2b + |\sigma|^2)t} |X_0|^2. \quad (1.30) \]

**Remark 1.2.11.** Consider the case of the non-scalar real linear SDE with multiplicative real noise

\[ dY_t = AY_t \, dt + \sum_{j=1}^m B_j Y_t \, dW_t^j, \quad (1.31) \]

where \( W_t \in \mathbb{R}^m \) and \( A, B_j \in \mathbb{R}^{d \times d} \) are constant matrices and commute, i.e.

\[ [A, B_j] := AB_j - B_j A = 0, \quad [B_j, B_k] = 0, \quad \forall k, j = 1, \ldots, m. \quad (1.32) \]

The exact solution of \( (1.31) \) is then (see [6])

\[ Y_t = \exp \left( \left( A - \frac{1}{2} \sum_{j=1}^m B_j^2 \right) t + \sum_{j=1}^m B_j W_t^j \right) Y_0. \quad (1.33) \]

**Remark 1.2.12.** Since every complex SDE in \( \mathbb{C}^d \) with Brownian motion in \( \mathbb{R}^m \) can be rewritten as a real SDE in \( \mathbb{R}^{2d} \), an exact solution can be found through \( (1.33) \) for complex linear SDEs of the type

\[ dX_t = AX_t \, dt + \sum_{j=1}^m B_j X_t \, dW_t^j, \text{ with } W_t \in \mathbb{R}^m, \quad A, B_j \in \mathbb{C}^{d \times d}, \quad (1.34) \]

provided \( (1.32) \) is satisfied.

**Proof of Remark 1.2.12** first rewrite \( (1.34) \) as a real system by defining

\[ Y_t := \begin{pmatrix} X_r \\ X_i \end{pmatrix} \in \mathbb{R}^{2d}, \quad \tilde{A} := \begin{pmatrix} A_r & -A_i \\ A_i & A_r \end{pmatrix} \in \mathbb{R}^{2d \times 2d}, \quad \tilde{B}_j := \begin{pmatrix} B^j_r \\ B^j_i \end{pmatrix} \in \mathbb{R}^{2d \times 2d}, \quad j = 1, \ldots, m, \]

\[ Y_t = \exp \left( \tilde{A} Y_t \, dt + \sum_{j=1}^m \tilde{B}_j Y_t \, dW_t^j \right) Y_0. \quad (1.35) \]

It is easy to see that from \([A, B_j] = [B_j, B_k] = 0\) follows immediately \([\tilde{A}, \tilde{B}_j] = [\tilde{B}_j, \tilde{B}_k] = 0, \quad k, j = 1, \ldots, m.\) Therefore, using Remark 1.2.11 the solution of \( (1.35) \) is

\[ Y_t = \exp \left( \tilde{A} - \frac{1}{2} \sum_{j=1}^m \tilde{B}_j^2 \right) t + \sum_{j=1}^m \tilde{B}_j W_t^j \right) Y_0. \]
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The matrix \( R \in \mathbb{R}^{2d \times 2d} \) has the same blockwise skew symmetric structure as \( \tilde{A}, \tilde{B}_j \), namely

\[
R =: \begin{pmatrix}
M & -N \\
N & M
\end{pmatrix},
\]

where in this case

\[
M = \left\{ \begin{array}{c}
A_r + \frac{1}{2} \sum_{j=1}^{m} \left[ \left( B^j_i \right)^2 - \left( B^j_r \right)^2 \right] \\
t + \sum_{j=1}^{m} B^j_i W^j_t \end{array} \right\} \in \mathbb{R}^{d \times d},
\]

\[
N = \left\{ \begin{array}{c}
A_i - \frac{1}{2} \sum_{j=1}^{m} \left( B^j_i B^j_l + B^j_l B^j_i \right) \\
t + \sum_{j=1}^{m} B^j_i W^j_t \end{array} \right\} \in \mathbb{R}^{d \times d}.
\]

Any power of a blockwise skew symmetric matrix stays blockwise skew symmetric. Therefore, it holds that

\[
e^R =: \begin{pmatrix}
S & -T \\
T & S
\end{pmatrix},
\]

where \( S(t, W_t), T(t, W_t) \in \mathbb{R}^{d \times d} \), and the solution of the complex SDE (1.34) is

\[
X_t = (S + iT)X_0.
\]

Proof: the complex Brownian motion \( W \) obviously satisfies the SDE

\[
dW_t = 0 \cdot dt + I_m \, dW_t.
\]
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Now define

\[ Z_t = U(t, W_t) = \exp \left( At + \sum_{j=1}^{m} B_j W_t^j \right) Z_0 \]  

(1.40)

and compute its derivatives

\[ \frac{\partial U}{\partial t} = AZ_t, \quad \frac{\partial U}{\partial W^k} = B_k Z_t. \]

Since \( A, B_1, \ldots, B_m \) all commute with each other, one can write for any \( k = 1, \ldots, m, \quad \ell = 1, \ldots, d \):

\[ U^\ell(t, W) = \left( e^{At + \sum_{j \neq k} B_j W^j} \right)_\ell \cdot e^{B_k W^k} Z_0, \]

where \( M_\ell, \cdot \) denotes the \( \ell \)th row of the matrix \( M \). From this form, it is obvious that \( U^\ell \)

is holomorphic in \( W^k \) for every \( k, \ell \), hence

\[ \frac{\partial U^\ell}{\partial W^k} = 0, \quad \frac{\partial U^\ell}{\partial W^k} = \frac{\partial U^\ell}{\partial W^k}, \quad \frac{\partial U^\ell}{\partial W^k} = -\frac{\partial U^\ell}{\partial W^k}. \]

Since \( U \) is componentwise holomorphic, use Theorem 1.2.9 to check the SDE for \( Z_t \):

\[ dZ_t = \left\{ \frac{\partial U}{\partial t} + \sum_{k=1}^{m} a^k \frac{\partial U}{\partial W^k} \right\} dt + \sum_{j=1}^{m} \sum_{k=1}^{m} b_{kj} \frac{\partial U}{\partial W^k} dW_t^j \]

\[ = A Z_t dt + \sum_{j=1}^{m} B_j Z_t dW_t^j. \]

1.2.3. Stratonovich stochastic differential equations

So far, only Itô SDEs were considered, yet the second integral in (1.14) does not have to be an Itô stochastic integral. In fact, it can be argued that other choices make more sense depending on the context, see for example the discussion in Section 3.3 of [69]. If one interprets the stochastic integral in (1.14) as a Stratonovich stochastic integral, the corresponding Stratonovich SDE is written as

\[ X_t = X_{t_0} + \int_{t_0}^{t} a(s, X_s) \, ds + \int_{t_0}^{t} b(s, X_s) \, dW_s \]

(1.41)
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in its integral form, respectively as

\[ \text{d}X_t = a(t, X_t) \text{d}t + b(t, X_t) \circ \text{d}W_t \tag{1.42} \]

in its differential form. As opposed to the Itô integral, the Stratonovich integral is not a martingale. However, it has the advantage of satisfying the chain rule of classical calculus, hence the Itô rule (real or complex) does not hold for Stratonovich SDEs. Instead, if \( X_t \) is the solution of (1.42) and \( U \in C([0, T] \times \mathbb{R}^d, \mathbb{R}^N) \), the process defined by \( Y_t = U(t, X_t) \) satisfies the following Stratonovich SDE

\[ \text{d}Y^\ell_t = \left\{ \frac{\partial U^\ell}{\partial t} + \sum_{k=1}^{d} a_k(t, X_t) \frac{\partial U^\ell}{\partial x_k} \right\} \text{d}t + \sum_{j=1}^{m} \sum_{k=1}^{d} b^{k,j}(t, X_t) \frac{\partial U^\ell}{\partial x_k} \circ \text{d}W^j_t, \quad \ell = 1, \ldots, N. \tag{1.43} \]

Note that the Itô and Stratonovich formulations represent different interpretations of the meaning of (1.14), hence (1.13) and (1.42) have different solution processes. But if the process \( X_t \) satisfies the Itô SDE (1.13), it is also a solution to the Stratonovich SDE

\[ \text{d}X_t = a(t, X_t) \text{d}t + b(t, X_t) \circ \text{d}W_t, \tag{1.44} \]

with modified drift

\[ a^\ell(t, X) = a^\ell(t, X) - \frac{1}{2} \sum_{j=1}^{m} \sum_{k=1}^{d} b^{k,j}(t, X) \frac{\partial b^{\ell,j}}{\partial x_k}(t, X), \quad \ell = 1, \ldots, N. \tag{1.45} \]

The same holds of course in the opposite direction: if \( X_t \) satisfies the Stratonovich SDE (1.44), it is also a solution to the Itô SDE (1.13) with

\[ a^\ell(t, X) = a^\ell(t, X) + \frac{1}{2} \sum_{j=1}^{m} \sum_{k=1}^{d} b^{k,j}(t, X) \frac{\partial b^{\ell,j}}{\partial x_k}(t, X), \quad \ell = 1, \ldots, N. \tag{1.46} \]

Therefore, once the choice of the interpretation of the integral has been made, only one type of SDE needs to be discussed, as the other can be derived from it. For the rest of this thesis, unless specified otherwise, all SDEs will be Itô SDEs.

For more details about Itô and Stratonovich calculus, see [57] and [59].

1.3. A short introduction to coherent states

In this section, the quantum mechanics notation necessary for the next chapters will be briefly introduced. Coherent states were first mentioned by Glauber in [45] in the field of quantum optics, and have since then been investigated by many authors. In this thesis however, only the boson case will be considered, and the coherent states of interest (indeed, the only ones that will be looked into) are the canonical coherent states, i.e. those generated by the ladder operators. For a broader overview about coherent states, the author recommends looking into [41], [55], [56] and [75].
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**Definition 1.3.1.** The ladder operators $\hat{a}^\dagger, \hat{a}$ are the creation and annihilation operators (also known as raising and lowering operators) of the boson field, which are associative and satisfy the relation

$$[\hat{a}, \hat{a}^\dagger] = \hat{a} \hat{a}^\dagger - \hat{a}^\dagger \hat{a} = 1,$$

(1.47)

where the bracket $[\cdot, \cdot]$ is the commutator.

**Remark 1.3.2.** In this thesis, normal ordering will not be used, hence $\hat{a}$ and $\hat{a}^\dagger$ are not commutative, as follows from (1.47). For a definition of normal ordering, see [52].

**Definition 1.3.3.** Following the Dirac notation, a quantum state will be denoted by a ket, which is a notation for a vector $|\psi\rangle$ in a Hilbert space (or state space) $\mathcal{H}$ with inner product $(\cdot, \cdot)_{\mathcal{H}}$, where $\psi$ is an element of the corresponding label space $\mathcal{L}$ (which is $\mathbb{C}$ for the one-mode case covered by this thesis). Of particular interest are the number states (or Fock states)

$$|k\rangle := \frac{1}{\sqrt{k!}} (\hat{a}^\dagger)^k |0\rangle,$$

where $k \in \mathbb{N}$ and $|0\rangle$ is the vacuum state. Every ket $|\psi\rangle$ has a dual bra $\langle \psi |$, a linear functional defined by

$$\langle \psi | : \mathcal{H} \to \mathbb{C}, \langle \psi | (|\varphi\rangle) = \langle \psi | |\varphi\rangle := (|\psi\rangle, |\varphi\rangle)_{\mathcal{H}},$$

(1.48)

if the physics convention about inner products is respected, i.e. $(\cdot, \cdot)_{\mathcal{H}}$ is linear in the second argument. The following short-hand notation will be used:

$$\langle \psi | \varphi \rangle := \langle \psi | |\varphi\rangle.$$

(1.49)

The bra corresponding to the number state $|k\rangle$ is

$$\langle k | = \frac{1}{\sqrt{k!}} (0| \hat{a})^k.$$

Since kets are elements of a Hilbert space, it obviously follows from the vector space properties that they commute with any scalar (in the case seen here: with any complex number). For any $\psi \in \mathcal{L}$ the bra $\langle \psi |$ is the dual (also called Hermitian conjugate) of the ket $|\psi\rangle$, i.e. $|\psi\rangle^\dagger = \langle \psi |$ where $\langle \psi |$ is defined by (1.48).

**Remark 1.3.4.** Note that the number states $|k\rangle$, $k = 0, \ldots, \infty$, are the eigenstates of the quantum harmonic oscillator and form an orthonormal basis for the one-mode Hilbert space. The following properties hold

$$\langle 0 | 0 \rangle = 1,$$

$$\hat{a} | 0 \rangle = 0,$$

and its Hermitian conjugate

$$\langle 0 | \hat{a}^\dagger = 0,$$

(1.50)

(1.51)

(1.52)
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from which can be derived

\[ \hat{a} (\hat{a}^\dagger)^k |0\rangle = k (\hat{a}^\dagger)^{k-1} |0\rangle, \text{ for } k \geq 0, \]  
\[ (\langle 0| \hat{a}^\dagger (\hat{a}^\dagger)^{\ell} |0\rangle = k! \delta_{k\ell}, \text{ for } k, \ell \geq 0, \]  
\[ \hat{a} |k\rangle = \sqrt{k} |k-1\rangle, \text{ for } k \geq 1, \]  
\[ \hat{a}^\dagger |k\rangle = \sqrt{k+1} |k+1\rangle, \text{ for } k \geq 0, \]  
\[ (\hat{a}^\dagger)^k |k\rangle = k^k |k\rangle, \text{ for } k, \ell \geq 0, \text{ thus } \]  
\[ e^{\eta (\hat{a}^\dagger \hat{a})^2} |k\rangle = e^{\eta k^2} |k\rangle, \text{ for } k \geq 0, \eta \in \mathbb{C} \text{ and therefore } \]  
\[ e^{-iHt/\hbar} |k\rangle = e^{-ik^2t/2} |k\rangle, \text{ for } k \geq 0, \]  

where \( \hat{H} = \frac{\hbar}{2} (\hat{a}^\dagger \hat{a})^2 \) is the one-mode version of the BEC Hamiltonian (see Chapter 2), \( \hbar \) is Planck's constant and \( \hat{n} := \hat{a}^\dagger \hat{a} \) is the number operator, so called because

\[ \hat{n} |n\rangle \overset{1.57}{=} n |n\rangle, \text{ for } n \in \mathbb{N}. \]  

Proof of (1.53): Induction over \( k \): \( k = 0 \) follows immediately from (1.51).

\[ k \rightarrow k + 1 : \hat{a} (\hat{a}^\dagger)^k |0\rangle \overset{1.49}{=} (1 + \hat{a}^\dagger \hat{a}) (\hat{a}^\dagger)^k |0\rangle = (\hat{a}^\dagger)^k |0\rangle + \hat{a}^\dagger \hat{a} (\hat{a}^\dagger)^k |0\rangle \overset{\text{Ind.}}{=} ((\hat{a}^\dagger)^k + \hat{a}^\dagger k (\hat{a}^\dagger)^{k-1}) |0\rangle = (k+1)(\hat{a}^\dagger)^k |0\rangle \]  

Proof of (1.54):

- **Case** \( k = \ell \geq 0 \): one needs to show:

\[ \langle 0| \hat{a}^k (\hat{a}^\dagger)^k |0\rangle = k! \]  

Induction over \( k \): case \( k = 0 \) trivial as \( \langle 0|0\rangle = 1 \), for \( k = 1 \) it holds

\[ \langle 0| \hat{a} \hat{a}^\dagger |0\rangle \overset{1.49}{=} \langle 0|0\rangle + \langle 0| \hat{a}^\dagger \hat{a} |0\rangle \overset{1.50, 1.51}{=} 1. \]  

Induction step \( k \rightarrow k + 1 \):

\[ \langle 0| \hat{a}^{k+1} (\hat{a}^\dagger)^{k+1} |0\rangle \overset{1.47}{=} \langle 0| \hat{a}^{k} (\hat{a}^\dagger)^{k} |0\rangle + \langle 0| \hat{a}^{k} \hat{a}^\dagger (\hat{a}^\dagger)^{k} |0\rangle \overset{\text{(Ind.)}, 1.53}{=} k! + k \langle 0| \hat{a}^{k} (\hat{a}^\dagger)^{k} |0\rangle \overset{\text{(Ind.)}}{=} (k+1)! \]  

- **Case** \( \ell > k \): one has to show that

\[ \langle 0| \hat{a}^{k} (\hat{a}^\dagger)^{\ell} |0\rangle = 0, \forall \ell > k. \]  

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Induction over \( k \): \( k = 0 \) obvious because of (1.52) and \( \ell \geq 1 \).

Induction step \( k \to k + 1 \): consider \( \ell + 1 > k + 1 \), thus

\[
\langle 0 | \hat{a}^{k+1} \left( \hat{a}^\dagger \right)^{\ell+1} | 0 \rangle \overset{(\text{Ind.})}{=} \langle 0 | \hat{a}^k \left( \hat{a}^\dagger \right)^{\ell} \hat{a} \left( \hat{a}^\dagger \right)^{\ell} | 0 \rangle
\]

\[
\overset{(\text{Ind.})}{=} 0.
\]

- **Case** \( \ell < k \): similarly, one has to show that

\[
\langle 0 | \hat{a}^k \left( \hat{a}^\dagger \right)^{\ell} | 0 \rangle = 0, \forall \ell < k.
\]

Induction over \( \ell \): \( \ell = 0 \) obvious because of (1.51) and \( k \geq 1 \).

Induction step \( \ell \to \ell + 1 \): identical as the proof of the \( \ell > k \) case. \( \Box \)

Proof of (1.55): By the definition of \( |k\rangle \), it follows

\[
\hat{a} |k\rangle = \hat{a} \frac{1}{\sqrt{k!}} \left( \hat{a}^\dagger \right)^k |0\rangle \overset{(1.53)}{=} \sqrt{k} |k - 1\rangle.
\]

The relation (1.56) follows directly from the definition of \( |k\rangle \); (1.57) can be shown by using (1.55) and (1.56) recursively. By using (1.57), one can show easily that (1.58) and (1.59) hold, and see that the Fock states are orthonormal:

\[
\langle k | \ell \rangle = \delta_{k\ell}, \forall k, \ell \in \mathbb{N}.
\]

For \( \alpha \in \mathbb{C} \), the expression \( \|\alpha\rangle \), defined by

\[
\|\alpha\rangle := \exp \left( \alpha \hat{a}^\dagger \right) |0\rangle,
\]

is an unnormalized coherent state (or Bargmann states). Since

\[
\hat{a} \|\alpha\rangle = \alpha \|\alpha\rangle
\]

holds, it is an eigenvector (or eigenstate) of the annihilation operator, hence it is a minimal uncertainty state (see the connection in [56], Section 7.1). Similarly, its dual \( \langle \alpha \| := \langle 0 | \exp (\overline{\alpha} \hat{a}) \) satisfies

\[
\langle \alpha \| \hat{a}^\dagger = \overline{\alpha} \langle \alpha \|.
\]

Proof of (1.66):

\[
\hat{a} \|\alpha\rangle = \hat{a} \exp (\alpha \hat{a}^\dagger) |0\rangle = \sum_{j=0}^{\infty} \frac{\alpha^j}{j!} \hat{a} \left( \hat{a}^\dagger \right)^j |0\rangle \overset{(1.63)}{=} \sum_{j=0}^{\infty} \frac{\alpha^j}{j!} j! (\hat{a}^\dagger)^{j-1} |0\rangle
\]

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\[ \ell = j - 1 = \alpha \sum_{\ell=0}^{\infty} \frac{\alpha^{\ell}}{\ell!} (\hat{a}^\dagger)^{\ell} |0\rangle = \alpha \exp(\alpha \hat{a}^\dagger) |0\rangle = \alpha |\alpha\rangle. \]

Property (1.67) can be shown easily by taking the Hermitian conjugate of (1.66) and using the fact that scalars and kets/bras commute.

The normalized coherent state

\[ |\alpha\rangle := \exp\left(-\frac{1}{2} |\alpha|^2\right) |\alpha\rangle \]  

and its dual \( \langle \alpha | \) also displays the properties (1.66) and (1.67), respectively, as well as

\[ \langle \alpha | \alpha \rangle = e^{-|\alpha|^2} \sum_{k,\ell \geq 0} \frac{\alpha^k}{k!} \frac{\alpha^{\ell}}{\ell!} \langle 0 | \hat{a}^k \hat{a}^{\dagger \ell} | 0 \rangle = e^{-|\alpha|^2} \sum_{k \geq 0} \frac{|\alpha|^{2k}}{k!} = 1. \]

Remark 1.3.5. The coherent state representation displays some interesting properties. One of them is the partition of unity (also called resolution of unity or completeness), which is the fact that the identity operator \( I \) on \( \mathcal{H} \) can be represented as

\[ I = \frac{1}{\pi} \int |\alpha\rangle \langle \alpha | \ d\alpha, \]  

see [41] for a proof. From (1.69), it is easy to see that any arbitrary state \( |\psi\rangle \) can be represented as

\[ |\psi\rangle = \frac{1}{\pi} \int |\alpha\rangle \langle \alpha | \psi \rangle \ d\alpha, \]

which means that only the diagonal elements of the density matrix

\[ \rho = \int |\alpha\rangle \langle \beta | P(\alpha, \beta) \ d\alpha \ d\beta \]

are actually needed as a basis. This is known as the overcompleteness of the coherent states basis.

Remark 1.3.6. For any \( m \geq 1 \), the following relations hold:

\[ \left( \hat{a}^\dagger \hat{a} \right)^m |\alpha\rangle = \left( \alpha \frac{\partial}{\partial \alpha} \right)^m |\alpha\rangle, \]  

\[ \langle \alpha | \left( \hat{a}^\dagger \hat{a} \right)^m = \left( \alpha \frac{\partial}{\partial \alpha} \right)^m \langle \alpha | \]

Proof of (1.70): Induction over \( m \) (note that any combination of \( \hat{a}^\dagger \) and \( \hat{a} \) commute with \( \alpha \in \mathbb{C} \)):

\[ m = 1 : \quad \hat{a}^\dagger \hat{a} |\alpha\rangle \]  

\[ m \rightarrow m + 1 : \quad \left( \hat{a}^\dagger \hat{a} \right)^{m+1} |\alpha\rangle \]  

\[ \boxed{\hat{a}^\dagger \alpha \exp(\alpha \hat{a}^\dagger) |0\rangle = \alpha \frac{\partial}{\partial \alpha} \exp(\alpha \hat{a}^\dagger) |0\rangle = \alpha \frac{\partial}{\partial \alpha} |\alpha\rangle} \]

\[ = \left( \alpha \frac{\partial}{\partial \alpha} \right)^{m+1} |\alpha\rangle \]  

□

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1. Preliminaries

The validity of (1.71) can be demonstrated in the same way.

In this thesis, the Schrödinger picture will be used. This means that, in an isolated system, the states are evolving in time, rather than the observables operators (see below) like in the Heisenberg picture. The time-evolution operator $U(t,t_0)$ yields the ket $|\psi(t)\rangle$ by acting on $|\psi(t_0)\rangle$, such that $|\psi(t)\rangle = U(t,t_0)|\psi(t_0)\rangle$ is the solution to the Schrödinger equation

$$i\hbar \frac{\partial |\psi(t)\rangle}{\partial t} = \hat{H} |\psi(t)\rangle$$

(1.72)

with initial condition $|\psi(t_0)\rangle$ at $t = t_0$. In the case where the system Hamiltonian $\hat{H}$ is time-independent (as for the one-mode version of the BEC Hamiltonian considered in the next chapters), one has

$$U(t,t_0) = \exp(-i\hat{H}(t-t_0)/\hbar),$$

hence the time-evolution of $|\alpha_0\rangle = |\alpha(0)\rangle$ is

$$|\alpha(t)\rangle := \exp(-i\hat{H}t/\hbar)|\alpha_0\rangle.$$  

Of particular importance in later chapters is the notion of observables. An observable is a physical property of the system (e.g. energy, position, momentum, spin, etc.), described mathematically by a self-adjoint linear operator $\hat{O}$ on the separable Hilbert space $\mathcal{H}$, i.e. satisfying $\hat{O}^\dagger = \hat{O}$. The expectation value of the observable described by $\hat{O}$ can be computed in two different ways. The expectation value of $\hat{O}$ in the state $|\alpha(t)\rangle$ is

$$\langle \hat{O}\rangle_{t,\alpha} := \langle \alpha(t)|\hat{O}|\alpha(t)\rangle.$$  

(1.73)

It can also be computed using the density matrix, a positive definite Hermitian operator which, in the cases treated in this thesis, can be written in the form

$$\hat{\rho} = \int P(C,t)\hat{\Lambda}(C)\,dC,$$  

(1.74)

where $C$ is a set of configuration variables, $P$ is a probability density function (pdf) and $\hat{\Lambda}$ is called the kernel (see [27]). Note that density matrices satisfy the von Neumann’s equation

$$\frac{\partial \hat{\rho}}{\partial t} = -\frac{i}{\hbar} \left[\hat{H},\hat{\rho}\right],$$

(1.75)

which will also be called the master equation later on. The expectation value of $\hat{O}$ is then

$$\langle \hat{O}\rangle_{\hat{\rho}} := \text{Tr}[\hat{O}\hat{\rho}]/\text{Tr}[\hat{\rho}],$$

(1.76)
where one recalls that the trace of an operator $\hat{O} : \mathcal{H} \to \mathcal{H}$ can be computed as described in [73] using any countable orthonormal basis $|\varphi_k\rangle$ of $\mathcal{H}$ as

$$\text{Tr}[\hat{O}] = \sum_k \langle \varphi_k | \hat{O} | \varphi_k \rangle.$$  \hspace{1cm} (1.77)

In particular, when considering the one-mode Hilbert space with the number states as a basis, one obtains

$$\text{Tr}[\hat{O}] = \sum_{k=0}^{\infty} \langle k | \hat{O} | k \rangle.$$  \hspace{1cm} (1.78)

Note that (1.73) only is valid when $|\alpha(t)\rangle$ is a pure state (i.e. a state that can be described by a ket and whose time-evolution is governed by the Schrödinger equation (1.72)), while (1.76) is a more general definition. However, whenever defined, both expressions yield the same expectation value.

In this thesis, the importance of observables will be primarily as reference solutions to which the numerical approximations to the solutions of SDEs will be compared (how to derive these SDEs will be explained in Chapter 2), since in the cases considered, $\langle \hat{O}(t)_{t,\alpha_0}(a \text{ function of the time } t \text{ and the initial value } \alpha_0) \rangle$ and $\langle \hat{O} \rangle_{\rho}$ (a function of $C$) can be computed explicitly. A more convenient variant of (1.76) for our simulation purposes is

$$\langle \hat{O} \rangle_{\rho} = \frac{\text{Tr}[\hat{O} \hat{\Lambda}(C)]}{\text{Tr}[\hat{\Lambda}(C)]} \frac{\int \text{Tr}[\hat{\Lambda}(C)] P(C) \, dC}{\int \text{Tr}[\hat{\Lambda}(C)] P(C) \, dC} = \frac{E\text{Tr}[\hat{\Lambda}]}{E\text{Tr}[\hat{\Lambda}]}.$$  \hspace{1cm} (1.79)

where the last equality only holds true when $P$ is a probability density function. In the context of SDEs, (1.79) can be approximated as

$$\mathcal{O} = \frac{1}{N} \sum_{j=1}^{N} \text{Tr}[\hat{\Lambda}(C_j)]$$  \hspace{1cm} (1.80)

where the samples $C_j$ are $N$ simulated paths of the corresponding SDE.

**Remark 1.3.7.** Note that in the numerical discussions of Chapter 3, the shorthand notation

$$\hat{O}_t := \langle \hat{O} \rangle_{t,\alpha_0}$$  \hspace{1cm} (1.81)

will be used.
1. Preliminaries
2. The Simulation of Bose-Einstein condensation using stochastic differential equations

The simulation of Bose-Einstein condensation (BEC) through related SDEs has the advantage of allowing the consideration of a few bulk properties without having to deal with the enormous size of the associate Hilbert space. The price to pay for this is that the obtained SDEs are very unstable numerically, even for a simplified case such as the one-mode case described in [31]. In this chapter, it will be shown how, starting from the master equation (1.75), the various SDEs for the one-mode BEC that are investigated in this thesis can be derived. A discussion about the stability issues one has to expect when solving the SDEs are included in Section 2.2.2 and Section 2.4.1. A selection of metrics used to assess the accuracy of the simulations will be introduced in Section 2.5.

2.1. The Deuar and Drummond SDE

In [31], Deuar and Drummond derived the following gauge-modified autonomous SDE describing the evolution of the one-mode BEC anharmonic oscillator:

\[ d\phi = [n(1 - i) - 2G(T + i)] dt + \sqrt{2} dW^1, \quad (2.1) \]
\[ d\psi = [\overline{n}(1 - i) - 2\overline{G}(T - i)] dt + \sqrt{2} dW^2, \quad (2.2) \]
\[ d\bar{\theta} = -2T[G^2 + \overline{G}^2] dt + \sqrt{2} (\overline{G} dW^2 - G dW^1), \quad (2.3) \]

where \( W^1, W^2 \) are i.i.d. real Brownian motions, \( \phi, \psi \in \mathbb{C}, \bar{\theta} \in \mathbb{R}, T = \tan(\bar{\theta}), n = \alpha \beta \) with

\[ \alpha = \exp \left( \frac{1 - i}{2} \phi \right), \quad (2.4) \]
\[ \beta = \exp \left( \frac{1 - i}{2} \psi \right), \quad (2.5) \]

and \( G, \overline{G} \) are the following functions with free parameter \( \mu \in \mathbb{R} \):

\[ G = \frac{\mu}{2} [n_i - n_r + |\alpha|^2], \quad (2.6) \]
2. Simulation of Bose-Einstein condensation

\[ \mathcal{G} = \frac{\mu}{2} [n_i + n_r - |\beta|^2]. \]  

(2.7)

In order to stick to the notation of Chapter 1, one introduces the following variables:

\[ X_t^1 := \text{Re} (\phi_t), \ X_t^2 := \text{Im} (\phi_t), \ X_t^3 := \text{Re} (\psi_t), \ X_t^4 := \text{Im} (\psi_t), \ X_t^5 := \tilde{\theta}_t. \]

Using this notation, one can write (2.1)-(2.3) as

\[ dX_t = a(X_t) \, dt + b(X_t) \, dW_t, \]

(2.8)

where \( W_t = (W^1, W^2)^\top \), and the drift vector \( a(X_t) := (a_1(X_t), \ldots, a_5(X_t))^\top \) and diffusion matrix \( b(X_t) \in \mathbb{R}^{5 \times 2} \) are defined as follows (where \( \delta := \frac{1}{4}(X_t^2 - X_t^1 + X_t^3 - X_t^4) \)):

\[
a_1(X_t) = \exp \left( \frac{1}{2} \sum_{j=1}^{4} X_t^j \right) (\cos(\delta) + \sin(\delta)) \]

\[- \mu \tan(X_t^5) \left[ \exp \left( \frac{1}{2} \sum_{j=1}^{4} X_t^j \right) (\sin(\delta) - \cos(\delta)) + \exp(X_t^1 + X_t^2) \right], \]

(2.9)

\[
a_2(X_t) = \exp \left( \frac{1}{2} \sum_{j=1}^{4} X_t^j \right) (\sin(\delta) - \cos(\delta)) (1 - \mu) - \mu \exp(X_t^1 + X_t^2), \]

(2.10)

\[
a_3(X_t) = \exp \left( \frac{1}{2} \sum_{j=1}^{4} X_t^j \right) (\cos(\delta) - \sin(\delta)) \]

\[- \mu \tan(X_t^5) \left[ \exp \left( \frac{1}{2} \sum_{j=1}^{4} X_t^j \right) (\cos(\delta) + \sin(\delta)) - \exp(X_t^3 + X_t^4) \right], \]

(2.11)

\[
a_4(X_t) = \exp \left( \frac{1}{2} \sum_{j=1}^{4} X_t^j \right) (\cos(\delta) + \sin(\delta)) (\mu - 1) - \mu \exp(X_t^3 + X_t^4), \]

(2.12)

\[
a_5(X_t) = - \frac{\mu^2}{2} \tan(X_t^5) \left[ 2 \exp \left( \sum_{j=1}^{4} X_t^j \right) \right] \]

\[ + 2 \exp \left( \frac{1}{2} \sum_{j=1}^{4} X_t^j \right) \left( (\sin(\delta) - \cos(\delta)) \exp(X_t^1 + X_t^2) \right. \]

\[- (\sin(\delta) + \cos(\delta)) \exp(X_t^3 + X_t^4) \left] + \exp(2(X_t^1 + X_t^2)) + \exp(2(X_t^3 + X_t^4)) \right], \]

(2.13)

\[
b_{1,1}^{1,1}(X_t) = b_{3,2}^{3,2}(X_t) = \sqrt{2}, \]

(2.14)
2.2. The $\alpha, \beta$-SDE

$$b^{5,1}(X_t) = -\frac{\mu}{\sqrt{2}} \left( \exp \left( \frac{1}{2} \sum_{j=1}^{4} X^j_t \right) (\sin(\delta) - \cos(\delta)) + \exp \left( X^1_t + X^2_t \right) \right), \quad (2.15)$$

$$b^{5,2}(X_t) = \frac{\mu}{\sqrt{2}} \left( \exp \left( \frac{1}{2} \sum_{j=1}^{4} X^j_t \right) (\sin(\delta) + \cos(\delta)) - \exp \left( X^3_t + X^4_t \right) \right), \quad (2.16)$$

$$b^{i,j}(X_t) = 0, \text{ for all other } i, j. \quad (2.17)$$

When solving (2.1)-(2.3) numerically, it quickly became clear that standard SDE solvers where not giving the results one could expect based on the order of the used method alone. For the case when $\alpha_0 = \beta_0 = 3$, all tested explicit stochastic Taylor methods diverged in finite time (always before $t = 1$) while implicit and semi-implicit, although returning bounded results, failed to give reliable results after $t \approx 0.3$ (see Chapter 3 for more discussion about this behaviour), even for the (empirically) optimal parameter $\mu = 0.001$. The quality of the simulation was assessed based on the metrics derived in Section 2.5.1 and on various plots which all showed that the paths were spreading out very fast.

The results of simulations using the linear and 4-1 splitting method (see Section 3.1) are shown in Figures 3.9-3.16. In particular, the results for the optimal $\mu$-value depicted in Figure 3.16 show how unstable the solution is when attempting long-time numerical integration for the $\phi, \psi, \tilde{\theta}$-SDE.

Note that (2.1)-(2.3) is in fact a transformation from an SDE in the variables $\alpha, \beta, \theta$ (see Section 2.2 for its derivation) using (2.4)-(2.5) and

$$\theta = \tilde{\theta} - n_i. \quad (2.18)$$

One advantage of this change of coordinates is the resulting additive noise in (2.1)-(2.2); yet the drift depends on $\tan(\tilde{\theta})$, which makes the simulations unstable when $\tilde{\theta} \approx (k + \frac{1}{2})\pi$, $k \in \mathbb{Z}$. Whenever simulating the $\phi, \psi, \tilde{\theta}$-SDE, the variable $\tilde{\theta}$ was therefore controlled by keeping its absolute value smaller than $g < \frac{\pi}{2}$ for all paths, usually choosing $g = 1.5$. This did not affect the simulation very much, where most realizations of $\tilde{\theta}$ were found to stay relatively close to zero anyway, but it still felt a tad artificial to do so.

This led therefore not only to new numerical methods (presented in Chapter 3), but also to the derivation of alternative SDE representations (see the next sections).

2.2. The $\alpha, \beta$-SDE

Since solving $\phi, \psi, \tilde{\theta}$-SDE (2.1)-(2.3) numerically does not yield satisfying results even for the optimal parameter choice $\mu = 0.001$ (see Section 3.1), alternative SDE representations were considered. Of particular interest is the following $\alpha, \beta$-SDE, which
2. Simulation of Bose-Einstein condensation

corresponds to the gauge choice \( \mu = 0 \) in (2.6)-(2.7):
\[
\begin{align*}
\mathrm{d} \alpha &= -i(n + \frac{1}{2}) \alpha \, \mathrm{d}t + \frac{1 - i}{\sqrt{2}} \alpha \, \mathrm{d}W^1_t, \\
\mathrm{d} \beta &= -i(\pi + \frac{1}{2}) \beta \, \mathrm{d}t + \frac{1 - i}{\sqrt{2}} \beta \, \mathrm{d}W^2_t,
\end{align*}
\]
where \( n = \alpha \cdot \beta \). These equations can also be written as a real SDE
\[
\begin{align*}
\mathrm{d} \alpha_r &= (-\alpha_r^2 \beta_i + 2 \alpha_r \alpha_i \beta_r + \alpha_i^2 \beta_i + \frac{\alpha_i}{2}) \, \mathrm{d}t + \frac{\alpha_r + \alpha_i}{\sqrt{2}} \, \mathrm{d}W^1_t =: e^1 \, \mathrm{d}t + F^{1,1} \, \mathrm{d}W^1_t, \\
\mathrm{d} \alpha_i &= (-\alpha_i^2 \beta_r + 2 \alpha_i \alpha_r \beta_i + \alpha_r^2 \beta_i + \frac{\alpha_r}{2}) \, \mathrm{d}t + \frac{\alpha_i - \alpha_r}{\sqrt{2}} \, \mathrm{d}W^1_t =: e^2 \, \mathrm{d}t + F^{2,1} \, \mathrm{d}W^1_t, \\
\mathrm{d} \beta_r &= (-\alpha_r^2 \beta_i + 2 \alpha_r \beta_r \beta_i + \alpha_i \beta_i^2 + \frac{\beta_i}{2}) \, \mathrm{d}t + \frac{\beta_r + \beta_i}{\sqrt{2}} \, \mathrm{d}W^2_t =: e^3 \, \mathrm{d}t + F^{3,2} \, \mathrm{d}W^2_t, \\
\mathrm{d} \beta_i &= (-\alpha_i^2 \beta_r + 2 \alpha_i \beta_i \beta_r + \alpha_r \beta_r^2 + \frac{\beta_r}{2}) \, \mathrm{d}t + \frac{\beta_i - \beta_r}{\sqrt{2}} \, \mathrm{d}W^2_t =: e^4 \, \mathrm{d}t + F^{4,2} \, \mathrm{d}W^2_t.
\end{align*}
\]
This SDE will be derived directly from the master equation in the next subsection.

To obtain the full \( \mu \)-dependent \( \alpha, \beta, \theta \)-SDE corresponding to the Deuar and Drummond \( \phi, \psi, \tilde{\theta} \)-SDE (2.1)-(2.3), the Itô formula (1.17) has to be applied on the transformations (2.4), (2.5) and (2.18). As mentioned above, the equations (2.19)-(2.20) correspond to the gauge choice \( \mu = 0 \), which leads to
\[
\mathrm{d} \tilde{\theta} = 0.
\]
Since \( \tilde{\theta} \) does not appear in (2.19)-(2.20), this SDE for \( \tilde{\theta} \) will mostly be ignored in the rest of this thesis.

2.2.1. Derivation of the \( \alpha, \beta \)-SDE

From Section 1.3 one knows that the density matrix of the one-mode BEC anharmonic oscillator described in [31] has to satisfy the master equation
\[
\frac{\partial \hat{\rho}}{\partial t} = -\frac{i}{\hbar} \left[ \hat{H}, \hat{\rho} \right],
\]
where
\[
\hat{H} = \frac{\hbar}{2} (\hat{a}^\dagger \hat{a})^2
\]
is the BEC Hamiltonian and \( \hat{\rho} \) the density matrix. In this section, a Fokker-Planck equation (FPE) and a corresponding SDE will be derived from (2.25). The density matrix in this case is
\[
\hat{\rho} = \int \hat{\Lambda}_N \, \mathrm{d} \alpha \mathrm{d} \beta \mathrm{d} \theta
\]
(2.27)
2.2. The $\alpha,\beta$-SDE

with configuration variables $\alpha, \beta \in \mathbb{C}$, $\theta \in \mathbb{R}$, joint probability density function $P$ and normalized kernel $\hat{\Lambda}_N := e^{-g\hat{\Lambda}}$, where $\hat{\Lambda}$ is given by

$$\hat{\Lambda} = e^{i\theta \|\alpha\rangle\langle\beta\|} + e^{-i\theta \|\beta\rangle\langle\alpha\|},$$

(2.28)

and satisfies

$$\text{Tr} [\hat{\Lambda}] = \sum_{k=0}^{\infty} \langle k | \hat{\Lambda} | k \rangle = \sum_{k=0}^{\infty} \frac{1}{k!} \langle 0 | \hat{a}^k (e^{i\theta \|\alpha\rangle\langle\beta\|} + e^{-i\theta \|\beta\rangle\langle\alpha\|} ) \left( \hat{a}^\dagger \right)^k | 0 \rangle$$

(1.67)

$$\sum_{k=0}^{\infty} \frac{1}{k!} \left[ e^{i\theta \alpha \hat{a}^\dagger \hat{a}^k} + e^{-i\theta \beta \hat{a}^\dagger \hat{a}^k} \right] = e^{i\theta \alpha} e^{\beta \hat{a}^\dagger} + e^{-i\theta \beta} e^{\alpha \hat{a}}$$

(2.29)

Note that since $P$ is real, it must also depend on $\alpha$ and $\beta$. This can be seen as follows: assuming $\frac{\partial P}{\partial \alpha} \neq 0$, one sees from

$$\frac{\partial P}{\partial r} \frac{1}{2} \begin{pmatrix} \frac{\partial P}{\partial \alpha} & +i \frac{\partial P}{\partial \beta} \\ i & 0 \end{pmatrix}$$

that $\frac{\partial P}{\partial \alpha}$ can only be zero if $\frac{\partial P}{\partial \alpha} = \frac{\partial P}{\partial \beta} = 0$, hence if $\frac{\partial P}{\partial \alpha} = 0$. The same argument can be used for $\beta$. From the master equation (2.25), one can derive (using the short-hand notation $d\mu := d\alpha d\beta d\theta$)

$$\frac{\partial \hat{\rho}}{\partial t} = \int \frac{\partial P}{\partial t} \hat{\Lambda} e^{-g} d\mu - \frac{i}{\hbar} \int \Lambda e^{-g} [\hat{\Lambda}, \hat{H}] d\mu,$$

(2.30)

where the commutator $[\hat{\Lambda}, \hat{H}]$ satisfies

$$[\hat{\Lambda}, \hat{H}] = \hbar \left[ \left( \alpha \frac{\partial}{\partial \alpha} \right)^2 + \left( \beta \frac{\partial}{\partial \beta} \right)^2 - \left( \alpha \frac{\partial}{\partial \alpha} \right)^2 - \left( \beta \frac{\partial}{\partial \beta} \right)^2 \right] \hat{\Lambda}.$$  

(2.31)

This identity will then be used to derive a partial differential equation (PDE) from (2.30).

Proof of (2.31): It follows from (2.28) and (2.26) that

$$[\hat{\Lambda}, \hat{H}] = \frac{\hbar}{2} \left[ e^{i\theta \|\alpha\rangle\langle\beta\|} \left( \hat{a}^\dagger \hat{a} \right)^2 + e^{-i\theta \|\beta\rangle\langle\alpha\|} \left( \hat{a}^\dagger \hat{a} \right)^2 \right] = (I)$$

$$- e^{i\theta} \left( \hat{a}^\dagger \hat{a} \right)^2 \|\alpha\rangle\langle\beta\| - e^{-i\theta} \left( \hat{a}^\dagger \hat{a} \right)^2 \|\beta\rangle\langle\alpha\| \right] = (IV).$$
Using (1.71), one can easily see that

\[(I) = e^{i\theta} \langle \alpha \| \beta \rangle \left( \frac{\partial}{\partial \beta} \right)^2 \hat{\Lambda}, \]

since the \(\frac{\partial}{\partial \beta} e^{-i\theta} \langle \beta \| \alpha \rangle \) part of \(\hat{\Lambda} \) does not depend on \(\beta\). Similarly, one obtains

\[(II) = \left( \frac{\partial}{\partial \alpha} \right)^2 \hat{\Lambda}, \quad (III) = \left( \frac{\partial}{\partial \alpha} \right)^2 \hat{\Lambda}, \quad (IV) = \left( \frac{\partial}{\partial \beta} \right)^2 \hat{\Lambda}, \]

which yield (2.31). □

From (2.30) and (2.31), it follows immediately that

\[
\int \frac{\partial P}{\partial t} \hat{\Lambda} e^{-g} d\mu = \frac{i}{2} \left[ \int Pe^{-g} \left( (\pi \frac{\partial}{\partial \alpha})^2 + (\bar{\beta} \frac{\partial}{\partial \beta})^2 - (\alpha \frac{\partial}{\partial \alpha})^2 - (\beta \frac{\partial}{\partial \beta})^2 \right) \hat{\Lambda} d\mu \right].
\]

(2.33)

Using partial integration, the summands in (2.33) can be rewritten as

\[
\int Pe^{-g} \left( \frac{\partial}{\partial \alpha} \right)^2 \hat{\Lambda} d\mu = - \int \frac{\partial}{\partial \alpha} (\pi Pe^{-g}) \frac{\partial}{\partial \alpha} \hat{\Lambda} d\mu + \text{boundary terms}
\]

(2.34)

\[
\int Pe^{-g} \left( \frac{\partial}{\partial \beta} \right)^2 \hat{\Lambda} d\mu = - \int \frac{\partial}{\partial \beta} (\bar{\beta} Pe^{-g}) \frac{\partial}{\partial \beta} \hat{\Lambda} d\mu + \text{boundary terms}
\]

(2.35)

\[
\int Pe^{-g} \left( \frac{\partial}{\partial \alpha} \right)^2 \hat{\Lambda} d\mu = - \int \frac{\partial}{\partial \alpha} (\alpha Pe^{-g}) \frac{\partial}{\partial \alpha} \hat{\Lambda} d\mu + \text{boundary terms}
\]

(2.36)

\[
\int Pe^{-g} \left( \frac{\partial}{\partial \beta} \right)^2 \hat{\Lambda} d\mu = - \int \frac{\partial}{\partial \beta} (\beta Pe^{-g}) \frac{\partial}{\partial \beta} \hat{\Lambda} d\mu + \text{boundary terms}
\]

(2.37)

The terms in (2.34) and (2.36) are complex conjugates of each other, as are obviously (2.35) and (2.37), too. Thus, by assuming that the boundary values vanish (which is
certainly the case for \( t = 0 \) and as long as \( \alpha, \beta, \theta \) are bounded w.p.1) and using the fact that \( (\tau - z) = -2i \bar{z}_i \), one obtains

\[
\int \frac{\partial P}{\partial t} \Delta e^{-g} \, d\mu = \int \left( \text{Im} \left\{ \frac{\partial}{\partial \alpha} \left( \alpha \frac{\partial}{\partial \alpha} (\alpha P e^{-g}) \right) \right\} + \text{Im} \left\{ \frac{\partial}{\partial \beta} \left( \beta \frac{\partial}{\partial \beta} (\beta P e^{-g}) \right) \right\} \right) \Lambda \, d\mu. \tag{2.38}
\]

In order to obtain an SDE for the \( \alpha, \beta \)-variables, the derived PDE for the probability density function \( P \) must first be written as a Fokker-Planck equation. As will be seen, this requires the use of gauges.

**Remark 2.2.1.** The Fokker-Planck equation, also known as the Kolmogorov forward equation, has the form

\[
\frac{\partial P}{\partial t} = \frac{1}{2} \sum_{i,j=1}^{d} \frac{\partial^2}{\partial x_i \partial x_j} (d_{i,j}(t, x) P) - \sum_{i=1}^{d} \frac{\partial}{\partial x_i} (a_i(t, x) P), \tag{2.39}
\]

with drift \( a(t, x) \in \mathbb{R}^d \) and diffusion matrix \( d(t, x) = b(t, x) b(t, x)^\top \in \mathbb{R}^{d \times d} \), where \( b(t, x) \in \mathbb{R}^{d \times m} \). The matrix \( d(t, x) \) is symmetric and positive semidefinite, in particular

\[
d_{i,i}(t, x) \geq 0, \forall x \in \mathbb{R}^d, \forall t \in \mathbb{R}_+, i = 1, \ldots, d. \tag{2.40}
\]

Assuming that \( a \in C^2(\mathbb{R}_+ \times \mathbb{R}^d, \mathbb{R}^d) \), \( b \in C^2(\mathbb{R}_+ \times \mathbb{R}^d, \mathbb{R}^{d \times m}) \) and \( P \in C^2(\mathbb{R}_+^d \times \mathbb{R}^d, \mathbb{R}^d) \) and \( P(x, t) \) is a probability density function in \( x \) for all \( t \geq 0 \), one can show (see [40], Section 4.3.4) that the solution \( P \) of (2.39) corresponds to the pdf of the solution process \( X_t \) of the SDE

\[
dX_t = a(t, X_t) \, dt + b(t, X_t) \, dW_t, \tag{2.41}
\]

where \( W_t \) is a Brownian motion in \( \mathbb{R}^m \). This equivalence between the Fokker-Planck equation and its corresponding SDE(s) (the SDE representation is not necessarily unique: \( b(t, x) \) and \( m \) are arbitrary, provided \( d = b b^\top \in C^2(\mathbb{R}_+ \times \mathbb{R}^d, \mathbb{R}^{d \times d}) \)) will be used to derive the sought-after SDEs.

In order to be able to rewrite (2.38) in the wished form, however, one needs the following identities:

\[
\frac{\partial}{\partial \alpha} \left( \alpha \frac{\partial}{\partial \alpha} (\alpha P e^{-g}) \right) = \frac{\partial^2}{\partial \alpha^2} (\alpha^2 P e^{-g}) - \frac{\partial}{\partial \alpha} (\alpha P e^{-g}), \tag{2.42}
\]

\[
\frac{\partial}{\partial \beta} \left( \beta \frac{\partial}{\partial \beta} (\beta P e^{-g}) \right) = \frac{\partial^2}{\partial \beta^2} (\beta^2 P e^{-g}) - \frac{\partial}{\partial \beta} (\beta P e^{-g}), \tag{2.43}
\]

\[
\alpha_i \frac{\partial}{\partial \alpha_i} (e^{-g}) - \alpha_r \frac{\partial}{\partial \alpha_r} (e^{-g}) = - \beta_i \frac{\partial}{\partial \beta_i} (e^{-g}) + \beta_r \frac{\partial}{\partial \beta_r} (e^{-g}), \tag{2.44}
\]

\[
\left( \frac{\alpha_i \alpha_i}{2} \frac{\partial^2}{\partial \alpha_i^2} - \frac{\partial^2}{\partial \alpha_i \partial \alpha_r} \right) (e^{-g}) + \frac{\alpha_i^2 - \alpha_r^2}{2} \frac{\partial^2}{\partial \alpha_r \partial \alpha_i} (e^{-g})
\]
2. Simulation of Bose-Einstein condensation

\[
-\left(\frac{\beta_2}{2} \left[ \frac{\partial^2}{\partial \beta^2} - \frac{\partial^2}{\partial z^2} \right] + \frac{\beta_i^2 - \beta_r^2}{2} \frac{\partial^2}{\partial \beta_r \partial \beta_i} \right) (e^{-g}).
\]  

(2.45)

Using (2.42) and remembering that for \( z \in \mathbb{C} \)

\[
\frac{\partial}{\partial z} := \frac{1}{2} \left( \frac{\partial}{\partial z_r} - i \frac{\partial}{\partial z_i} \right),
\]

(2.46)

one derives

\[
\text{Im} \left\{ \frac{\partial}{\partial \alpha} \left( \frac{\partial}{\partial \alpha} (\alpha P e^{-g}) \right) \right\} = \text{Im} \left\{ \frac{\partial^2}{\partial \alpha^2} (\alpha^2 P e^{-g}) - \frac{\partial}{\partial \alpha} (\alpha Pe^{-g}) \right\}
\]

\[
= \frac{\partial^2}{\partial \alpha^2} \left( \frac{\partial}{\partial \alpha} (\alpha^2 Pe^{-g}) \right) - \frac{\partial^2}{\partial \alpha_i \partial \alpha_i} \left( \frac{\text{Im} \{i \alpha^2\}}{2} Pe^{-g} \right) - \frac{\partial^2}{\partial \alpha_r^2} \left( \frac{\text{Im} \{\alpha^2\}}{4} Pe^{-g} \right)
\]

\[
- \frac{\partial}{\partial \alpha_r} \left( \frac{\alpha_i}{2} Pe^{-g} \right) + \frac{\partial}{\partial \alpha_i} \left( \frac{\alpha_r}{2} Pe^{-g} \right)
\]

\[
= \frac{\partial^2}{\partial \alpha^2} \left( \frac{\alpha_r \alpha_i}{2} Pe^{-g} \right) - \frac{\partial^2}{\partial \alpha_i^2} \left( \frac{\alpha_r \alpha_i}{2} Pe^{-g} \right) + \frac{\partial^2}{\partial \alpha_r \partial \alpha_i} \left( \frac{\alpha_i^2 - \alpha_r^2}{2} Pe^{-g} \right)
\]

\[
- \frac{\partial}{\partial \alpha_r} \left( \frac{\alpha_i}{2} Pe^{-g} \right) + \frac{\partial}{\partial \alpha_i} \left( \frac{\alpha_r}{2} Pe^{-g} \right),
\]

(2.47)

which of course holds for its \( \beta \)-counterpart as well. It follows that

\[
\text{Im} \left\{ \frac{\partial}{\partial \beta} \left( \frac{\partial}{\partial \beta} (\beta Pe^{-g}) \right) \right\}
\]

\[
\left[ 2 \alpha_i \frac{\partial}{\partial \alpha_r} (e^{-g}) - 2 \alpha_r \frac{\partial}{\partial \alpha_i} (e^{-g}) + 2 \beta_i \frac{\partial}{\partial \beta_r} (e^{-g}) - 2 \beta_r \frac{\partial}{\partial \beta_i} (e^{-g}) \right]
\]

\[
\left[ \frac{\alpha_r \alpha_i}{2} \left[ \frac{\partial^2}{\partial \alpha_i^2} - \frac{\partial^2}{\partial \alpha_i^2} \right] + \frac{\alpha_i^2 - \alpha_r^2}{2} \frac{\partial^2}{\partial \alpha_r \partial \alpha_i} + \frac{\beta_r \beta_i}{2} \left[ \frac{\partial^2}{\partial \beta_r^2} - \frac{\partial^2}{\partial \beta_i^2} \right] + \frac{\beta_i^2 - \beta_r^2}{2} \frac{\partial^2}{\partial \beta_r \partial \beta_i} \right] (e^{-g}) \right] P
\]

\[
= 0
\]

\[
\left[ \frac{\alpha_r \alpha_i}{2} \frac{\partial}{\partial \alpha_r} (e^{-g}) + \frac{\alpha_i^2 - \alpha_r^2}{2} \frac{\partial}{\partial \alpha_i} (e^{-g}) \right] \frac{\partial P}{\partial \alpha_r}
\]

\[
= \beta
\]

\[
\left[ \frac{\alpha_r \alpha_i}{2} \frac{\partial}{\partial \alpha_i} (e^{-g}) + \frac{\alpha_i^2 - \alpha_r^2}{2} \frac{\partial}{\partial \alpha_i} (e^{-g}) \right] \frac{\partial P}{\partial \alpha_i}
\]

\[
= \gamma
\]

\[
\left[ \beta_r \beta_i \frac{\partial}{\partial \beta_r} (e^{-g}) + \frac{\beta_i^2 - \beta_r^2}{2} \frac{\partial}{\partial \beta_i} (e^{-g}) \right] \frac{\partial P}{\partial \beta_r}
\]

\[
= \delta
\]

\[
= \epsilon
\]
2.2. The $\alpha, \beta$-SDE

$$+ \left[ \beta_r \beta_i \frac{\partial}{\partial \beta_i} (e^{-g}) + \frac{\beta_i^2 - \beta_r^2}{2} \frac{\partial}{\partial \beta_r} (e^{-g}) \right] \frac{\partial P}{\partial \beta_i}$$

$$+ \frac{1}{2} \left[ -\alpha_i \frac{\partial}{\partial \alpha_i} (e^{-g}) + \alpha_r \frac{\partial}{\partial \alpha_i} (e^{-g}) - \beta_i \frac{\partial}{\partial \beta_r} (e^{-g}) + \beta_r \frac{\partial}{\partial \beta_i} (e^{-g}) \right] P$$

$$+ \frac{e^{-g}}{2} \left\{ -\frac{\partial}{\partial \alpha_i} (\alpha_r P) + \frac{\partial}{\partial \alpha_i} (\alpha_r P) - \frac{\partial}{\partial \beta_r} (\beta_i P) + \frac{\partial}{\partial \beta_i} (\beta_r P) \right\} (2.48)$$

It can be shown that

$$\tilde{a} = e^{-g} \left[ -\alpha_r \alpha_i (\beta_r + \beta_i \tan(\tilde{\theta})) + \frac{\alpha_r^2 - \alpha_i^2}{2} (\beta_r - \beta_i \tan(\tilde{\theta})) \right], \quad (2.49)$$

$$\tilde{b} = e^{-g} \left[ \alpha_r \alpha_i (\beta_i - \beta_r \tan(\tilde{\theta})) + \frac{\alpha_r^2 - \alpha_i^2}{2} (\beta_i + \beta_r \tan(\tilde{\theta})) \right], \quad (2.50)$$

$$\tilde{c} = e^{-g} \left[ -\beta_r \beta_i (\alpha_r - \alpha_i \tan(\tilde{\theta})) + \frac{\beta_r^2 - \beta_i^2}{2} (\alpha_r + \alpha_i \tan(\tilde{\theta})) \right], \quad (2.51)$$

and that it holds

$$\frac{\partial}{\partial \alpha_i} (e^g \tilde{a}) + \frac{\partial}{\partial \alpha_i} (e^g \tilde{b}) + \frac{\partial}{\partial \beta_i} (e^g \tilde{c}) + \frac{\partial}{\partial \beta_i} (e^g \tilde{d}) = 0, \quad (2.53)$$

from which follows

$$\tilde{a} \frac{\partial P}{\partial \alpha_i} + \tilde{b} \frac{\partial P}{\partial \alpha_i} + \tilde{c} \frac{\partial P}{\partial \beta_i} + \tilde{d} \frac{\partial P}{\partial \beta_i} \quad (2.54)$$

This yields with $(2.38)$ and $(2.48)$ the following PDE:

$$\frac{\partial P}{\partial t} = \frac{\partial^2}{\partial \alpha_i^2} \left\{ \frac{\alpha_r \alpha_i}{2} P \right\} + \frac{\partial^2}{\partial \alpha_i^2} \left\{ -\frac{\alpha_r \alpha_i}{2} P \right\}$$

$$+ \frac{\partial^2}{\partial \beta_i^2} \left\{ \beta_r \beta_i \frac{1}{2} P \right\} + \frac{\partial^2}{\partial \beta_i^2} \left\{ -\beta_r \beta_i \frac{1}{2} P \right\}$$

$$+ \frac{\partial^2}{\partial \alpha_i \partial \alpha_i} \left\{ \frac{\alpha_i^2 - \alpha_r^2}{2} P \right\} + \frac{\partial^2}{\partial \beta_i \partial \beta_i} \left\{ \frac{\beta_i^2 - \beta_r^2}{2} P \right\}$$

$$+ \frac{\partial}{\partial \alpha_r} \left\{ \left( \frac{\alpha_i}{2} + \tilde{a} e^g \right) P \right\} + \frac{\partial}{\partial \alpha_i} \left\{ \left( \frac{\alpha_r}{2} + \tilde{b} e^g \right) P \right\}$$

$$+ \frac{\partial}{\partial \beta_i} \left\{ \left( \frac{\beta_i}{2} + \tilde{c} e^g \right) P \right\} + \frac{\partial}{\partial \beta_i} \left\{ \left( \frac{\beta_r}{2} + \tilde{d} e^g \right) P \right\}. \quad (2.55)$$
2. Simulation of Bose-Einstein condensation

So far, the PDE \( (2.55) \) is (ultra)hyperbolic and the resulting diffusion matrix \( d \) is not positive semidefinite, since \( d_{1,1} = -d_{2,2} = \alpha_r \alpha_i \) and \( d_{3,3} = -d_{4,4} = \beta_r \beta_i \). In order to ensure that \( d_{ii} \geq 0 \), one makes use of the following identities (or gauges):

\[
\begin{align*}
\left( \frac{\partial^2}{\partial \theta^2} + 1 \right) \hat{\Lambda} &= 0, \\
\left( \frac{\partial^2}{\partial \theta \partial \alpha_i} + \frac{\partial}{\partial \alpha_r} \right) \hat{\Lambda} &= 0, \\
\left( \frac{\partial^2}{\partial \theta \partial \beta_i} + \frac{\partial}{\partial \beta_r} \right) \hat{\Lambda} &= 0, \\
\left( \frac{\partial^2}{\partial \alpha_i^2} + \frac{\partial^2}{\partial \beta_i^2} \right) \hat{\Lambda} &= 0, \\
\left( \frac{\partial^2}{\partial \theta \partial \alpha_r} - \frac{\partial}{\partial \alpha_i} \right) \hat{\Lambda} &= 0, \\
\left( \frac{\partial^2}{\partial \theta \partial \beta_r} + \frac{\partial}{\partial \beta_i} \right) \hat{\Lambda} &= 0.
\end{align*}
\]

(2.56) (2.57) (2.58) (2.59) (2.60) (2.61) (2.62)

These can be multiplied with arbitrary functions \( G_1, \ldots, G_7 \) and rewritten into zero-integrals. This yields, respectively,

\[
0 = \int G_1 P e^{-g} \left( \frac{\partial^2}{\partial \theta^2} + 1 \right) \hat{\Lambda} \, d\mu = \int \left( \frac{\partial^2}{\partial \theta^2} + 1 \right) \left( e^{-g} G_1 P \right) \hat{\Lambda} \, d\mu
\]

(2.63)

\[
= \int \left[ \left( e^{-g} + \frac{\partial e^{-g}}{\partial \theta^2} \right) G_1 P + 2 \frac{\partial e^{-g}}{\partial \theta} \frac{\partial}{\partial \theta} \left\{ G_1 P \right\} + e^{-g} \frac{\partial^2}{\partial \theta^2} \left\{ G_1 P \right\} \right] \hat{\Lambda} \, d\mu
\]

(2.63)

\[
= \int \left[ 2(1 + \tan^2(\tilde{\theta})) e^{-g} G_1 P + 2 \tan(\tilde{\theta}) e^{-g} \frac{\partial}{\partial \theta} \left\{ G_1 P \right\} + e^{-g} \frac{\partial^2}{\partial \theta^2} \left\{ G_1 P \right\} \right] \hat{\Lambda} \, d\mu
\]

(2.63)

\[
0 = \int G_2 P e^{-g} \left( \frac{\partial^2}{\partial \theta \partial \alpha_i} + \frac{\partial}{\partial \alpha_r} \right) \hat{\Lambda} \, d\mu = \int \left( \frac{\partial^2}{\partial \theta \partial \alpha_i} + \frac{\partial}{\partial \alpha_r} \right) \left( G_2 P e^{-g} \right) \hat{\Lambda} \, d\mu
\]

(2.63)

\[
= \int \left[ \left( \frac{\partial e^{-g}}{\partial \alpha_i \partial \theta} - \frac{\partial e^{-g}}{\partial \alpha_r} \right) G_2 P + \frac{\partial e^{-g}}{\partial \alpha_i} \frac{\partial}{\partial \theta} \left\{ G_2 P \right\} + \frac{\partial e^{-g}}{\partial \theta} \frac{\partial}{\partial \alpha_i} \left\{ G_2 P \right\} \right. \\
\left. + \left( \frac{\partial^2}{\partial \alpha_i \partial \theta} \left\{ G_2 P \right\} - \frac{\partial}{\partial \alpha_r} \left\{ G_2 P \right\} \right) e^{-g} \right] \hat{\Lambda} \, d\mu
\]
\[ 2.2. \text{The } \alpha, \beta\text{-SDE} \]

\[
0 = \int \left[ 2\beta_r (1 + \tan^2(\tilde{\theta})) G_2 P + \tan(\tilde{\theta}) \frac{\partial}{\partial \alpha_i} \left\{ G_2 P \right\} \right. \\
+ \left. (-\beta_i + \beta_r \tan(\tilde{\theta})) \frac{\partial}{\partial \theta} \left\{ G_2 P \right\} + \frac{\partial^2}{\partial \alpha_i \partial \theta} \left\{ G_2 P \right\} - \frac{\partial}{\partial \alpha_r} \left\{ G_2 P \right\} \right] e^{-g} \hat{\Lambda} d\mu \\
= \int \left[ \frac{\partial^2}{\partial \alpha_i \partial \theta} \left\{ G_2 P \right\} - \frac{\partial}{\partial \alpha_r} \left\{ G_2 P \right\} + \frac{\partial}{\partial \alpha_i} \left\{ \tan(\tilde{\theta}) G_2 P \right\} \\
+ \frac{\partial}{\partial \theta} \left\{ (-\beta_i + \beta_r \tan(\tilde{\theta})) G_2 P \right\} \right] e^{-g} \Lambda d\mu ,
\tag{2.64}
\]

\[
0 = \int G_3 P e^{-g} \left( \frac{\partial^2}{\partial \theta \partial \beta_i} - \frac{\partial}{\partial \beta_r} \right) \hat{\Lambda} d\mu = \int \left( \frac{\partial^2}{\partial \theta \partial \beta_i} + \frac{\partial}{\partial \beta_r} \right) (G_3 P e^{-g}) \hat{\Lambda} d\mu \\
= \int \left[ \left( \frac{\partial^2}{\partial \theta \partial \beta_i} + \frac{\partial}{\partial \beta_r} \right) \frac{e^{-g}}{G_3 P} G_3 P + \frac{\partial}{\partial \theta} \left\{ \frac{e^{-g}}{G_3 P} G_3 P \right\} + \frac{\partial}{\partial \beta_i} \left\{ \frac{e^{-g}}{G_3 P} G_3 P \right\} \\
+ \left( \frac{\partial^2}{\partial \beta_i \partial \theta} \left\{ G_3 P \right\} + \frac{\partial}{\partial \beta_r} \left\{ G_3 P \right\} \right) e^{-g} \right] \hat{\Lambda} d\mu \\
= \int \left[ -2\alpha_r (1 + \tan^2(\tilde{\theta})) G_3 P + \tan(\tilde{\theta}) \frac{\partial}{\partial \beta_i} \left\{ G_3 P \right\} \\
- (\alpha_i + \alpha_r \tan(\tilde{\theta})) \frac{\partial}{\partial \theta} \left\{ G_3 P \right\} + \frac{\partial^2}{\partial \beta_i \partial \theta} \left\{ G_3 P \right\} + \frac{\partial}{\partial \beta_i} \left\{ \tan(\tilde{\theta}) G_3 P \right\} \\
+ \frac{\partial}{\partial \theta} \left\{ (-\alpha_i - \alpha_r \tan(\tilde{\theta})) G_3 P \right\} \right] e^{-g} \Lambda d\mu ,
\tag{2.65}
\]

\[
0 = \int G_4 P e^{-g} \left( \frac{\partial^2}{\partial \alpha^2} + \frac{\partial^2}{\partial \alpha_i^2} \right) \hat{\Lambda} d\mu = \int \left( \frac{\partial^2}{\partial \alpha_i^2} + \frac{\partial^2}{\partial \alpha^2} \right) (G_4 P e^{-g}) \hat{\Lambda} d\mu \\
= \int \left[ \left( \frac{\partial^2}{\partial \alpha_i^2} + \frac{\partial^2}{\partial \alpha^2} \right) \frac{e^{-g}}{G_4 P} G_4 P + \frac{\partial}{\partial \alpha_r} \left\{ \frac{e^{-g}}{G_4 P} G_4 P \right\} + 2 \frac{\partial}{\partial \alpha_i} \left\{ \frac{e^{-g}}{G_4 P} G_4 P \right\} \\
+ \left( \frac{\partial^2}{\partial \alpha_i^2} \left\{ G_4 P \right\} + \frac{\partial^2}{\partial \alpha^2} \left\{ G_4 P \right\} \right) e^{-g} \right] \hat{\Lambda} d\mu \\
= \int \left[ 2 \beta_r^2 + \frac{\beta_i^2}{\cos^2(\tilde{\theta})} G_4 P + 2 (-\beta_r - \beta_i \tan(\tilde{\theta})) \frac{\partial}{\partial \alpha_r} \left\{ G_4 P \right\} \\
+ 2 (-\beta_i + \beta_r \tan(\tilde{\theta})) \frac{\partial}{\partial \alpha_i} \left\{ G_4 P \right\} + \frac{\partial^2}{\partial \alpha_i^2} \left\{ G_4 P \right\} + \frac{\partial^2}{\partial \alpha^2} \left\{ G_4 P \right\} \right] e^{-g} \Lambda d\mu 
\]
2. Simulation of Bose-Einstein condensation

\begin{equation}
0 = \int G_5 P e^{-g} \left( \frac{\partial^2}{\partial \beta_i^2} + \frac{\partial^2}{\partial \beta_r^2} \right) \Lambda \, d\mu = \int \left( \frac{\partial^2}{\partial \beta_i^2} + \frac{\partial^2}{\partial \beta_r^2} \right) \left( G_5 P e^{-g} \right) \Lambda \, d\mu
\end{equation}

\begin{equation}
= \int \left[ \left( \frac{\partial^2 e^{-g}}{\partial \beta_i^2} + \frac{\partial^2 e^{-g}}{\partial \beta_r^2} \right) G_5 P + 2 \frac{\partial e^{-g}}{\partial \beta_i} \frac{\partial}{\partial \beta_i} \left\{ G_5 P \right\} + 2 \frac{\partial e^{-g}}{\partial \beta_r} \frac{\partial}{\partial \beta_r} \left\{ G_5 P \right\} \right] e^{-g} \Lambda \, d\mu
\end{equation}

\begin{equation}
= \int \left[ 2 \frac{\alpha_i^2 + \alpha_r^2}{\cos^2(\theta)} G_5 P + 2(-\alpha_r + \alpha_i \tan(\tilde{\theta})) \frac{\partial}{\partial \beta_i} \left\{ G_5 P \right\} \right] e^{-g} \Lambda \, d\mu
\end{equation}

\begin{equation}
= \int \left[ \frac{\partial^2}{\partial \beta_i^2} \left\{ G_5 P \right\} + \frac{\partial^2}{\partial \beta_r^2} \left\{ G_5 P \right\} + \frac{\partial}{\partial \beta_i} \left\{ 2(-\alpha_r + \alpha_i \tan(\tilde{\theta})) G_5 P \right\} \right] e^{-g} \Lambda \, d\mu
\end{equation}

\begin{equation}
= \int \left[ \frac{\partial^2}{\partial \beta_i^2} \left\{ G_5 P \right\} + \frac{\partial^2}{\partial \beta_r^2} \left\{ G_5 P \right\} + \frac{\partial}{\partial \beta_i} \left\{ -2(\alpha_i + \alpha_r \tan(\tilde{\theta})) G_5 P \right\} \right] e^{-g} \Lambda \, d\mu,
\end{equation}

(2.67)

\begin{equation}
0 = \int G_6 P e^{-g} \left( \frac{\partial^2}{\partial \theta \partial \alpha_r} - \frac{\partial}{\partial \alpha_i} \right) \Lambda \, d\mu = \int \left( \frac{\partial^2}{\partial \alpha_i \partial \theta} + \frac{\partial}{\partial \alpha_i} \right) \left( G_6 P e^{-g} \right) \Lambda \, d\mu
\end{equation}

\begin{equation}
= \int \left[ \left( \frac{\partial e^{-g}}{\partial \alpha_r \partial \theta} + \frac{\partial e^{-g}}{\partial \alpha_i} \right) G_6 P + \frac{\partial e^{-g}}{\partial \alpha_r} \frac{\partial}{\partial \alpha_r} \left\{ G_6 P \right\} + \frac{\partial e^{-g}}{\partial \theta} \frac{\partial}{\partial \alpha_r} \left\{ G_6 P \right\} \right]
\end{equation}

\begin{equation}
= \int \left[ -2 \beta_r (1 + \tan^2(\tilde{\theta})) G_6 P + \tan(\tilde{\theta}) \frac{\partial}{\partial \alpha_r} \left\{ G_6 P \right\} \right] e^{-g} \Lambda \, d\mu
\end{equation}

\begin{equation}
= \int \left[ \frac{\partial^2}{\partial \alpha_i \partial \theta} \left\{ G_6 P \right\} + \frac{\partial}{\partial \alpha_r} \left\{ \tan(\tilde{\theta}) G_6 P \right\} + \frac{\partial}{\partial \alpha_i} \left\{ G_6 P \right\} \right] e^{-g} \Lambda \, d\mu
\end{equation}

\begin{equation}
= \int \left[ \frac{\partial^2}{\partial \alpha_i \partial \theta} \left\{ G_6 P \right\} + \frac{\partial}{\partial \alpha_r} \left\{ \tan(\tilde{\theta}) G_6 P \right\} + \frac{\partial}{\partial \alpha_i} \left\{ G_6 P \right\} \right] e^{-g} \Lambda \, d\mu,
\end{equation}

(2.68)
Hence, one obtains the following gauge-modified FPE:

\[
0 = \int G_T e^{-g} \left( \frac{\partial^2}{\partial \theta^2} + \frac{\partial}{\partial \beta_i} \right) \hat{\Lambda} \, d\mu = \int \left( \frac{\partial^2}{\partial \beta_i \partial \theta} - \frac{\partial}{\partial \beta_i} \right) \left( G_T e^{-g} \right) \hat{\Lambda} \, d\mu \\
= \int \left[ \left( \frac{\partial^2 e^{-g}}{\partial \beta_i \partial \theta} - \frac{\partial e^{-g}}{\partial \beta_i} \right) G_T P + \frac{\partial e^{-g}}{\partial \theta} \left\{ G_T P \right\} + \frac{\partial e^{-g}}{\partial \beta} \left\{ G_T P \right\} \right] \hat{\Lambda} \, d\mu \\
+ \left( \frac{\partial^2}{\partial \beta_i \partial \theta} \left\{ G_T P \right\} - \frac{\partial}{\partial \beta_i} \left\{ G_T P \right\} \right) e^{-g} \hat{\Lambda} \, d\mu \\
= \int \left[ \frac{\partial^2}{\partial \beta_i \partial \theta} \left\{ G_T P \right\} + \frac{\partial}{\partial \beta_i} \left\{ \tan(\bar{\theta}) G_T P \right\} - \frac{\partial}{\partial \beta_i} \left\{ G_T P \right\} \right] e^{-g} \hat{\Lambda} \, d\mu \\
+ \frac{\partial}{\partial \theta} \left\{ \left( -\alpha_r + \alpha_i \tan(\bar{\theta}) \right) G_T P \right\} \right] e^{-g} \hat{\Lambda} \, d\mu. \quad (2.69)
\]

Hence, one obtains the following gauge-modified FPE:

\[
\frac{\partial P}{\partial t} = \frac{1}{2} \left[ \frac{\partial^2}{\partial \alpha_i^2} \left\{ (\alpha_r \alpha_i + 2G_4) P \right\} + \frac{\partial^2}{\partial \alpha_r \partial \alpha_i} \left\{ (\alpha_r^2 - \alpha_i^2) P \right\} + \frac{\partial^2}{\partial \alpha_r \partial \theta} \left\{ 2G_6 P \right\} \right.
\]
\[
+ \frac{\partial^2}{\partial \alpha_i^2} \left\{ (-\alpha_r \alpha_i + 2G_4) P \right\} + \frac{\partial^2}{\partial \alpha_i \partial \theta} \left\{ 2G_2 P \right\} + \frac{\partial^2}{\partial \beta_i^2} \left\{ (\beta_r \beta_i + 2G_5) P \right\} \right.
\]
\[
+ \frac{\partial^2}{\partial \beta_i \partial \beta_r} \left\{ 2G_3 P \right\} + \frac{\partial^2}{\partial \theta^2} \left\{ 2G_1 P \right\} \right.
\]
\[
+ \frac{\partial}{\partial \alpha_r} \left\{ \left( -\frac{\alpha_i}{2} + \bar{a} \bar{e}^g - G_2 - 2(\beta_r + \beta_i \tan(\bar{\theta})) G_4 + \tan(\bar{\theta}) G_6 \right) P \right\} \right.
\]
\[
+ \frac{\partial}{\partial \alpha_i} \left\{ \left( \frac{\alpha_r}{2} + \bar{b} \bar{e}^g + G_2 \tan(\bar{\theta}) + 2(-\beta_i + \beta_r \tan(\bar{\theta})) G_4 + G_6 \right) P \right\} \right.
\]
\[
+ \frac{\partial}{\partial \beta_r} \left\{ \left( -\frac{\beta_i}{2} + \bar{c} \bar{e}^g + G_3 + 2(-\alpha_r + \alpha_i \tan(\bar{\theta})) G_5 + \tan(\bar{\theta}) G_7 \right) P \right\} \right.
\]
\[
+ \frac{\partial}{\partial \beta_i} \left\{ \left( \frac{\beta_r}{2} + \bar{d} \bar{e}^g + \tan(\bar{\theta}) G_3 - 2(-\alpha_r + \alpha_i \tan(\bar{\theta})) G_5 - G_7 \right) P \right\} \right.
\]
\[
+ \frac{\partial}{\partial \theta} \left\{ \left( 2 \tan(\bar{\theta}) G_1 + (-\beta_i + \beta_r \tan(\bar{\theta})) G_2 - (\alpha_i + \alpha_r \tan(\bar{\theta})) G_3 \right. \right.
\]
\[
- (\beta_r + \beta_i \tan(\bar{\theta})) G_6 + (-\alpha_r + \alpha_i \tan(\bar{\theta})) G_7 \right) P \right\} \]
\]

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\[ = \frac{1}{2} \sum_{i,j=1}^{5} \frac{\partial^2}{\partial x_i \partial x_j} (d^{i,j}(x) P) - \sum_{i=1}^{5} \frac{\partial}{\partial x_i} (a_i(x) P) . \tag{2.70} \]

The diffusion matrix is thus

\[
d = \begin{pmatrix}
\alpha_r \alpha_i + 2G_4 & \frac{\alpha_i^2 - \alpha_r^2}{2} & 0 & 0 & G_6 \\
\frac{\alpha_i^2 - \alpha_r^2}{2} & -\alpha_r \alpha_i + 2G_4 & 0 & 0 & G_2 \\
0 & 0 & \beta_r \beta_i + 2G_5 & \frac{\beta_i^2 - \beta_r^2}{2} & G_7 \\
0 & 0 & \frac{\beta_i^2 - \beta_r^2}{2} & -\beta_r \beta_i + 2G_5 & G_3 \\
G_6 & G_2 & G_7 & G_3 & 2G_1
\end{pmatrix},
\]

and one can now impose the conditions that \( d^{i,i} \geq 0, \forall i = 1, \ldots, 5 \), which implies that \( G_1, G_4 \) and \( G_5 \) have to satisfy

\[
G_4 \geq \frac{\alpha_r^2 + \alpha_i^2}{4}, \tag{2.71}
\]

\[
G_5 \geq \frac{\beta_r^2 + \beta_i^2}{4}, \tag{2.72}
\]

\[
G_1 \geq 0. \tag{2.73}
\]

The eigenvalues of \( d \) are \( \lambda_1 = 2G_1, \lambda_{2,3} = 2G_4 \pm \frac{\alpha_i^2 + \alpha_r^2}{2}, \lambda_{4,5} = 2G_5 \pm \frac{\beta_i^2 + \beta_r^2}{2} \), which are all non-negative iff \( \text{(2.71)-(2.73) hold} \).

There are now several choices of \( b \in \mathbb{R}^{5 \times m} \) such that \( d = bb^\top \), depending on the coefficient functions \( G_1, \ldots, G_7 \). A natural choice for \( G_1, G_5 \) is

\[
G_4 = \frac{\alpha_r^2 + \alpha_i^2}{4}, \tag{2.74}
\]

\[
G_5 = \frac{\beta_r^2 + \beta_i^2}{4}, \tag{2.75}
\]

which obviously satisfies \( \text{(2.71)-(2.72)} \) and leads to

\[
d = \begin{pmatrix}
\frac{(\alpha_r + \alpha_i)^2}{\sqrt{2}} & \frac{\alpha_i^2 - \alpha_r^2}{\sqrt{2}} & 0 & 0 & G_6 \\
\frac{\alpha_i^2 - \alpha_r^2}{\sqrt{2}} & \frac{(\alpha_i - \alpha_r)^2}{\sqrt{2}} & 0 & 0 & G_2 \\
0 & 0 & (\beta_r + \beta_i)^2 & \frac{\beta_i^2 - \beta_r^2}{\sqrt{2}} & G_7 \\
0 & 0 & \frac{\beta_i^2 - \beta_r^2}{\sqrt{2}} & (\beta_r - \beta_i)^2 & G_3 \\
G_6 & G_2 & G_7 & G_3 & 2G_1
\end{pmatrix}.
\]

By selecting

\[
b = \begin{pmatrix}
\frac{\alpha_r + \alpha_i}{\sqrt{2}} & 0 \\
\frac{\alpha_i - \alpha_r}{\sqrt{2}} & 0 \\
0 & \frac{\beta_r + \beta_i}{\sqrt{2}} \\
0 & \frac{\beta_i - \beta_r}{\sqrt{2}} \\
b_5,1 & b_5,2
\end{pmatrix}, \tag{2.76}
\]
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with $b^{5.1}, b^{5.2}$ yet to be chosen, it follows that

\begin{align*}
G_1 &= \frac{1}{2} \left[ (b^{5.1})^2 + (b^{5.2})^2 \right], \\
G_2 &= b^{5.1} \frac{\alpha_i - \alpha_r}{\sqrt{2}}, \\
G_3 &= b^{5.2} \frac{\beta_i - \beta_r}{\sqrt{2}}, \\
G_6 &= b^{5.1} \frac{\alpha_r + \alpha_i}{\sqrt{2}}, \\
G_7 &= b^{5.2} \frac{\beta_r + \beta_i}{\sqrt{2}},
\end{align*}

(2.77)

(2.78)

(2.79)

(2.80)

(2.81)

and from (2.77) it is obvious that condition (2.73) holds. It can be seen that the four first rows of $b$ from equation (2.76) match the diffusion coefficient matrix $F$ from the SDE (2.21)-(2.24). To have the first four rows of $a$ match with the drift $e$ from (2.21)-(2.24) as well, one needs to pick

\begin{align*}
b^{5.1} &= \frac{1}{\sqrt{2}} \left[ (\alpha_r + \alpha_i)\beta_i + (\alpha_r - \alpha_i)\beta_r \right] = \frac{n_r - n_i}{\sqrt{2}}, \\
b^{5.2} &= \frac{1}{\sqrt{2}} \left[ (\beta_i - \beta_r)\alpha_r - (\beta_r + \beta_i)\alpha_i \right] = -\frac{n_r + n_i}{\sqrt{2}}.
\end{align*}

(2.82)

(2.83)

Note that all the terms in (2.70) containing the variable $\tilde{\theta}$ vanish with this choice. Thus, put into the SDE form, one obtains (2.21)-(2.24), as well as

\[ d\theta = \frac{n_r - n_i}{\sqrt{2}} dW_1^1 - \frac{n_r + n_i}{\sqrt{2}} dW_2^1. \]

(2.84)

By considering the variable $\tilde{\theta} = \theta + n_i$ and the SDE for $n_i$ (see Section 2.3), i.e.

\[ dn_i = \frac{n_i - n_r}{\sqrt{2}} dW_1^1 + \frac{n_r + n_i}{\sqrt{2}} dW_2^1, \]

(2.85)

it is clear that

\[ d\tilde{\theta} = d\theta + dn_i = 0. \]

(2.86)

This is consistent with picking $\mu = 0$ in (2.3).

**Remark 2.2.2.** Since $\theta$ is not present in (2.21)-(2.24), its SDE (2.84) will not be considered in numerical simulations of $\alpha$ and $\beta$.

2.2.2. The stability of the $\alpha, \beta$-SDE

The stability of differential equations is far from being a clear-cut notion. In fact, many definitions of stability can be found in the literature for both ODEs and SDEs, see for example [5], [10], [12], [47], [49] and [89]. A common definition of stability in the context of ODEs is the following one, which is given in [5].
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**Definition 2.2.3.** Consider the \(d\)-dimensional ODE

\[
\dot{X}_t = f(t, X_t), \quad X_{t_0} = x_0, \quad t \geq t_0,
\]

(2.87)

where it is assumed that there exists a unique solution \(X_t(x_0)\) for every \(t \geq t_0\) and every initial condition \(x_0 \in \mathbb{R}^d\), and that \(f\) is continuous in \(t\). Assume further that

\[
f(t, 0) = 0,
\]

(2.88)

meaning that \(X_t \equiv 0\) is a solution of (2.87) under the initial condition \(X_{t_0} = 0\). The solution \(X_t \equiv 0\) is said to be **stable**, if for every \(\varepsilon > 0\) there exists a \(\delta = \delta(\varepsilon, t_0) > 0\) such that for \(\|x_0\|_2 \leq \delta\), it follows that

\[
\sup_{t \in [t_0, \infty)} \|X_t(x_0)\|_2 \leq \varepsilon.
\]

(2.89)

If not, the solution \(X_t \equiv 0\) is called **unstable**.

Considering complex ODEs is not a problem, as they can easily be rewritten a real ODE system which fits the framework of Definition 2.2.3. In the SDEs treated in this chapter, the link to their corresponding real SDE is considered to be clear enough to leave them in complex form.

Note that checking directly whether (2.89) holds for a given ODE can be tricky, since the exact solution of (2.87) is generally not known. Luckily, the exact solution can be found explicitly (hence the method of Lyapunov functions described in \([5]\) can be avoided) in the case of the noiseless \(\alpha, \beta\)-SDE, i.e. the following ODE

\[
d\alpha(t) = -i(n + \frac{1}{2})\alpha\, dt,
\]

(2.90)

\[
d\beta(t) = -i(n + \frac{1}{2})\beta\, dt.
\]

(2.91)

Note that the solution of the \(\alpha\)-ODE (2.90) will be denoted by \(\alpha(t)\) to help distinguish it from the solution \(\alpha_t\) of the SDE (2.19). The same holds of course for \(\beta\) and \(n\). In order to find the solution of the ODE (2.90)-(2.91), it helps to see that \(n(t) = \alpha(t) \cdot \overline{\beta(t)}\) is a constant in this case, since

\[
dn(t) = \overline{\beta} \, d\alpha + \alpha \, d\overline{\beta} = -i(n + \frac{1}{2})n\, dt - i(n + \frac{1}{2})n\, dt = 0.
\]

(2.92)

Hence, \(n(t) \equiv n_0 = \alpha_0\overline{\beta_0}\), meaning that (2.90) and (2.91) are linear. Their solution is therefore

\[
\alpha(t) = e^{-i(n_0 + \frac{1}{2})t}\alpha_0,
\]

(2.93)

\[
\beta(t) = e^{-i(n_0 + \frac{1}{2})t}\beta_0.
\]

(2.94)
Thus, as long \( n_0 \) is strictly real, the solution processes simply orbit around zero at respective distances \(|\alpha_0|\) and \(|\beta_0|\). If \( n_0' := \text{Im} \ n_0 > 0 \), however, then \(|\alpha(t)| = e^{n_0't}|\alpha_0| \to \infty\) and \(|\beta(t)| = e^{-n_0't}|\beta_0| \to 0\) as \( t \to \infty\). Similarly, \(|\alpha(t)| \to 0\) and \(|\beta(t)| \to \infty\) as \( t \to \infty\) for \( n_0' < 0 \).

In order to put the ODE (2.90)-(2.91) into the framework of Definition 2.2.3, one needs to rewrite it as a real system in \( \mathbb{R}^4 \), e.g. by writing \( X = (\alpha_r, \alpha_i, \beta_r, \beta_i)^\top \). It is, however, not hard to see from the solution given by (2.93)-(2.94) that if \( n_0' = x_{00}^2x_0^2 - x_{00}^4 \neq 0 \), the condition (2.89) will not hold. The ODE (2.90)-(2.91) is therefore unstable.

Note that when starting with \( \alpha_0 = \beta_0 \) as an initial condition, \( n_0 = |\alpha_0|^2 \) is real, which means that \( \alpha(t) \) and \( \beta(t) \) should stay bounded, at least when solved exactly using the formulae (2.93)-(2.94). But adding stochastic noise to the ODE will automatically lead to the perturbation of the orbits through a non-vanishing \( n_i \) (in fact, \( n_i \neq 0 \) w.p.1 for \( t > 0 \), as will be shown in Section 2.3) and thus to the divergence of a growing number of paths. Hence one should expect an unstable behaviour in the context of the \( \alpha, \beta \)-SDE (2.19)-(2.20). Indeed, this is what happens when solving the SDE numerically, as can be seen throughout Chapter 3.

**Remark 2.2.4.** The ODEs (2.90)-(2.91) and SDEs (2.19)-(2.20) for \( \alpha \) and \( \beta \) have the same **critical points** 0 and \( \infty \). Note that (2.93)-(2.94) does not describe the complete picture of the dynamics of the solution to the \( \alpha, \beta \)-SDE, despite hinting at one of the causes of the instability. Indeed, when solving the SDE **numerically**, the growth of the magnitude of \( \alpha \) or \( \beta \) will for instance **not necessarily** lead to the convergence towards zero of the other variable (although it is likely). When computing one step of a method with time step \( h << 1 \), if \( |n_{t_k}| \) is very large at time \( t_k \) (say, such that \( |n_{t_k}|h > 2 \)), it is possible that the magnitude of the approximations at time \( t_{k+1} = t_k + h \) will be both larger than at time \( t_k \), i.e. \( |\alpha_{t_{k+1}}| > |\alpha_{t_k}| \) and \( |\beta_{t_{k+1}}| > |\beta_{t_k}| \).

**Remark 2.2.5.** Although zero is not a stable solution of the ODE (2.90)-(2.91), it is still an **attracting point** of both separate \( \alpha \)-SDE (2.19) and \( \beta \)-SDE (2.20), i.e. if \( \alpha^2 = 0 \) for the path labelled by \( j \) at any time \( \tau \), then for that particular path, \( \alpha^2 = 0 \) for every \( t > \tau \). For the same path \( j \), the SDE for \( \beta^j \) and \( t > \tau \) is

\[
d\beta^j_t = -\frac{i}{2} \beta^j_t \, dt + \frac{1 - i}{\sqrt{2}} \beta^j_t \, dW^2_t. \tag{2.95}
\]

Since (2.95) is linear, its solution is

\[
\beta^j_t = e^{\sqrt{-1}(W^2_t - W^2_{t-})} \beta^j_0, \tag{1.26}
\]

where \( W^2_t \) denotes the value of the \( j \)th path of the Brownian motion \( W^2 \) at time \( t \geq \tau \). Furthermore, one expects from (1.27) and (1.30) that

\[
E[\beta^j_t] = e^{-\frac{1}{2}(t-\tau)} \beta^j_0, \\
E[|\beta^j_t|^2] = e^{(t-\tau)} |\beta^j_0|^2.
\]
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So while the magnitude of the expected value of $\beta^j_t$ is constant and the expected value of its magnitude grows exponentially fast, $\beta^j_t$ can still decrease in magnitude, since $W^2_{\tau,j} - W^2_\tau$ can be negative (and will be at some time w.p.1). This illustrates again the difference between ODEs and SDEs. The same argument can of course be made for $\alpha^j_t$ if $\beta^j_\tau = 0$.

This tendency of paths to diverge (in magnitude) is of course problematic to deal with numerically, where one has to simulate a finite number of samples paths, hence one single (nearly) unbounded path is enough to render the mean of the whole sample useless, unless discarding the paths that are too large. Yet ignoring them is clearly is not the right way to go, since the presence of these paths mostly points out that the solution of the SDE is intrinsically unstable. Indeed, it is often a sign that the boundary terms dismissed so conveniently in the derivation of (2.38) cannot be ignored anymore, hence invalidating the SDE representation. This is discussed in detail in [44], where four ‘signatures’ are presented whose presence indicate non-vanishing boundary conditions. The four signatures are

1. the presence of (numerically) diverging paths,
2. an increase in the statistical error (this will of course follow if 1. holds),
3. the probability distribution function (or its numerical approximation through binning of a large sample) develops power-law tails,
4. adding a linear damping term (as in Section 3.6) helps to avoid the manifestation of the signatures 1.-3.

In the case of the $\alpha,\beta$-SDE, the first two signatures are present in every simulation (unless specific methods are used to control the simulations as done in Section 3.4.1 or Section 3.5 in which case ‘only’ signature 2. is apparent). The third and fourth items mentioned need more effort to spot and were not investigated in detail (although the linear damping case was investigated in Section 3.6 and did not seem to be able to prevent the large statistical error, see Figure 3.41).

In this thesis, one does not concern oneself so much about the validity of the model in itself. The fact that growing boundary values might break the validity of the connection between the SDE and the FPE (2.41) at some time $t_B$ does not affect the validity of (2.19)-(2.20) as an SDE on its own (although it might mean that the metrics computed in Section 2.5.1 will not be valid approximations of the moments of the process after the time of break $t_B$). The focus is on exploring methods to find reliable solutions to SDEs whose solution process is unstable, not to solve the anharmonic oscillator case physically.

One should bear in mind that SDEs which do not satisfy both Lipschitz and linear growth conditions might have no solution, no unique solution, or more interestingly, a solution existing only up to a random time $t_{dep}$ (which will be called time of departure). This is illustrated by the following example given in [44].
Example 2.2.6. The exact solution of the real one-dimensional SDE
\[ dX_t = X_t^3 \, dt - X_t^2 \, dW_t \]  \hspace{1cm} (2.96)
with initial value \( X_0 \neq 0 \) at \( t = 0 \) is given by
\[ X_t = \left( \frac{1}{X_0} + W_t \right)^{-1}. \] \hspace{1cm} (2.97)
Hence for any sample path, the solution \( X_t \) exists only until the Brownian motion hits \(-X_0^{-1}\). This can happen at any time \( t > 0 \), since \( W_t \sim N(0, t) \). In fact, the probability that it will happen eventually is 1 for any \( X_0 \neq 0 \).

Remark 2.2.7. When considering a sample of \( N \) independent simulated paths of an SDEs where the time of departure is known to be finite and random, the larger the sample, the earlier will one of the paths blow up, making the mean value of the whole sample unbounded. This is problematic, since large samples are required for meaningful statistics. The time of departure of a sample is therefore defined as the minimum \( t_{dep} \) of all its paths. If there is a minimal possible value for \( t_{dep} \) for an SDE with given conditions, one will call that value \( t_{theo} \) the theoretical first time of departure.

It would of course be possible to investigate the stability of the \( \alpha, \beta \)-SDE using other criteria (e.g. a stochastic extension of the notion of stability with respect to a property \( P \) and perturbations presented in \cite{10}, where the property \( P \) could be the boundedness of the solution). Extensive theory and various definitions of stability for SDEs exist in the literature (see e.g. \cite{4}, \cite{19}, \cite{35}), yet (as far as the author can tell) only when the drift and diffusion coefficient satisfy some variants of the Lipschitz condition and linear growth bound needed to establish the existence and uniqueness of a strong solution (see the corresponding theorem in Section 4.5 of \cite{57}). But the drift of the \( \alpha, \beta \)-SDE (2.19)-(2.20) clearly does not satisfy any non-local Lipschitz condition nor linear growth bound conditions, meaning some other fitting stability concepts would have to be found. However, the arguments shown earlier be more precise in this section combined with the ample supply of diverging results when solving the SDE numerically were deemed sufficient to convince the author of the inherent instability of the problem and of the need for new methods to stabilise its numerical solution.

In Section 2.3 the behaviour of \( n \) in the stochastic case will be investigated more carefully. Note that the importance of the imaginary part of \( n \) in the growth/decay of the solution is what motivated the methods presented in Section 3.4 and Section 3.5.

2.3. The \( n \)-SDE

Due to the crucial role of \( n = \alpha \beta \) in the (in)stability considerations of the solution of the \( \alpha, \beta \)-SDE (and its presence in the drift of both \( \alpha, \beta \)-SDE and \( \phi, \psi, \theta \)-SDE), it is logical
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to consider its corresponding SDE, which can be derived using (2.21)-(2.24) and the Itô formula. Since

\[ n = \alpha_r \beta_r + \alpha_i \beta_i + i(\alpha_i \beta_r - \alpha_r \beta_i), \]

\[ \frac{\partial n}{\partial \alpha_r} = \beta_r, \quad \frac{\partial n}{\partial \alpha_i} = i \beta_i, \quad \frac{\partial n}{\partial \beta_r} = \alpha_r, \quad \frac{\partial n}{\partial \beta_i} = -i \alpha_i. \]

it is easy to see that

\[ \frac{\partial n_r}{\partial \alpha_r} = \beta_r, \quad \frac{\partial n_r}{\partial \alpha_i} = \beta_i, \quad \frac{\partial n_r}{\partial \beta_r} = \alpha_r, \quad \frac{\partial n_r}{\partial \beta_i} = \alpha_i, \quad (2.98) \]

\[ \frac{\partial n_i}{\partial \alpha_r} = -\beta_i, \quad \frac{\partial n_i}{\partial \alpha_i} = \beta_r, \quad \frac{\partial n_i}{\partial \beta_r} = \alpha_i, \quad \frac{\partial n_i}{\partial \beta_i} = -\alpha_r. \quad (2.99) \]

Furthermore, \( \partial_t n = 0 \) and (using the notation \( x = (\alpha_r, \alpha_i, \beta_r, \beta_i)^T \in \mathbb{R}^4 \))

\[ F^{1,2} = F^{2,2} = F^{3,1} = F^{4,1} = 0, \]

\[ \frac{\partial^2 n}{\partial x_i \partial x_j} = 0, \text{ if } i,j \in \{1, 2\} \text{ or } i,j \in \{3, 4\}. \]

Therefore it holds

\[ \sum_{j=1}^{2} \sum_{i,k=1}^{4} F^{i,j} F^{k,j} \frac{\partial^2 n}{\partial x_i \partial x_k} = 0 \quad (2.100) \]

and with (2.98)-(2.100) and the real Itô formula (applied simultaneously on the real and imaginary components of \( n \))

\[ d n = \left[ 0 + e^1 \frac{\partial n}{\partial \alpha_r} + e^2 \frac{\partial n}{\partial \alpha_i} + e^3 \frac{\partial n}{\partial \beta_r} + e^4 \frac{\partial n}{\partial \beta_i} + \frac{1}{2} \cdot 0 \right] d t \]

\[ + \left( F^{1,1} \frac{\partial n}{\partial \alpha_r} + F^{2,1} \frac{\partial n}{\partial \alpha_i} \right) d W_t^1 + \left( F^{3,2} \frac{\partial n}{\partial \beta_r} + F^{4,2} \frac{\partial n}{\partial \beta_i} \right) d W_t^2 \]

\[ = \left( \frac{n_r + n_i}{\sqrt{2}} + i \frac{-n_r + n_i}{\sqrt{2}} \right) d W_t^1 + \left( \frac{n_r - n_i}{\sqrt{2}} + i \frac{n_r + n_i}{\sqrt{2}} \right) d W_t^2 \]

\[ = \frac{1 - i}{\sqrt{2}} n d W_t^1 + \frac{1 + i}{\sqrt{2}} n d W_t^2. \]

(2.101)\n
(2.102)\n
(2.103)

Defining

\[ \xi_1 = \frac{1}{\sqrt{2}} \left( W_t^1 + W_t^{2*} \right), \]

\[ \xi_2 = \frac{1}{\sqrt{2}} \left( W_t^2 - W_t^1 \right), \]

(2.104)\n
(2.105)
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one can rewrite (2.103) as

\[
dn = n \, d\xi^1_t + i \, n \, d\xi^2_t,
\]  
\( (2.106) \)

where \( \xi^1_t, \xi^2_t \) are i.i.d. real Brownian motions. Furthermore, \( n \) can be written as

\[
n_t = e^{\xi^1_t + i \xi^2_t} n_0,
\]  
\( (2.107) \)

with mean

\[
\mathbb{E}[n_t] = n_0
\]  
\( (2.108) \)

and variance

\[
\text{Var}(n_t) = |n_0|^2 \left(e^{2t} - 1\right).
\]  
\( (2.109) \)

**Remark 2.3.1.** For \( p \in \mathbb{N} \), it holds

\[
\mathbb{E}[|n|^p] = |n_0|^p e^{p^2 t/2}.
\]  
\( (2.110) \)

**Proof of Remark 2.3.1** With the definition (2.107) of \( n \), it follows that

\[
\mathbb{E}[|n|^p] = \frac{1}{2\pi t} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{px_1} |n_0|^p e^{-\frac{x_1^2}{2t}} e^{-\frac{x_2^2}{2t}} \, dx_1 \, dx_2
\]

\[
= |n_0|^p \frac{1}{\sqrt{2\pi t}} \int_{-\infty}^{\infty} e^{-\frac{(x_1-m)^2}{2t}} e^{p^2 t/2} \, dx_1
\]

\[
= |n_0|^p e^{p^2 t/2}, \quad \forall p \in \mathbb{N}. \quad \square
\]

**Proof of (2.107):** Consider

\[
B_1 = \begin{pmatrix}
-1/\sqrt{2} & 1/\sqrt{2} \\
-1/\sqrt{2} & 1/\sqrt{2}
\end{pmatrix}, \quad B_2 = \begin{pmatrix}
1/\sqrt{2} & -1/\sqrt{2} \\
1/\sqrt{2} & 1/\sqrt{2}
\end{pmatrix}.
\]

By defining \( \mathbf{n} = (n_r, n_i) \), one can thus rewrite (2.102) as

\[
d\mathbf{n} = B_1 \, dW^1_t + B_2 \, dW^2_t.
\]  
\( (2.111) \)

This is a linear real SDE with constant matrices \( B_1 \) and \( B_2 \) which commute. Therefore, from Remark 1.2.11 one knows that the solution of (2.111) is

\[
\mathbf{n}_t = \exp \left( -\frac{1}{2} \sum_{j=1}^{2} B_j^2 \, t + \sum_{j=1}^{2} B_j W^j_t \right) \mathbf{n}_0 = \exp \left( B_1 W^1_t + B_2 W^2_t \right) \mathbf{n}_0
\]

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\[
= \exp \left( \begin{pmatrix} \xi_1^1 & -\xi_2^1 \\ \xi_2^1 & \xi_1^1 \end{pmatrix} \right) n_0
\]

\[
= \begin{pmatrix} -i & i \\ 1 & 1 \end{pmatrix} \begin{pmatrix} \exp(\xi_1^1 - i\xi_2^2) & 0 \\ 0 & \exp(\xi_1^1 + i\xi_2^2) \end{pmatrix} \begin{pmatrix} -i & i \\ 1 & 1 \end{pmatrix}^{-1} n_0
\]

\[
= e^{\xi_1^1} \begin{pmatrix} \cos(\xi_2^1) & -\sin(\xi_2^1) \\ \sin(\xi_2^1) & \cos(\xi_2^1) \end{pmatrix} n_0, \tag{2.112}
\]

which is equivalent to (2.107) when rewritten as a complex expression. \(\Box\)

Proof of (2.108): Using (2.107) and remembering that \(\xi_1^1, \xi_2^1\) are i.i.d \(N(0,t)\), one can compute

\[
E[n] = \frac{1}{2\pi t} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{x_1 + x_2} n_0 e^{-\frac{x_1^2}{4t}} e^{-\frac{x_2^2}{4t}} dx_1 dx_2
\]

\[
= n_0 \frac{1}{\sqrt{2\pi t}} \int_{-\infty}^{\infty} e^{-\frac{(x_2 - iw)^2}{2t}} \left( \frac{1}{\sqrt{2\pi t}} \int_{-\infty}^{\infty} e^{-\frac{(x_1 - iw)^2}{2t}} dx_1 \right) dx_2
\]

\[
= n_0 \frac{1}{\sqrt{2\pi t}} \int_{-\infty}^{\infty} e^{-\frac{(x_2 - iw)^2}{2t}} dx_2 \tag{2.113}
\]

Proof of (2.109): From Remark 2.3.1 it follows that

\[
E[|n_t|^2] = |n_0|^2 e^{2t},
\]

thus

\[
\text{Var}(n_t) = E[|n_t - E[n_t]|^2] = E[|n_t|^2] - |E[n_t]|^2 = |n_0|^2 (e^{2t} - 1). \tag*{\Box}
\]

Remark 2.3.2. For initial conditions \(\alpha_0 = \beta_0\), it follows that \(\text{Im}[n_0] = 0\), thus (2.108) implies \(E[n_t] \in \mathbb{R}, t \geq 0\). However, even if \(n_0 \in \mathbb{R}\), it is clear from (2.107) that \(P(n_t = 0) = 0\) for any \(t > 0\) if \(n_0 \neq 0\). This does not bode well for the stability of the \(\alpha, \beta\)-SDE.

Remark 2.3.3. Note that one knows from the proof of (2.109) that

\[
E[|n_t - n_0|^2] = |n_0|^2 (e^{2t} - 1).
\]

Hence, despite the fact that \(E[n_t] = n_0\), the sample paths of \(n_t\) will quickly spread. Indeed, at time \(t = \frac{1}{2} \log(2) \approx 0.35\), the expected size of \(|n_t - n_0|^2\) is \(|n_0|^2\). At \(t = 2\pi\), one expects \(E[|n_t - n_0|^2] \approx 2.86 \cdot 10^5 |n_0|^2\). In short: one can expect a significant amount of simulated paths of both \(\alpha, \beta\)-SDE and \(n\)-SDE to grow very large.

2.4. The \(\alpha\)-SDE

The lack of stability of the \(\alpha, \beta\)-SDE (2.19)-(2.20) (see Section 2.2.2 and Chapter 3) motivated the investigation of what SDE would follow from a different representation
2.4. The $\alpha$-SDE

for the density matrix kernel. Consider the kernel

\[ \hat{\Lambda}_\alpha := \|\alpha\rangle \langle \alpha\|, \]  

(2.114)

where $\alpha \in \mathbb{C}$. The corresponding density matrix is

\[ \hat{\rho}_\alpha := \int \|\alpha\rangle \langle \alpha\| e^{-\hbar P(\alpha,t)} d\alpha. \]  

(2.115)

where the normalization factor $e^{-\hbar}$ follows from

\[ e^{\hbar} := \text{Tr}[\hat{\Lambda}_\alpha] = \sum_{k=0}^{\infty} \langle k | \hat{\Lambda}_\alpha | k \rangle = \sum_{k=0}^{\infty} \frac{1}{k!} \langle 0 | \hat{a}^k \| \alpha \| \langle \alpha | \hat{a}^k \rangle \langle 0 \rangle = \sum_{k=0}^{\infty} \frac{1}{k!} \langle 0 \langle 0 | [\hat{\Lambda}_\alpha, (\hat{a}^\dagger \hat{a})^2] d\alpha. \]  

(2.116)

Since $\hat{\rho}_\alpha$ has to satisfy the master equation

\[ \frac{d\hat{\rho}_\alpha}{dt} = -\frac{i}{\hbar} [\hat{H}, \hat{\rho}_\alpha], \]  

(2.117)

it follows that

\[ \frac{d\hat{\rho}_\alpha}{dt} = \int \frac{\partial P}{\partial t} \hat{\Lambda}_\alpha e^{-|\alpha|^2} d\alpha \]  

(2.118)

Using (1.70) and (1.71), it follows that

\[ [\hat{\Lambda}_\alpha, (\hat{a}^\dagger \hat{a})^2] = \left( \left( \frac{\alpha}{\alpha} \frac{\partial}{\partial \alpha} \right)^2 - \left( \frac{\alpha}{\alpha} \frac{\partial}{\partial \alpha} \right)^2 \right) \|\alpha\rangle \langle \alpha\|, \]  

(2.119)

which, combined with (2.118), yields

\[ \int \frac{\partial P}{\partial t} \hat{\Lambda}_\alpha e^{-|\alpha|^2} d\alpha = \frac{i}{2} \int P e^{-|\alpha|^2} \left( \left( \frac{\alpha}{\alpha} \frac{\partial}{\partial \alpha} \right)^2 - \left( \frac{\alpha}{\alpha} \frac{\partial}{\partial \alpha} \right)^2 \right) \|\alpha\rangle \langle \alpha\| d\alpha. \]  

(2.120)

As in Section 2.2.1 one can derive the following

\[ \int P e^{-|\alpha|^2} \left( \frac{\alpha}{\alpha} \frac{\partial}{\partial \alpha} \right)^2 \hat{\Lambda}_\alpha d\alpha = -\int \frac{\partial}{\partial \alpha} \left( \alpha P e^{-|\alpha|^2} \right) \frac{\alpha}{\alpha} \frac{\partial}{\partial \alpha} \hat{\Lambda}_\alpha d\alpha + \text{boundary terms} \]

\[ = \int \frac{\partial}{\partial \alpha} \left( \frac{\alpha}{\alpha} \frac{\partial}{\partial \alpha} \left( \alpha P e^{-|\alpha|^2} \right) \right) \hat{\Lambda}_\alpha d\alpha + \text{boundary terms}, \]  

(2.121)

\[ \int P e^{-|\alpha|^2} \left( \frac{\alpha}{\alpha} \frac{\partial}{\partial \alpha} \right)^2 \hat{\Lambda}_\alpha d\alpha = -\int \frac{\partial}{\partial \alpha} \left( \alpha P e^{-|\alpha|^2} \right) \frac{\alpha}{\alpha} \frac{\partial}{\partial \alpha} \hat{\Lambda}_\alpha d\alpha + \text{boundary terms} \]

\[ = \int \frac{\partial}{\partial \alpha} \left( \alpha P e^{-|\alpha|^2} \right) \hat{\Lambda}_\alpha d\alpha + \text{boundary terms}. \]  

(2.122)
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If the boundary terms vanish, plugging (2.121) and (2.122) into (2.120) and using the fact that \((z - z) = -2i \text{Im} \{z\}\) yields

\[
\int \frac{\partial}{\partial t} \hat{\Lambda}_\alpha e^{-|\alpha|^2} d\alpha = \int \text{Im} \left\{ \frac{\partial}{\partial \alpha} \left( \alpha \frac{\partial}{\partial \alpha} \left( \alpha Pe^{-|\alpha|^2} \right) \right) \right\} \hat{\Lambda}_\alpha d\alpha,
\]

(2.123)

from which follows immediately

\[
\frac{\partial}{\partial t} e^{-|\alpha|^2} = \text{Im} \left\{ \frac{\partial}{\partial \alpha} \left( \alpha \frac{\partial}{\partial \alpha} \left( \alpha Pe^{-|\alpha|^2} \right) \right) \right\}.
\]

(2.124)

In order to obtain a Fokker-Planck equation, i.e. an equation of the type (2.39), one uses the following identity (which holds for sufficiently smooth functions \(Q\))

\[
\frac{\partial}{\partial \alpha} \left( \alpha \frac{\partial}{\partial \alpha} \left( \alpha Q \right) \right) = \frac{\partial}{\partial \alpha} \left( \alpha \frac{\partial}{\partial \alpha} \left( \alpha P \right) e^{-|\alpha|^2} \right) - \frac{\partial}{\partial \alpha} \left( \alpha Pe^{-|\alpha|^2} \right).
\]

(2.125)

Thus, in the same way as in (2.47), one derives

\[
e^{-|\alpha|^2} \frac{\partial}{\partial t} = \text{Im} \left\{ \frac{\partial}{\partial \alpha} \left( \alpha \frac{\partial}{\partial \alpha} \left( \alpha Pe^{-|\alpha|^2} \right) \right) \right\} = \text{Im} \left\{ \frac{\partial^2}{\partial \alpha^2} \left( \alpha^2 Pe^{-|\alpha|^2} \right) - \frac{\partial}{\partial \alpha} \left( \alpha Pe^{-|\alpha|^2} \right) \right\}
\]

\[
= \frac{\partial^2}{\partial \alpha_r^2} \left( \frac{\alpha_r \alpha_r}{2} Pe^{-|\alpha|^2} \right) - \frac{\partial^2}{\partial \alpha_i^2} \left( \frac{\alpha_i \alpha_i}{2} Pe^{-|\alpha|^2} \right) + \frac{\partial^2}{\partial \alpha_r \partial \alpha_i} \left( \frac{\alpha_i^2 - \alpha_r^2}{2} Pe^{-|\alpha|^2} \right)
\]

\[
- \frac{\partial}{\partial \alpha_r} \left( \frac{\alpha_r}{2} Pe^{-|\alpha|^2} \right) + \frac{\partial}{\partial \alpha_i} \left( \frac{\alpha_i}{2} Pe^{-|\alpha|^2} \right).
\]

(2.126)

The normalization term \(e^{-|\alpha|^2}\) still needs to be extracted on the right-hand side in (2.126) to cancel out with its left-hand side counterpart. With some more tedious yet straightforward algebra, one can show that (2.126) is equivalent to the FPE

\[
\frac{\partial P}{\partial t} = \frac{1}{2} \left( \frac{\partial^2}{\partial \alpha_r^2} - \frac{\partial^2}{\partial \alpha_i^2} \right) \left( \alpha_r \alpha_r \right) P + \frac{1}{2} \left( \frac{\partial^2}{\partial \alpha_r \partial \alpha_i} + \frac{\partial^2}{\partial \alpha_i \partial \alpha_r} \right) \left( \frac{\alpha_i^2 - \alpha_r^2}{2} \right)
\]

\[
- \frac{\partial}{\partial \alpha_r} \left[ \alpha_r \left( |\alpha|^2 + \frac{1}{2} \right) P \right] - \frac{\partial}{\partial \alpha_i} \left[ -\alpha_r \left( |\alpha|^2 + \frac{1}{2} \right) P \right].
\]

(2.127)

As in Section 2.2.1, the diffusion matrix corresponding to (2.127) is not positive definite, meaning that extracting the SDE directly from it is not allowed. Furthermore, the gauge approach used in Section 2.2.1 will not work in this case, as no nontrivial combination of the type

\[
G := \left( \frac{\partial^2}{\partial \alpha_r^2} f + \frac{\partial^2}{\partial \alpha_i^2} g + \frac{\partial^2}{\partial \alpha_r \partial \alpha_i} h + \frac{\partial}{\partial \alpha_r} \phi + \frac{\partial}{\partial \alpha_i} \psi \right) \hat{\Lambda}_\alpha,
\]

(2.128)

where \(f, g, h, \phi, \psi\) are any \(C^2(\mathbb{R}^2, \mathbb{C})\)-functions of \(\alpha_r, \alpha_i\) will ever give \(G = 0\). This can be seen as follows:

\[
\frac{\partial}{\partial \alpha_r} \phi \hat{\Lambda}_\alpha + \frac{\partial}{\partial \alpha_i} \phi \hat{\Lambda}_\alpha + \frac{\partial}{\partial \alpha_i} \phi \hat{\Lambda}_\alpha \hat{\alpha},
\]

(2.129)
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\[
\frac{\partial}{\partial \alpha_i} \psi \hat{\Lambda}_\alpha^{(1.65)} = \left( \frac{\partial \psi}{\partial \alpha_i} + i \psi \hat{a}^\dagger \right) \hat{\Lambda}_\alpha - i \psi \hat{\Lambda}_\alpha \hat{a},
\]
\[
\frac{\partial^2}{\partial \alpha_i \partial \alpha_i} f \hat{\Lambda}_\alpha^{(2.129)} = \left( \frac{\partial^2 f}{\partial \alpha_r \partial \alpha_r} + 2 \frac{\partial f}{\partial \alpha_r} \hat{a}^\dagger + f \left( \hat{a}^\dagger \right)^2 \right) \hat{\Lambda}_\alpha + \hat{\Lambda}_\alpha \left( 2 \frac{\partial f}{\partial \alpha_r} \hat{a} + f \hat{a}^2 \right) + 2 f \hat{a}^\dagger \hat{\Lambda}_\alpha \hat{a},
\]
\[
\frac{\partial^2}{\partial \alpha_i \partial \alpha_i} g \hat{\Lambda}_\alpha^{(2.130)} = \left( \frac{\partial^2 g}{\partial \alpha_i \partial \alpha_i} + 2i \frac{\partial g}{\partial \alpha_i} \hat{a}^\dagger - g \left( \hat{a}^\dagger \right)^2 \right) \hat{\Lambda}_\alpha - \hat{\Lambda}_\alpha \left( 2i \frac{\partial g}{\partial \alpha_i} \hat{a} + g \hat{a}^2 \right) + 2g \hat{a}^\dagger \hat{\Lambda}_\alpha \hat{a},
\]
\[
\frac{\partial^2}{\partial \alpha_r \partial \alpha_i} h \hat{\Lambda}_\alpha^{(2.129)} = \left( \frac{\partial^2 h}{\partial \alpha_r \partial \alpha_i} \hat{\alpha}^\dagger + i \frac{\partial h}{\partial \alpha_r} \hat{a}^\dagger \left( \hat{a}^\dagger \right)^2 \hat{\Lambda}_\alpha + \hat{\Lambda}_\alpha \left( \frac{\partial h}{\partial \alpha_i} - i \frac{\partial h}{\partial \alpha_r} \right) \hat{a} - i \hat{a}^2 \right).
\]

In order for $G$ as defined in (2.128) to be zero, each of the individual coefficients of $\hat{\Lambda}_\alpha (= ||\alpha|| \langle \alpha \rangle |)$, $\hat{a}^\dagger \hat{\Lambda}_\alpha \hat{a}$, $\hat{a}^\dagger \hat{\Lambda}_\alpha \hat{a}$, $(\hat{a}^\dagger)^2 \hat{\Lambda}_\alpha$ and $\hat{\Lambda}_\alpha \hat{a}^2$ have to be zero, since the latter terms cannot cancel each other by linear combination alone. Hence, setting $G \equiv 0$ would mean that $f = g = h = \phi = \psi = 0$.

Although the transition from FPE to SDE is not possible directly, the passage is possible if the problem is perturbed slightly. It is easy to see that adding $\frac{\alpha^2 + \alpha^2 r}{2} I_2$ to the diffusion matrix of (2.127) yields the following SDE

\[
da = -i(\langle |\alpha|^2 + \frac{1}{2} \rangle |\alpha|^2 + \sqrt{-i} \alpha \, dW_t.
\]

Of course, this SDE does not correspond to the FPE (2.127) exactly, yet it it still an interesting problem to play with. When experimenting with it, it was seen (see Figures 3.3-3.6) that halving the diffusion coefficient in (2.134) gave results that were closer to the solution one wants to approximate (based on the metrics from Section 2.5.2 for the density matrix representation (2.115)). To reflect the fact that the solution process of (2.134) is just an arbitrary approximation to the $\alpha$ described by (2.115), consider the more general SDE with arbitrary parameter $\zeta \in \mathbb{C}$:

\[
da = -i(\langle |\alpha|^2 + \frac{1}{2} \rangle |\alpha|^2 + \zeta \sqrt{-i} \alpha \, dW_t.
\]

Using the real Itô rule (1.17), one finds the following SDE for $|\alpha|^2$

\[
d|\alpha|^2 = |\zeta|^2 |\alpha|^2 dt + \sqrt{2} (\zeta_r + \zeta_i) |\alpha|^2 dW_t,
\]

which has the exact solution

\[
|\alpha_t|^2 = |\alpha_0|^2 e^{-2\zeta_r t + \sqrt{2}(\zeta_r + \zeta_i) W_t}
\]

and expected value

\[
\mathbb{E} [|\alpha_t|^2] = |\alpha_0|^2 e^{2|\zeta|^2 t}.
\]
2. Simulation of Bose-Einstein condensation

Note that although the choice $\zeta = \frac{1}{2}$ yields reasonable results (when compared to the metrics from Section 2.5.2), its corresponding SDE (2.135) is still not a valid description of the process described by $\hat{\rho}_\alpha$, and this for any $\zeta \in \mathbb{C}$.

Whenever talking about the $\alpha$-SDE later on, the SDE (2.134) will be meant, unless otherwise specified.

2.4.1. The stability of the generalized $\alpha$-SDE

The noiseless ODE corresponding to the (generalized) $\alpha$-SDE (2.135) is

$$\, d\alpha(t) = -i(|\alpha|^2 + \frac{1}{2})\alpha \, dt. \tag{2.139}$$

As in Section 2.2.2 an exact solution can be found through the fact that

$$\, d|\alpha(t)|^2 = 0, \tag{2.140}$$

from which follows $|\alpha(t)|^2 \equiv |\alpha_0|^2$. Thus, (2.139) is linear and has solution

$$\alpha(t) = e^{-i(|\alpha_0|^2 + \frac{1}{2})t}\alpha_0. \tag{2.140}$$

Since $|\alpha(t)| \equiv |\alpha_0|$ for every $\alpha_0$, the zero solution of (2.139) is clearly stable in the sense of Definition 2.2.3 (choose $\delta = \epsilon$).

Interestingly, removing the diffusion term in the $|\alpha|^2$-SDE (2.136) yields

$$\, d|\alpha|^2(t) = |\zeta|^2 |\alpha|^2(t) \, dt, \tag{2.141}$$

which is not the same as (2.140). This might be counterintuitive, yet it is a consequence of the Itô rule, since through it the diffusion coefficient in (2.135) causes the term $|\zeta|^2 |\alpha|^2$ to appear in the drift of the SDE (2.136). The exact solution of (2.141) is

$$|\alpha|^2(t) = e^{t|\zeta|^2}|\alpha_0|^2, \tag{2.142}$$

hence the $|\alpha|^2(t) \equiv 0$ is not a stable solution of (2.141), as its solution is unbounded for any $\alpha_0 \neq 0$.

These ambiguous results should be taken as a warning about placing too much trust in one lone concept of stability, especially when dealing with SDEs for which no existence of solution or uniqueness can be proven. The generalized $\alpha$-SDE might not have the $\alpha, \beta$-SDE equivalent of the $n_t$ term in its drift (see Section 2.2.2), yet from (2.138) one expects an exponential growth for the mean of $|\alpha|^2$. Considering that and the argument below, hoping that the simulated $\alpha_t$ will stay bounded might be overoptimistic, as will be seen in Section 3.1.

One way to explain the fact that the numerical solution of the (generalized) $\alpha$-SDE (2.135) diverges is the following heuristic argument. For a short time interval $[\tau, \tau + h]$,
2.4. The $\alpha$-SDE

one can approximate the solution of (2.135) locally with a linear SDE if considering the value $|\alpha_t|^2$ to be fixed, i.e. $|\alpha_t|^2 = |\alpha_\tau|^2$, $\forall t \in [\tau, \tau + h]$. Under that assumption, from (1.26) one knows that the exact solution is

$$
\alpha_{\tau+h} = e^{-i(|\alpha_\tau|^2 + \frac{1}{2})h + \zeta \sqrt{\frac{2}{h}}(W_{\tau+h} - W_{\tau})} \alpha_{\tau},
$$

(2.143)

hence one expects from (1.27) that

$$
E[\alpha_{\tau+h}] = e^{-i(|\alpha_\tau|^2 + \frac{1}{2})h} \alpha_{\tau},
$$

(2.144)

i.e. the expected value of $\alpha_{\tau+h}$ is simply a rotation of $\alpha_{\tau}$ around the origin. However, one can also predict using (1.30) that the solution (2.143) will satisfy

$$
E[|\alpha_t|^2] = |\alpha_0|^2 e^{\frac{1}{2}t}.
$$

(2.145)

Note that interestingly, (2.145) matches the prediction for the exact $|\alpha_t|^2$ as given by (2.138). Hence, $|\alpha_t|^2$ can be expected to grow exponentially. Numerically, this will be a problem since the discretization used in most SDE methods usually involves similar local approximations of the solution. The difficulty will be illustrated for the Euler method given in Example 1.2.4. The Euler estimate of $\alpha_{\tau+h}$ is

$$
\alpha_{\text{euler}} = \alpha_{\tau} - i(|\alpha_\tau|^2 + \frac{1}{2})h \alpha_{\tau} + \zeta \sqrt{\frac{2}{h}}(W_{\tau+h} - W_{\tau}).
$$

(2.146)

If $(|\alpha_\tau|^2 + \frac{1}{2})h \approx 1$ (which is bound to happen eventually for some path) and $h << 1$, one can expect $(|\alpha_\tau|^2 + \frac{1}{2})h \gg |\zeta \sqrt{\frac{2}{h}}(W_{\tau+h} - W_{\tau})|$ and thus $\alpha_{\text{euler}} \approx \alpha_{\tau} - i\alpha_{\tau}$, i.e. $|\alpha_{\text{euler}}| \approx \sqrt{2}|\alpha_{\tau}|$. At the next step, the magnitude of the next estimate would thus be approximatively

$$
|\alpha_{\text{euler}} - i2\alpha_{\text{euler}}| = \sqrt{5}|\alpha_{\text{euler}}| \approx \sqrt{10}|\alpha_{\tau}|
$$

hence an exponential growth of the magnitude would follow (unless the phenomenon is prevented through very unlikely realizations of the Brownian motion, since $P(|W_{\tau+h} - W_{\tau}| > 8\sqrt{h}) \approx 10^{-15}$, so if $h = 10^{-3}$, $P(|W_{\tau+h} - W_{\tau}| > 0.25) = 0$ in practice).

Of course, this phenomenon is well-known in the context of ODEs, where several specific methods have been designed to deal with it (in particular the class of symplectic methods, see [46]). Symplectic methods have been developed for SDEs (see [62], [63], [65] and [66]) and can improve the stability of simulations greatly for some SDEs, but not all.

Consider that the magnitude of the exact solution of the ODE (2.139) is conserved, while one knows from (2.138) that it is not so for $|\alpha_t|^2$ in the stochastic case. Hence wanting to keep $|\alpha_t|^2$ bounded forever is probably too much to ask for.
2. Simulation of Bose-Einstein condensation

2.5. Metrics for the one-mode BEC

Since the exact solutions of SDEs (including those introduced in Section 2.1, 2.2 and 2.4) are generally not known, any available information about the stochastic processes involved is useful in order to assess the quality of the numerical solution. In the following subsections, various functionals of the solution process described in this chapter will be derived for this purpose (using either observables or more general metrics). Unfortunately, a common feature of these metrics is that they only give some information about moments of functionals of the process, and thus do not allow the reconstruction of the individual paths of the exact solutions.

Consider a general linear operator \( \hat{O} \) acting on the one-mode Hilbert space \( \mathcal{H} \) introduced in Section 1.3. If \( \hat{O} \) is not self-adjoint, it is not an observable in the sense of Section 1.3, and the quantities \( \langle \hat{O} \rangle_{t,\alpha,0} \) and \( \langle \hat{O} \rangle_{\hat{\rho}} \) (as defined in (1.73) and (1.76)) might not have any physical meaning. However, these expressions can still be computed and used to measure the quality of simulations.

The most obvious choice of operators is \( \hat{a} \) and \( \hat{a}^\dagger \) along with their respective powers \( \hat{a}^m, (\hat{a}^\dagger)^m, m \geq 1 \). Their expectations will be computed for the BEC case, depending on the kernel representation used.

2.5.1. Two states representation

In the two states representation used in Sections 2.1, 2.3 one recalls that

\[
\dot{\hat{\rho}} = \int P(\alpha, \beta, \theta, t) \hat{\Lambda}_N \, d\alpha \, d\beta \, d\theta \tag{2.147}
\]

with \( \alpha, \beta \in \mathbb{C}, \theta \in \mathbb{R} \), pdf \( P \) and normalized kernel \( \hat{\Lambda}_N := e^{-g\hat{\Lambda}}, \) where

\[
\hat{\Lambda} = e^{i\|\alpha\rangle \langle \beta\|} + e^{-i\|\beta\rangle \langle \alpha\|},
\]

\[
e^g := \text{Tr} [\hat{\Lambda}] = 2 e^{nr} \cos(\tilde{\theta}). \tag{2.149}
\]

Hence \( \text{Tr}[\hat{\Lambda}_N] = 1 \) and it follows from (1.79) that for any linear operator \( \hat{O} \)

\[
\langle \hat{O} \rangle_{\hat{\rho}} = \frac{\text{Tr}[\hat{O}\hat{\rho}]}{\text{Tr}[\hat{\rho}]} = \frac{\int \text{Tr}[\hat{O}\Lambda_N(C)] P(C) \, dC}{\int \text{Tr}[\Lambda_N(C)] P(C) \, dC} = \frac{\int \text{Tr}[\hat{O}\Lambda_N(C)] P(C) \, dC}{\int P(C) \, dC}.
\]

\[
= E \left[ \text{Tr}[\hat{\Lambda}_N] \right] = E \left[ \frac{\text{Tr}[\hat{O}\Lambda]}{\text{Tr}[\hat{\Lambda}]} \right] = E \left[ e^{-g} \text{Tr}[\hat{\Lambda}] \right]. \tag{2.150}
\]

which can be approximated by

\[
\overline{\hat{O}} \approx \frac{1}{N} \sum_{j=1}^{N} e^{-g}(C_j) \text{Tr}[\hat{O}\Lambda](C_j), \tag{2.151}
\]

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i.e. by taking the average over a sample of \( N \) simulated independent paths generated by some SDE method. Now compute

\[
\text{Tr}[\hat{a}^m \hat{A}] = \sum_{k=0}^{\infty} \langle k | \hat{a}^m \hat{A} | k \rangle = \sum_{k=0}^{\infty} \frac{1}{k!} \langle 0 | \hat{a}^{k+m} \left[ e^{i\theta} \langle \alpha | | \beta \rangle + e^{-i\theta} \langle \beta | | \alpha \rangle \right] (\hat{a}^\dagger)^k | 0 \rangle
\]

\[
= \sum_{k=0}^{\infty} \frac{1}{k!} \left[ e^{i\theta} \sum_{\ell=0}^{\infty} \frac{\alpha^\ell}{\ell!} (0) \hat{a}^{k+m} (\hat{a}^\dagger)^\ell | 0 \rangle \sum_{j=0}^{\infty} \frac{\beta^j}{j!} (0) \hat{a}^j (\hat{a}^\dagger)^k | 0 \rangle + e^{-i\theta} \sum_{\ell=0}^{\infty} \frac{\beta^\ell}{\ell!} (0) \hat{a}^{k+m} (\hat{a}^\dagger)^\ell | 0 \rangle \sum_{j=0}^{\infty} \frac{\alpha^j}{j!} (0) \hat{a}^j (\hat{a}^\dagger)^k | 0 \rangle \right]
\]

\[
= \alpha^m e^{i\theta} e^{\alpha\beta} + \beta^m e^{-i\theta} e^{\alpha\beta} \tan(\theta) + m_n \alpha e^{i\theta} e^{\alpha\beta} + \beta e^{-i\theta} e^{\alpha\beta} \tan(\theta), \quad (2.152)
\]

\[
\text{Tr}[\hat{a}^m \hat{A}] = \sum_{k=0}^{\infty} \langle k | \hat{a}^m \hat{A} | k \rangle
\]

\[
= \sum_{k=0}^{\infty} \frac{1}{k!} \langle 0 | \hat{a}^k (\hat{a}^\dagger)^m \left[ e^{i\theta} \langle \alpha | | \beta \rangle + e^{-i\theta} \langle \beta | | \alpha \rangle \right] (\hat{a}^\dagger)^k | 0 \rangle
\]

\[
= \sum_{k=0}^{\infty} \frac{1}{k!} \left[ e^{i\theta} \sum_{\ell=0}^{\infty} \frac{\alpha^\ell}{\ell!} (0) \hat{a}^k (\hat{a}^\dagger)^\ell | 0 \rangle \sum_{j=0}^{\infty} \frac{\beta^j}{j!} (0) \hat{a}^j (\hat{a}^\dagger)^k | 0 \rangle + e^{-i\theta} \sum_{\ell=0}^{\infty} \frac{\beta^\ell}{\ell!} (0) \hat{a}^k (\hat{a}^\dagger)^\ell | 0 \rangle \sum_{j=0}^{\infty} \frac{\alpha^j}{j!} (0) \hat{a}^j (\hat{a}^\dagger)^k | 0 \rangle \right]
\]

\[
= \beta^m e^{i\theta} e^{\alpha\beta} + \alpha^m e^{-i\theta} e^{\alpha\beta} \tan(\theta) + m_n \beta e^{i\theta} e^{\alpha\beta} + \alpha e^{-i\theta} e^{\alpha\beta} \tan(\theta). \quad (2.153)
\]

Hence, one obtains the expectations

\[
\langle \hat{A}^m \rangle \sim \mathbb{E} \left[ e^{-g \text{Tr}[\hat{a}^m \hat{A}]} \right] = \frac{1}{2} \mathbb{E} \left[ (\alpha^m + \beta^m) + i (\alpha^m - \beta^m) \tan(\theta) \right], \quad (2.154)
\]

\[
\langle \hat{D}^m \rangle \sim \mathbb{E} \left[ e^{-g \text{Tr}[\hat{a}^m \hat{A}]} \right] = \frac{1}{2} \mathbb{E} \left[ (\alpha^m - \beta^m) + i (\alpha^m + \beta^m) \tan(\theta) \right], \quad (2.155)
\]

which are easy to approximate numerically by taking the average over a sample of \( N \) simulated independent paths generated by some SDE method. These values can be compared with the expectations of their time-evolution. Starting with the initial condition \( \alpha_0 = \beta_0 \) at \( t = 0 \), it is possible to use (1.73) to determine \( \langle \hat{A}^m \rangle_{t, \alpha_0} \) and
2. Simulation of Bose-Einstein condensation

\[ \langle \hat{D}^m \rangle_{t,\alpha_0} \] exactly:

\[
\langle \hat{A}^m \rangle_{t,\alpha_0} = e^{-|\alpha_0|^2/2} \langle 0 | \hat{a}^m e^{\hat{a} \hat{a}^\dagger} | 0 \rangle
\]

\[
= e^{-|\alpha_0|^2} \sum_{k,\ell \geq 0} \frac{(\bar{\alpha}_0)^k}{k!} \frac{(\alpha_0)^\ell}{\ell!} \langle 0 | \hat{a}^k e^{\hat{a} \hat{a}^\dagger} \hat{a}^\ell e^{-\hat{a} \hat{a}^\dagger} | 0 \rangle
\]

\[
\rightarrow e^{-|\alpha_0|^2} \sum_{k,\ell \geq 0} \frac{(\bar{\alpha}_0)^k}{k!} \frac{(\alpha_0)^\ell}{\ell!} e^{im^2t/2} \langle 0 | \hat{a}^k \hat{a}^\ell e^{-\hat{a} \hat{a}^\dagger} | 0 \rangle
\]

\[
\rightarrow e^{-|\alpha_0|^2} e^{-im^2t/2} \sum_{\ell \geq 0} \frac{(\bar{\alpha}_0)^{k+m}}{\ell!} e^{im\ell t} \langle 0 | \hat{a}^\ell e^{-\hat{a} \hat{a}^\dagger} | 0 \rangle
\]

\[
= (\alpha_0)^m \exp \left( |\alpha_0|^2 (e^{-imt} - 1) - \frac{im^2t}{2} \right)
\]

\[
\langle \hat{D}^m \rangle_{t,\alpha_0} = e^{-|\alpha_0|^2/2} \langle 0 | \hat{a}^m e^{\hat{a} \hat{a}^\dagger} | 0 \rangle
\]

\[
= e^{-|\alpha_0|^2} \sum_{k,\ell \geq 0} \frac{(\bar{\alpha}_0)^k}{k!} \frac{(\alpha_0)^\ell}{\ell!} \langle 0 | \hat{a}^k e^{\hat{a} \hat{a}^\dagger} \hat{a}^\ell e^{-\hat{a} \hat{a}^\dagger} | 0 \rangle
\]

\[
\rightarrow e^{-|\alpha_0|^2} \sum_{k,\ell \geq 0} \frac{(\bar{\alpha}_0)^k}{k!} \frac{(\alpha_0)^\ell}{\ell!} e^{im^2t/2} \langle 0 | \hat{a}^k \hat{a}^\ell e^{-\hat{a} \hat{a}^\dagger} | 0 \rangle
\]

\[
\rightarrow e^{-|\alpha_0|^2} e^{-im^2t/2} \sum_{\ell \geq 0} \frac{(\bar{\alpha}_0)^{k+m}}{\ell!} e^{im\ell t} \langle 0 | \hat{a}^\ell e^{-\hat{a} \hat{a}^\dagger} | 0 \rangle
\]

\[
= (\bar{\alpha}_0)^m \exp \left( |\alpha_0|^2 (e^{-imt} - 1) + \frac{im^2t}{2} \right)
\]

One has thus a range of metrics at disposal to measure the accuracy of \( \alpha \) and \( \beta \), or even \( \phi, \psi, \tilde{\theta} \) when applying the transformations \( \phi \rightarrow \beta \), \( \psi \rightarrow \tilde{\theta} \).

**Remark 2.5.1.** Consider (2.19)–(2.20). By remembering that \( W^1 \) and \( W^2 \) are i.i.d. real Brownian motions and seeing that one SDE follows from the other by exchanging \( W^1 \leftrightarrow W^2 \), \( \alpha \leftrightarrow \beta \), it is easy to see that \( \alpha \) and \( \beta \) (and thus any moments thereof) have the same distribution when \( \alpha_0 = \beta_0 \) at \( t = 0 \) (or indeed if \( \alpha_0 = \beta_0 \) at any time \( t_0 \)). Therefore, one has the following approximation for the moments of \( \alpha \) and \( \beta \):

\[
\mathbb{E} [\alpha^m] = \mathbb{E} [\beta^m] = (\alpha_0)^m \exp \left( |\alpha_0|^2 (e^{-imt} - 1) - \frac{im^2t}{2} \right)
\]

One can then compute the characteristic function of \( \alpha \) as

\[
\mathbb{E} [e^{i\lambda \alpha}] = \mathbb{E} \left[ \sum_{m \geq 0} \frac{(i\lambda \alpha)^m}{m!} \right] = \sum_{m \geq 0} \left( \frac{(i\lambda)^m}{m!} \right) \mathbb{E} [\alpha^m]
\]

\[
= \sum_{m \geq 0} \left( \frac{(i\lambda)^m}{m!} \right) (\alpha_0)^m \exp \left( |\alpha_0|^2 (e^{-imt} - 1) - \frac{im^2t}{2} \right)
\]

It is of course easy to simulate the left hand side of (2.159) numerically by computing the mean of \( e^{i\lambda \alpha_j} \) for various simulated paths \( \alpha_j, j = 1, \ldots, N \). The right hand side can

50
also be approximated numerically, e.g. by summing only as long as $|\alpha(t)|^m > TOL$ (since $|E[|\alpha|^m]| \leq |\alpha|^m$, where $TOL << 1$ is chosen to be ‘sufficiently small’).

Using the results obtained for the operators $\hat{a}^m$ and $(\hat{a}^\dagger)^m$, it is now easy to compute the expectations of their various linear combinations. Among these possible choices, two observables are noteworthy: the $\hat{Y}$-observable

$$\hat{Y} := \frac{\hat{a} - \hat{a}^\dagger}{2i}$$

introduced in [31] and its counterpart

$$\hat{Z} := \frac{\hat{a} + \hat{a}^\dagger}{2}.$$  

By the linearity of the trace with respect to the operators $\hat{a}$ and $\hat{a}^\dagger$, it follows from (2.160) and (2.161) that

$$\Tr[\hat{Y} \hat{\Lambda}] = \frac{1}{2i} \left( \Tr[\hat{a} \hat{\Lambda}] - \Tr[\hat{a}^\dagger \hat{\Lambda}] \right) = e^{n_r} \frac{2i}{2} \left( \alpha e^{i\tilde{\theta}} + \beta e^{-i\tilde{\theta}} - \beta e^{i\tilde{\theta}} - \alpha e^{-i\tilde{\theta}} \right)$$

$$= e^{n_r} \Im \left[ e^{i\tilde{\theta}} (\alpha - \beta) \right],$$

$$\Tr[\hat{Z} \hat{\Lambda}] = \frac{1}{2} \left( \Tr[\hat{a} \hat{\Lambda}] + \Tr[\hat{a}^\dagger \hat{\Lambda}] \right) = e^{n_r} \frac{2i}{2} \left( \alpha e^{i\tilde{\theta}} + \beta e^{-i\tilde{\theta}} + \beta e^{i\tilde{\theta}} + \alpha e^{-i\tilde{\theta}} \right)$$

$$= e^{n_r} \Re \left[ e^{i\tilde{\theta}} (\alpha + \beta) \right].$$

Combining (2.151) and (2.162) yields

$$\hat{Y} = \frac{1}{N} \sum_{j=1}^{N} \frac{\Im \left[ e^{i\tilde{\theta}_j (\alpha_j - \beta_j) } \right]}{2e^{n_r} \cos(\theta)} = \frac{1}{2N} \sum_{j=1}^{N} \frac{(\alpha_i + \beta_i) j \cos(\tilde{\theta}_j) + (\alpha_i - \beta_i) j \sin(\tilde{\theta}_j)}{\cos(\tilde{\theta}_j)}$$

(2.164)

$$\hat{Z} = \frac{1}{2N} \sum_{j=1}^{N} \frac{(\alpha_i + \beta_i) j \cos(\tilde{\theta}_j) - (\alpha_i - \beta_i) j \sin(\tilde{\theta}_j)}{\cos(\tilde{\theta}_j)}$$

(2.165)

where the subscript $j$ denotes the $j$-th sample path. For the initial condition $\alpha_0 = \beta_0$ at $t = 0$, it is possible to use (1.73) to determine $\langle \hat{Y} \rangle_{t,\alpha_0}$ and $\langle \hat{Z} \rangle_{t,\alpha_0}$ exactly:

$$\langle \hat{Y} \rangle_{t,\alpha_0} = \langle \alpha(t) \hat{Y} | \alpha(t) \rangle = \frac{1}{2i} \left( \langle \hat{A} \rangle_{t,\alpha_0} - \langle \hat{D} \rangle_{t,\alpha_0} \right)$$

$$= Im \left[ \alpha_0 \exp \left( |\alpha_0|^2 (e^{-it} - 1) - \frac{it}{2} \right) \right]$$

(2.166)

which is the formula given in [31]. One can however rewrite (2.166) as a more explicit formula:

$$\langle \hat{Y} \rangle_{t,\alpha_0} = Im \left[ \alpha_0 e^{i|\alpha_0|^2 (\cos t - 1) - i(\cos |\alpha_0|^2 \sin t + \frac{1}{2})} \right]$$

(2.167)
2. Simulation of Bose-Einstein condensation

\[ e^{\alpha_0^2 \cos t - 1} \left[ \text{Im} \left( \alpha_0 \right) \cos \left( |\alpha_0|^2 \sin t + \frac{t}{2} \right) - \text{Re} \left( \alpha_0 \right) \sin \left( |\alpha_0|^2 \sin t + \frac{t}{2} \right) \right]. \]

Similarly,

\[ \langle \hat{Z} \rangle^t_{\alpha, \alpha_0} = \langle \alpha(t) | \hat{Z} | \alpha(t) \rangle = \frac{1}{2} \left( \langle \hat{A} \rangle^t_{\alpha, \alpha_0} + \langle \hat{D} \rangle^t_{\alpha, \alpha_0} \right) \]

\[ = e^{\alpha_0^2 (\cos t - 1)} \left[ \text{Re} \left( \alpha_0 \right) \cos \left( |\alpha_0|^2 \sin t + \frac{t}{2} \right) + \text{Im} \left( \alpha_0 \right) \sin \left( |\alpha_0|^2 \sin t + \frac{t}{2} \right) \right]. \]

Figure 2.1.: Real and imaginary part of $E[\alpha_t] = E[\beta_t]$ for the $\alpha, \beta$-SDE from Section 2.2. The full $4\pi$-period is displayed.

Using the same argument as in Remark 2.5.1, provided $\alpha_0 = \beta_0$ at $t = 0$, one expects

\[ E[\alpha_r] = E[\beta_r] = \text{Re} \left[ \alpha_0 \exp \left( |\alpha_0|^2 (e^{-it} - 1) - \frac{it}{2} \right) \right], \]  

\[ E[\alpha_i] = E[\beta_i] = \text{Im} \left[ \alpha_0 \exp \left( |\alpha_0|^2 (e^{-it} - 1) - \frac{it}{2} \right) \right], \]

hence $E[\alpha] = E[\beta]$ is $4\pi$-periodic, see Figure 2.1.
2.5. Metrics for the one-mode BEC

2.5.2. One state representation

Since the value of $\langle \hat{O} \rangle_{t,\alpha_0}$ is independent of the choice of the kernel (but not of the Hamiltonian), the values of $\langle \hat{A} \rangle_{t,\alpha_0}$ and $\langle \hat{D} \rangle_{t,\alpha_0}$ are already given in Subsection 2.5.1. Using the normalized kernel

$$\hat{\Lambda}_{N,\alpha} = e^{-|\alpha|^2} \langle \alpha | \langle \alpha |,$$

it follows that

$$\langle \hat{A} \rangle_{\hat{\rho}_\alpha} = \mathbb{E} \left[ \text{Tr} \left[ \hat{a}^m \hat{\Lambda}_{N,\alpha} \right] \right] = \mathbb{E} \left[ e^{-|\alpha|^2} \sum_{k=0}^{\infty} \frac{1}{k!} \langle 0 | \hat{a}^{k+m} | \alpha \rangle \langle \alpha | \left( \hat{a}^\dagger \right)^k | 0 \rangle \right]$$

$$= \mathbb{E} \left[ e^{-|\alpha|^2} \sum_{k=0}^{\infty} \frac{1}{k!} \sum_{\ell \geq 0} \frac{\alpha^\ell}{\ell!} \langle 0 | \hat{a}^{k+m} \left( \hat{a}^\dagger \right)^\ell | 0 \rangle \sum_{j \geq 0} \frac{\bar{\alpha}^j}{j!} \langle 0 | \hat{a}^j \left( \hat{a}^\dagger \right)^k | 0 \rangle \right]$$

$$= \mathbb{E} \left[ e^{-|\alpha|^2} \alpha^m \sum_{k=0}^{\infty} \frac{|\alpha|^{2k}}{k!} \right] = \mathbb{E} \left[ \alpha^m \right], \quad (2.171)$$

$$\langle \hat{D} \rangle_{\hat{\rho}_\alpha} = \mathbb{E} \left[ \text{Tr} \left[ \left( \hat{a}^\dagger \right)^m \hat{\Lambda}_{N,\alpha} \right] \right]$$

$$= \mathbb{E} \left[ e^{-|\alpha|^2} \sum_{k=0}^{\infty} \frac{1}{k!} \sum_{\ell \geq 0} \frac{\alpha^\ell}{\ell!} \langle 0 | \hat{a}^{k+m} \left( \hat{a}^\dagger \right)^\ell | 0 \rangle \sum_{j \geq 0} \frac{\bar{\alpha}^j}{j!} \langle 0 | \hat{a}^j \left( \hat{a}^\dagger \right)^k | 0 \rangle \right]$$

$$= \mathbb{E} \left[ e^{-|\alpha|^2} \alpha^m \sum_{k=0}^{\infty} \frac{|\alpha|^{2k}}{k!} \right] = \mathbb{E} \left[ \bar{\alpha}^m \right]. \quad (2.172)$$

Hence, comparing (2.156)-(2.157) with (2.171)-(2.172), one has

$$\mathbb{E} \left[ \alpha^m \right] = (\alpha_0)^m \exp \left( |\alpha_0|^2 (e^{-imt} - 1) - \frac{im^2 t}{2} \right), \quad (2.173)$$

as expected from Subsection 2.5.1. Hence, the expected results for $\alpha$ are independent of the choice of the kernel representation among the variants (2.28) and (2.114), although the corresponding numerical results are not.
2. Simulation of Bose-Einstein condensation
3. Numerical schemes and experiments

Several schemes were used on the $\phi, \psi, \tilde{\theta}$-SDE (2.1)-(2.3) and the $\alpha, \beta$-SDE (2.19)-(2.20) to see if the results from [31] could be improved. The standard explicit methods tested (e.g. the Euler, Milstein, explicit weak and strong Taylor schemes presented in [57]) all yielded solutions diverging much faster than the semi-implicit method used in [31].

Naturally, this led to the use of more sophisticated numerical schemes. In Sections 3.1.1-3.2, drift (and diffusion coefficient) splitting methods will be presented which allow SDEs to be solved semi-implicitly. Split-step methods are introduced in Section 3.3, where the idea is to treat the deterministic and stochastic terms differently, allowing the use of existing robust ODEs solvers to deal with the noiseless SDE. The schemes from Sections 3.4-3.7 were derived specifically for the $\alpha, \beta$-SDE (but are not restricted to it), either making explicit use on the information about the distribution of $n$ acquired in Chapter 2 or by keeping the simulated paths of $\alpha$ and $\beta$ bounded artificially. Section 3.8.1 will show how Wick-rotating an SDE through a complex change of time can lead to a significant improvement of the stability and quality of the numerical results under suitable conditions.

Unless otherwise specified, SDEs in this chapter will be considered in their autonomous form

$$dX_t = a(X_t) \, dt + b(X_t) \, dW_t,$$

with drift $a(X_t) \in \mathbb{C}^d$, diffusion matrix $b(X_t) \in \mathbb{C}^{d \times m}$ and Brownian motion $W_t \in \mathbb{C}^m$.

In most cases treated, the SDE (and hence the Brownian motion) will be real.

In this chapter, there will be mentions of stable methods, results, variables or SDEs. Unless a specific concept is referenced (e.g. the stability of the zero solution of Definition 2.2.3), the stability will have to be understood in the following non-formal way. If, using some numerical method, simulations of an SDE with known bounded moments (on a finite time interval) yield diverging paths and thus diverging moments in finite time (or simply if the error grows too much to be due to mere statistical error), the numerical method will be called (numerically) unstable for the given SDE. If this happens when using ‘reasonable’ schemes (e.g. stochastic Taylor methods with a small step size and large number of samples), the SDE and the variables for which the error is too large will also be called unstable.

In order to clarify the notation used within the Figures and algorithms throughout this chapter, the most frequent appellations are explained here. When solving an SDE in
autonomous form (3.1) numerically, the most straightforward approach is to simulate a sample of N independent (sample) paths of the solution. This means that for each path \( j = 1, \ldots, N \), starting from the (possibly random) initial value \( \hat{X}_0 \) at \( t_0 \), successive approximations \( \hat{X}_{j1}, \ldots, \hat{X}_{jM} \) of \( X_{t_1}, \ldots, X_{t_M} \) will be computed, where \( X_t \) is the exact solution at time \( t \) of the SDE (3.1) with initial value \( X_0 \) at \( t_0 \), \( k = 1, \ldots, M \). Of course, this means that \( t_0 < t_1 < \cdots < t_M =: T \). The quantity \( h_k := t_k - t_{k-1} \) is called the step size (at the step \( k \)). In most methods presented here, the step size is fixed, i.e. \( t_k = k \cdot h \) where \( h = (T - t_0)/M \) for all \( k = 1, \ldots, M \). If the step size is meant in general (i.e. for no particular step \( k \)), \( h \) might be used instead of \( h_k \), even when the step sized is not fixed.

Since the paths are independent, they can be split into \( N_B \) batches each containing \( N_S \) paths (i.e. \( N = N_B \cdot N_S \)) which allows to speed up the simulation through parallelization. The approximation (or numerical solution) \( \hat{X}_{jk} \) will often be written \( X_{jk} \) (or even \( X_k \)) when mentioned inside the figures.

### 3.1. Drift splitting methods

Drift splitting methods methods use an additive splitting of the drift to increase the numerical stability. One example is the order 2.0 weak method given in [71], which yields a semi-implicit one-step approximation for the solution of \( d \)-dimensional SDEs of the form (3.1). Based on a splitting of the drift

\[
a(x) = A(x) + B(x),
\]

one iteration for one path (whose index is dropped for readability) of the method is computed as

\[
X_{k+1}^\alpha = X_k^\alpha + \frac{h_k}{2} \left( A^\alpha(X_{k+1}) + B^\alpha(X_e) + a_k^\alpha \right)
+ \frac{1}{2} \sum_{\beta=1}^{m} \left( b^{\alpha\beta}(X_+) + b^{\alpha\beta}(X_-) \right) \xi^\beta_1
+ \frac{1}{2 \sqrt{h_k}} \sum_{\delta,\epsilon=1}^{m} \left( b^{\alpha\delta}(X^{(e)}_+) - b^{\alpha\delta}(X^{(e)}_-) \right) \Xi_{\epsilon\delta}, \quad \alpha = 1, \ldots, d,
\]

where \( a_k := a(X_k) \), \( b_k := b(X_k) \) and

\[
X_e = X_k + b_k \xi_1 + a_k h_k, \quad X_\pm = X_k + \frac{h}{2} a_k \pm \frac{1}{\sqrt{2}} b_k \xi_0, \quad X^{(e)}_\pm = X_k \pm \sqrt{h_k} b'_k.
\]

The \( \xi_0, \xi_1, \beta = 1, \ldots, m \), are i.i.d. approximations of the stochastic integrals \( \int_{t_k}^{t_{k+1}} dW^\beta_s \), while \( \Xi_{\epsilon\delta} \approx \int_{t_k}^{t_{k+1}} W^\epsilon_s dW^\delta_s \), see [71]. Note that \( b'_k \) denotes the \( \epsilon \)th column of \( b(X_k) \). Ideally, \( A(x) \) is such that for any right-hand side \( y \) the equation \( x - \frac{h}{2} A(x) = y \) is easy to solve for \( x \), e.g. with \( A \) linear, as below.
3.1. Drift splitting methods

3.1.1. Linear splitting

This scheme splits the drift of (3.1) into \( a(x) = Ax + B(x) \), where \( A \in \mathbb{C}^{d \times d} \) is constant (and real in all examples below).

Example 3.1.1 (Linear splitting for the \( \phi, \psi, \tilde{\theta} \)-SDE). Applied on the SDE (2.8), an intuitive choice (by selecting first order terms in the Taylor expansion of the drift) is

\[
A = \begin{pmatrix}
0 & 1 & 1 & 0 & 0 \\
-1 & -\mu & 0 & \mu - 1 & 0 \\
1 & 0 & 0 & 1 & 0 \\
0 & \mu - 1 & -1 & -\mu & 0 \\
0 & 0 & 0 & 0 & 0
\end{pmatrix}.
\] (3.5)

Since \( \det(I_5 - \frac{h}{2}A) = 1 + h\mu + \frac{1}{2}h^2\mu \geq 1 \) for all \( h > 0 \) and \( \mu \geq 0 \), the matrix \( I_5 - \frac{h}{2}A \) is invertible and its inverse can be computed exactly. Furthermore, its condition number (in the 2-norm) is low for reasonable values of \( h \) and \( \mu \) (e.g. \( \kappa_2(I_5 - \frac{h}{2}A) < 3 \) when \( h \in [0,1] \), \( \mu \in [0,0.4] \)). This makes the method (3.3) with \( A \) given by (3.5) convenient to use, as \( X_{k+1} \) is then easy to compute and unique. Results involving this splitting for the \( \phi, \psi, \tilde{\theta} \)-SDE can be found in Figures 3.9-3.17.

Example 3.1.2 (Linear splitting for the \( \alpha, \beta \)-SDE). For the SDE given by (2.21)-(2.24), the matrix corresponding to the splitting \( a(x) = \hat{A}x + B(x) \) and \( x = (\alpha_r, \alpha_i, \beta_r, \beta_i)^\top \) is

\[
A = \begin{pmatrix}
0 & \frac{1}{2} & 0 & 0 \\
-\frac{1}{2} & 0 & 0 & 0 \\
0 & 0 & 0 & \frac{1}{2} \\
0 & 0 & -\frac{1}{2} & 0
\end{pmatrix}.
\] (3.6)

Since \( \det(I_4 - \frac{h}{2}A) = 1 + \frac{1}{8}h^2 + \frac{1}{256}h^4 > 1 \) for \( h > 0 \), the matrix \( I_4 - \frac{h}{2}A \) is always regular. Additionally, \( \kappa_2(I_4 - \frac{h}{2}A) = 1 \), \( \forall h > 0 \), hence the linear splitting is safe to use with method (3.3). However, the fact that the matrix \( I_4 - \frac{h}{2}A \) is so close to the identity matrix also means that the linear implicitness will not improve the stability much. Indeed, the numerical results shown in Figure 3.1 were very similar (i.e. they diverge; compare with Figure 3.13) to those obtained with the ‘more implicit’ linear splitting derived in Example 3.1.1 for the \( \phi, \psi, \tilde{\theta} \)-SDE with \( \mu = 0 \). As the \( \alpha, \beta \)-SDE corresponds to the case \( \mu = 0 \), this is hardly surprising. Yet the divergence of the mean solution over the paths is obviously not desirable.

One crude way to keep the situation under control is to reject any path whose components are too large. In the simulation leading to Figure 3.2, the procedure was the following: if for the simulated sample path \( j \) the condition

\[
\|X_k^j\|_\infty > \text{TOL}
\] (3.7)
3. Numerical schemes and experiments

Figure 3.1: $\hat{Y}$- and $\hat{Z}$-observable simulations for the $\alpha, \beta$-SDE using the linear splitting method (3.6) with $h = 10^{-4}$ and 5000 sample paths. As with the corresponding $\mu = 0$ case shown in Figure 3.13 for the $\phi, \psi, \theta$-SDE, the results diverge.

holds for any $k$, the path was rejected. If not, it was accepted. The first time $t_k$ at which (3.7) holds for a rejected path is said to be its time of rejection. Note that if both TOL and the size of the sample are large enough, the minimum time of rejection will (probably) be a fairly good approximation of the theoretical first time of departure for that path.

The plots shown in the Figures 3.1, 3.2 come from the same simulation. Figure 3.1 shows the mean over all paths, while the mean over the accepted paths only are showed in Figure 3.2. In this case, the mean of the accepted paths is clearly not as good an approximation as the mean of all the simulated paths, at least for small $t$ values. After the time of departure of the sample (defined in Section 2.2.2), the absolute error is of course larger when the mean over all paths is considered, but the results in Figure 3.2 are so inaccurate that it scarcely matters. This is caused by the fact that sample paths with large values are necessary for a meaningful simulation (as long as they do not diverge). Indeed, from Section 2.2.2 one expects both quickly growing sample paths and samples converging toward zero. Hence, rejecting paths with large elements will bias the simulation towards zero, as paths with small values will be given more importance than they should.

Example 3.1.3 (Linear splitting for the $\alpha$-SDE). In the case of the general $\alpha$-SDE (2.135),
3.1. Drift splitting methods

Figure 3.2.: \(\hat{Y}\) - and \(\hat{Z}\) - observable simulations for the \(\alpha, \beta\)-SDE using the linear splitting method (3.6) with \(h = 10^{-4}\) and 5000 sample paths. Paths which did not satisfy (3.7) for TOL = 50 were rejected. The mean over the accepted paths is displayed.

The linear splitting matrix is

\[
A = \begin{pmatrix}
0 & \frac{1}{2} \\
-\frac{1}{2} & 0
\end{pmatrix},
\]

(3.8)

As in the case of its counterparts from Examples 3.1.1, 3.1.2, the matrix \(I_2 - \frac{h}{2}A\) is regular \((\det(I_2 - \frac{h}{2}A) = 1 + \frac{1}{16}h^2 > 1)\) and the condition number is low \((\kappa_2(I_2 - \frac{h}{2}A) = 1, \forall h > 0)\).

When solving the general \(\alpha\)-SDE (2.135) with the linear splitting method, it can be noticed (see Figures 3.5, 3.6) that although the results are more stable than those obtained for the \(\alpha, \beta\)-SDE, there is still a tendency for some of the paths to blow up (even if it occurs later). As for the \(\alpha, \beta\)-SDE, rejecting paths where \(\max(\{|\alpha_r|, |\alpha_i|\}) \geq \text{TOL}\) kept the mean values of \(\alpha_r\) and \(\alpha_i\) under control. Although it did not seem to affect the quality of the accepted sample when looking at Figure 3.3 or Figure 3.5 alone, comparing the mean \(|\alpha_t|^2\) to its exact expected value given by (2.138) (as opposed to the unknown \(E[\alpha_r]\) and \(E[\alpha_i]\), for which one can only hope that they will be close to the values predicted in Section 2.5.2) showed that the mean of the accepted paths fell short of the exact \(E[|\alpha_t|^2]\) (see Figures 3.4 and 3.6). This indicated again the statistical importance of the rejected large paths (before they blow off completely).

Note that setting TOL to \(10^5\) instead of 50 in the simulations leading to Figures 3.5, 3.6 did not change the number of rejected paths, since those paths, once large enough, grew to be virtually unbounded.
3. Numerical schemes and experiments

Figure 3.3.: Simulations of $E[\alpha_r]$ and $E[\alpha_i]$ (with and without path rejection) for the $\alpha$-SDE (2.134) using the linear splitting method (3.8) with $h = \frac{\pi}{3} \cdot 10^{-4}$ and 5000 sample paths. The mean values of the corresponding $|\alpha|^2$ are shown in Figure 3.4.

As mentioned in Section 2.4 and seen from Figures 3.3-3.6, choosing $\zeta = \frac{1}{2}$ led to results that were reasonably close to what would be expected from (2.173) for the quantity $\alpha$ derived from to the density matrix representation (2.115), i.e. having as pdf the solution of the one-state FPE (2.127). At least, the numerical solution looks decent up to $t \approx 5$ (when using path rejection), after which the numerical solution misses the turning points, as does the solution of the $\alpha, \beta$-SDE in Figure 3.15.

Note that increasing the number of time steps or simulated sample paths is not necessarily a good idea when dealing with such sensitive SDEs, as it increases the chance of having diverging paths in the simulation. In the simulation leading to Figures 3.7-3.8, only one path diverged. It could be seen that for this path, $|\alpha|^2$ stayed in [500, 1000] for more than a thousand time steps before suddenly diverging around $t \approx 3.11$, which illustrates the dangers involved when simulating unstable stochastic processes mentioned in Section 2.4.1.

Since the linear splitting method did not perform well on its own for both $\phi, \psi, \tilde{\theta}$-SDE (see Figures 3.9-3.17), $\alpha, \beta$-SDE and ($\zeta$-dependent) $\alpha$-SDE, further splittings and methods were investigated. Some of them are presented in the rest of this chapter.
3.1. Drift splitting methods

Expected vs mean of $|\alpha|^2$ for linear splitting solution of $d\alpha = -i(|\alpha|^2 + 1/2) \alpha dt + \sqrt{-i} \alpha dW_t$

Figure 3.4.: Simulations of $E[|\alpha|^2]$ (with and without path rejection) for the $\alpha$-SDE (2.134) using the linear splitting method (3.8) with $h = \frac{\pi}{3} \cdot 10^{-4}$ and 5000 sample paths. The mean values of the corresponding $\alpha_r, \alpha_i$ are shown in Figure 3.3.

Linear splitting solution of the SDE $d\alpha = -i(|\alpha|^2 + 1/2) \alpha dt + \sqrt{-i}/2 \alpha dW_t$

Figure 3.5.: Simulations of $E[\alpha_r]$ and $E[\alpha_i]$ (with and without path rejection) for the $\alpha$-SDE (2.135) with $\zeta = \frac{1}{2}$, using the linear splitting method (3.8) with $h = \frac{\pi}{3} \cdot 10^{-4}$ and 5000 sample paths. The mean values of the corresponding $|\alpha|^2$ are shown in Figure 3.6.
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Figure 3.6.: Simulations of $E[|\alpha_t|^2]$ (with and without path rejection) for the modified $\alpha$-SDE (2.135) with $\zeta = \frac{1}{2}$, using the linear splitting method (3.8) with $h = \pi \cdot 10^{-4}$ and 5000 sample paths. The mean values of the corresponding $\alpha_r, \alpha_i$ are shown in Figure 3.5.

Figure 3.7.: Simulations of $E[\alpha_r]$ and $E[\alpha_i]$ (with and without path rejection) for the $\alpha$-SDE (2.135) with $\zeta = \frac{1}{2}$, using the linear splitting method (3.8) with $h = \pi \cdot 10^{-4}$ and 5000 sample paths. The mean values of the corresponding $|\alpha|^2$ are shown in Figure 3.8.
3.1. Drift splitting methods

Figure 3.8.: Simulations of $E[|\alpha_t|^2]$ (with and without path rejection) for the modified \(\alpha\)-SDE (2.135) with \(\zeta = \frac{1}{2}\), using the linear splitting method (3.8) with \(h = \pi \cdot 10^{-4}\) and 5000 sample paths. The mean values of the corresponding \(\alpha_r, \alpha_i\) are shown in Figure 3.7.
3. Numerical schemes and experiments

3.1.2. 4-1 splitting

The 4-1 splitting scheme was only used for the \( \phi, \psi, \tilde{\theta} \)-SDE (2.8). As can be seen from (2.9)-(2.13), \( a_5(x) \) has no linear term in \( x^1, \ldots, x^4 \) and \( a_1, \ldots, a_4 \) have no linear term in \( x^5 \). However, \( a_5(x) \) has a linear term with respect to \( x^5 \), provided \( x^1, \ldots, x^4 \) are fixed. Hence, the terms \( X_{k+1}^1, X_{k+1}^2, X_{k+1}^3, X_{k+1}^4 \) can be evaluated first, followed by a decoupled linear splitting for the \( x^5 \)-component. At each time step, compute \( \tilde{X}_{k+1} := (X_{k+1}^1, X_{k+1}^2, X_{k+1}^3, X_{k+1}^4)^\top \) as a step of the splitting method (3.3) applied on the first four rows of the SDE (2.8) using the splitting

\[
\tilde{a}(x) = \tilde{A}\tilde{x} + \tilde{B}(\tilde{x}, x^5),
\]

where

\[
\tilde{A} = \begin{pmatrix}
0 & 1 & 1 & 0 \\
-1 & -\mu & 0 & \mu - 1 \\
1 & 0 & 0 & 1 \\
0 & \mu - 1 & -1 & -\mu
\end{pmatrix}, \quad \tilde{a} = \begin{pmatrix}
a_1 \\
a_2 \\
a_3 \\
a_4
\end{pmatrix} \quad \text{and} \quad \tilde{x} = \begin{pmatrix}
x^1 \\
x^2 \\
x^3 \\
x^4
\end{pmatrix}.
\]

Now split \( a^5(x) \) into

\[
a^5(x) \overset{(2.13)}{=} \tan(x^5)f(\tilde{x}) = f(\tilde{x})x^5 + B^5(x),
\]

where the Taylor expansion of \( \tan(x^5) \) was used, hence \( B^5(x) = f(\tilde{x})(\tan(x^5) - x^5) \).

When solving for \( x^5 \), compute \( X_\epsilon, X_\pm \) and \( X_\epsilon^{(c)} \) as in (3.10) and use \( \tilde{X}_{k+1} \) in \( f \) to find

\[
\tilde{X}_{k+1}^5 = \frac{1}{1 - \frac{h}{2} f(X_{k+1})} \left[ X_k^5 + \frac{h}{2} (B_5(X_\epsilon) + a_5(X_k)) \right]
\]

\[
+ \frac{1}{2} \sum_{\beta=1}^2 \left\{ b_{5\beta}(X_+) + b_{5\beta}(X_-) \right\} \xi_\beta^\beta
\]

\[
+ \frac{1}{2\sqrt{h_k}} \sum_{\delta=1}^m \left\{ b_{5\delta}(X_{\epsilon}^{(c)}) - b_{5\delta}(X_{\epsilon}^{(c)}) \right\} \zeta_\delta^\delta.
\]

In the case of the \( \phi, \psi, \tilde{\theta} \)-SDE (2.8), the results using the 4-1 splitting scheme are typically more accurate and less fluctuation-prone than those of the linear splitting method, see Figures 3.9, 3.14 for various \( \mu \)-values. The sample paths of the SDE being independent, the simulations were computed in \( N_B \) independent batches of \( N_S \) sample paths. Denote by \( \bar{Y}_k^{\ell,j} \) and \( \bar{Z}_k^{\ell,j} \) the \( j \)th path of the \( \ell \)th batch used in the \( \bar{Y} \)- and \( \bar{Z} \)-estimates (2.164)-(2.165) evaluated at time \( t_k := k \cdot h \), where one recalls from (2.4)-(2.5) that \( \alpha = \exp \left[ \frac{1}{2} (x^1 + i x^2) \right] \) and \( \beta = \exp \left[ \frac{1}{2} (x^3 + i x^4) \right] \). Define further

\[
\text{mse}_{Y_{\ell,t_k}} = \sqrt{\frac{1}{N_S} \sum_{j=1}^{N_S} \left( \bar{Y}_k^{\ell,j} - \hat{Y}_{\ell,t_k} \right)^2}
\]

(3.12)
3.1. Drift splitting methods

and

\[ \text{mse}_Z, t_k = \sqrt{\frac{1}{N_S} \sum_{j=1}^{N_S} \left( \bar{Z}_{k,j} - \hat{Z}_{t_k} \right)^2}, \]  \hspace{1cm} (3.13)

the respective mean square errors of \( \langle \hat{Y} \rangle \) and \( \langle \hat{Z} \rangle \) of batch number \( \ell \) at time \( t_k \), \( \ell = 1, \ldots, N_B \), \( k = 1, \ldots, M \).

The mean square errors \( \text{mse}_{\hat{Y}, t_k} \), \( \text{mse}_{\hat{Z}, t_k} \) of the 4-1 splitting method are found to be lower than their linear splitting counterparts for most batches \( \ell \) and times \( t_k \). Overall, both splitting methods yield results similar to those found in [31] for \( \alpha_0 = \beta_0 = 3 \), \( \mu = 0.001 \) (see Figures 3.9-3.10 and 3.15-3.16): the simulation data looks good until roughly \( t = 0.3 \) (or even earlier if higher moments are considered), and then, unfailingly, starts to be inaccurate. This is not just a question of sampling: in simulations with up to \( 1.25 \cdot 10^6 \) sample paths and \( h = 2 \cdot 10^{-5} \), the approximations of \( \langle \hat{Y} \rangle_\rho \) and \( \langle \hat{Z} \rangle_\rho \) were far from being in the 99% confidence interval of the expected values \( \hat{Y}_{t} \) and \( \hat{Z}_{t} \) after the samples’ time of departure \( t_{dep} \approx 0.3 \). Increasing the number of time steps and sample paths past the values in the following plots did not change the fact that the data was too inaccurate as a prediction past \( t_{dep} \approx 0.3 \).

Starting at a lower value of \( \alpha_0 = \beta_0 \) raised the time of departure, while increasing the starting value lowers it. Furthermore, although the results still look decent until \( t \approx 0.5-0.6 \), from then on the simulations of both \( \langle \hat{Y} \rangle_\rho \) and \( \langle \hat{Z} \rangle_\rho \) oscillate wildly around zero, missing the next curves of the exact solution completely. From the Figures 3.13-3.14 it is easy to see that both methods diverge numerically for \( \mu = 0 \), as in [31]. In fact, since \( \mu = 0 \) means that \( x^5 \) is constant, it is no surprise to see that in that situation the results for the linear and 4-1 schemes are almost the same. The same pseudorandom numbers were used for both methods in every simulation shown in Figures 3.9-3.14.

The difference in the magnitude between the absolute errors shown in Figures 3.9-3.14 and their average batch mean square errors is explained by the fact that the variances are large.
3. Numerical schemes and experiments

Figure 3.9.: \( \hat{Y} \)- and \( \hat{Z} \)-observable simulations with linear and 4-1 splitting methods, applied on the SDE (2.8) for the ‘optimal’ parameter \( \mu = 0.001 \), \( h = 10^{-4} \), \( 10^4 \) sample paths.

Figure 3.10.: Evolution in time of the mean square errors (3.12) and (3.13) using the linear and 4-1 splitting methods, applied on the SDE (2.8) for the ‘optimal’ parameter \( \mu = 0.001 \), \( h = 10^{-4} \), \( 10^4 \) sample paths.
3.1. Drift splitting methods

Figure 3.11: \( \hat{Y} \)- and \( \hat{Z} \)-observable simulations with linear and 4-1 splitting methods, applied on the SDE (2.8) for the ‘hermitian P’ \( \mu = 1 \) (see [31]), \( h = 10^{-4}, 10^4 \) sample paths.

Figure 3.12.: Evolution in time of the mean square errors (3.12) and (3.13) using the linear and 4-1 splitting methods, applied on the SDE (2.8) for the ‘hermitian P’ \( \mu = 1 \) (see [31]), \( h = 10^{-4}, 10^4 \) sample paths.
3. Numerical schemes and experiments

Figure 3.13: $\hat{Y}$- and $\hat{Z}$-observable simulations with linear and 4-1 splitting methods, applied on the SDE (2.8) for $\mu = 0$ (see [31]), $h = 10^{-4}$, $10^4$ sample paths. The results are practically identical and diverge.
3.1. Drift splitting methods

Figure 3.14.: Evolution in time of the mean square errors (3.12) and (3.13) using the linear and 4-1 splitting methods, applied on the SDE (2.8) for $\mu = 0$ (see [31]), $h = 10^{-4}$, 10^4 sample paths. As expected, the results are practically identical (up to the numerical cancelation error) and diverge.

Figure 3.15.: $\hat{Y}$- and $\hat{Z}$-observable simulations with linear and 4-1 splitting methods, applied on the SDE (2.8) for the ‘optimal’ $\mu = 0.001$, $h = \frac{2\pi}{3} \cdot 10^{-4}$, 5200 sample paths.
3. Numerical schemes and experiments

Figure 3.16.: Evolution in time of the mean square errors (3.12) and (3.13) using the linear and 4-1 splitting methods, applied on the SDE (2.8) for the ‘optimal’ $\mu = 0.001$, $h = \frac{2\pi}{3} \cdot 10^{-4}$, 5200 sample paths.
3.2. Drift and diffusion coefficient splitting method

Using the same techniques as in [71], a weak order 2.0 method was derived using splittings of both the drift and diffusion coefficient of the SDE (3.1). Consider

\[ a(x) = A(x) + B(x) \quad \text{and} \quad b(x) = C(x) + D(x), \]

where \( A \) and \( C \) are convenient functions (in the sense that the equation (3.16) is easy to solve for \( X_{k+1} \)) and

\[ \partial_\alpha \partial_\beta C(x) = 0 \quad \text{for} \quad \alpha, \beta = 1, \ldots, d. \]

(3.15)

Note that linear \( C \)'s satisfy the condition (3.15). The method for the splittings (3.14) is then

\[
X_{\alpha k+1} = X_{\alpha k} + \frac{h_k}{2} (A^\alpha (X_{k+1}) + B^\alpha (X_e) + a_k^\alpha) + \sum_{\epsilon=1}^d \sum_{\beta, \gamma=1}^m \left( \partial_\epsilon b^{\alpha \beta} (x) \right) \bigg|_{x = X_k} b_k^\epsilon \xi_1^\gamma \Xi_1^{\gamma \beta},
\]

(3.16)

where \( a_k := a(X_k) \), \( b_k := b(X_k) \),

\[ X_e = X_k + a_k h_k + b_k \xi_1, \quad X_{\pm} = X_k \pm b_k \xi_0, \quad \Xi = X_k + a_k h \]

and \( \xi_0^\beta, \xi_1^\beta, \Xi^\gamma \beta \) are defined as in section 3.1.

The method described by (3.16) can be shown to have an order of 2.0: writing

\[
\Delta C^{\alpha \beta} := \frac{1}{2} \left( b^{\alpha \beta} (X_+) + b^{\alpha \beta} (X_-) - 2b_k^{\alpha \beta} \right),
\]

\[
\Delta E^{\alpha \beta} := \frac{1}{2} \left( C^{\alpha \beta} (X_{k+1}) + D^{\alpha \beta} (\Xi) + b_k^{\alpha \beta} \right),
\]

\[
R^\alpha := \sum_{\beta, \gamma, \epsilon} \left( \partial_\epsilon C^{\alpha \beta} (x) \right) \bigg|_{x = X_k} b_k^\epsilon \xi_1^\gamma \xi^\beta_1,
\]

the stochastic (Itô-)Taylor expansion can be checked just as in [71].

Since the diffusion coefficient is partly implicit, the method is obviously to be handled with care (especially in the scalar case), as the randomness makes it hard to guarantee that (3.16) can be solved exactly (or even accurately) for each step and sample path. In
the case of the SDE (2.8), consider the choice of splitting where the \( j \)th column of \( C(x) \) is chosen as \( \tilde{C}^j x \) for \( x \in \mathbb{R}^5 \) and

\[
\tilde{C}^1 = -\tilde{C}^2 = \begin{pmatrix}
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
0 & -\frac{\mu}{\sqrt{2}} & 0 & \frac{\mu}{\sqrt{2}} & 0
\end{pmatrix},
\]

(3.17)

which correspond to the coefficients of the linear terms in the Taylor expansion of \( b^5,1 \) and \( b^5,2 \). Combining (3.17) with the linear drift splitting (3.5) yields the following linear iteration scheme:

\[
\begin{pmatrix}
I_5 - \frac{h}{2}A - \frac{1}{2} \sum_{j=1}^2 \tilde{C}^j \xi^j_1
\end{pmatrix} X_{k+1} = f(X_k, h, \xi_0, \xi_1).
\]

(3.18)

Figure 3.17: \( \hat{Y} \)- and \( \hat{Z} \)-observable simulations with the linear, 4-1 and double splitting methods, applied on the SDE (2.8) for \( \mu = 0.001 \) (see [31]), \( h = 10^{-4}, 10^4 \) sample paths. The results using the linear splitting and double splitting are almost identical.

Since \( \det(I_5 - \frac{h}{2}A - \frac{1}{2} \sum_{j=1}^2 \tilde{C}^j \xi^j_1) = 1 + h\mu + \frac{1}{2}h^2\mu \geq 1 \) for all \( h > 0 \) and \( \mu \geq 0 \) (and \( \xi_1 \)), there is a unique solution \( X_{k+1} \) of (3.18). However, using the same pseudorandom numbers for both methods, the numerical results obtained with this ‘double linear splitting’ were almost identical to those obtained with the linear splitting scheme presented in Section 3.1 for both \( \mu = 0.001 \) and \( \mu = 1 \) (see Figure 3.17), hence the method was not used further.
3.3. Split-step methods

The SDEs (2.1)-(2.3), (2.21)-(2.24) and (2.134) share the following structure: their drift is nonlinear, while their diffusion matrix is either linear or constant (except for the diffusion coefficients term in the SDE for \( \tilde{\theta} \)). This naturally led to the idea of treating the (explicitly) deterministic and stochastic parts of the SDEs separately, using split-step methods (following the terminology of [50]).

The idea is the following: consider an SDE of the type (3.1) with initial value \( X_0 \). Let \( S_1 \) be a given ODE numerical integrator and \( S_2 \) an SDE solver. The corresponding \( S_1-S_2 \) split-step method then works as follows. For \( k \geq 0 \), compute the numerical approximation \( X_{k+1} \) of \( X_{t_{k+1}} \) using the recursion below:

1. compute \( \tilde{X}_{k+1} \) as the numerical solution at time \( t_{k+1} \) of the initial value problem
   \[
   \frac{dx}{dt} = a(x), \quad x(t_k) = X_k
   \]  
   using the ODE integration scheme \( S_1 \).

2. compute \( X_{k+1} \) as one step (with step size \( h_k := t_{k+1} - t_k \)) of the modified SDE integration scheme \( S_2M \), applied on the SDE
   \[
   dX_t = a(X_t) \, dt + b(X_t) \, dW_t, \quad X(t_k) = \tilde{X}_{k+1},
   \]
   where the scheme \( S_2M \) is obtained from the SDE scheme \( S_2 \) by removing from it all the deterministic terms from the stochastic Taylor series (see [57]) that are already contained in the deterministic Taylor expansion of \( S_1 \).

Using ODE schemes does not only allow deterministic integration of a higher order than available with usual SDE methods, but also an easier use or implementation of features like adaptive time-stepping, many of them already included in available numerical ODE software (e.g. the adaptive Runge-Kutta methods \( \text{ode45} \) or \( \text{ode23s} \) in MATLAB).

**Remark 3.3.1.** Depending on the method \( S_1 \), the ODE time-stepping procedure may have to be done independently for each individual path (this is for instance the case when using \( \text{ode45} \) or \( \text{ode23s} \)), resulting in a much slower method than when using the stochastic method \( S_2 \) directly (assuming a step of \( S_2 \) can be done for all simulated paths simultaneously).

For \( j = 1, \ldots, N \), \( k = 0, \ldots, M \), denote by \( X^j_{k+1} \) the \( j \)th path of the approximation to \( X_{t_{k+1}} \) (set \( X^j_0 = X_0 \) for all \( j \)).

**Example 3.3.2 (ode45-Euler split-step scheme).** For \( k = 0, \ldots, M - 1 \), compute first each path of \( \tilde{X}_{k+1} \) separately using the MATLAB built-in Dormand-Prince integration scheme \( \text{ode45} \) applied on the corresponding initial value problem
   \[
   \frac{dx}{dt} = a(x), \quad x(t_k) = X^j_k.
   \]
3. Numerical schemes and experiments

The Dormand-Prince method has order four, hence it follows in particular that

$$\tilde{X}_{k+1}^j = X_k^j + h_k a(X_k^j) + \frac{h_k^2}{2} \sum_{\gamma=1}^d \left( \partial_\gamma a(X_k^j) \right) a^\gamma(X_k^j) + O(h_k^3). \quad (3.22)$$

The Euler-Maruyama method for \((3.1)\) is

$$X_{k+1}^j = X_k^j + h_k a(X_k^j) + b(X_k^j) \Delta W_k^j, \quad (3.23)$$

where \(\Delta W_k^1, \ldots, \Delta W_k^N\) are the simulated approximations to \(W_{k+1} - W_k\). Since the two first terms on the right-hand side of \((3.23)\) are already included in \((3.22)\), the \(j\)th path of the \((k+1)\)st step of the \textit{ode45-Euler split-step scheme} (or simply \textit{ode45-Euler scheme}) is then

$$X_{k+1}^j = \tilde{X}_{k+1}^j + b(\tilde{X}_{k+1}^j) \Delta W_k^j. \quad (3.24)$$

**Remark 3.3.3.** Note that \(X_{k+1}^j\) can be replaced by \(\tilde{X}_{k+1}^j\) or even \(\tilde{X}_{k+1}^j\) without changing the (stochastic) order of \((3.24)\).

**Example 3.3.4 (ode45-wpp split-step scheme).** The \textit{ode45-wpp split-step scheme} (or \textit{ode45-wpp scheme}) works in a similar way as the \textit{ode45-Euler scheme}. Compute \(\tilde{X}_{k+1}^j\) as the solution of \((3.21)\) using \texttt{ode45}. Then add the remaining terms from \((3.3)\) not included in \(\tilde{X}_{k+1}^j\):

$$X_{k+1}^j = \tilde{X}_{k+1}^j + \frac{h_k}{2} \left[ a \left( X_k^j + b(X_k^j) \Delta W_k^j \right) - a(X_k^j) \right] + \frac{1}{2} \left[ b \left( X_k^j \right) + b \left( X_k^j \right) \right] \Delta W_k^j + \frac{1}{2} \sqrt{h_k} \sum_{\delta,x=1}^m \left\{ b^\delta \left( X_+^{\delta,j} \right) - b^\delta \left( X_-^{\delta,j} \right) \right\} \Xi_{\delta}, \quad (3.25)$$

where

$$X_\pm = X_k^j + \frac{h_k}{2} a(X_k^j) \pm \frac{1}{\sqrt{2}} b(X_k^j) \Delta W_{k,0}, \quad X_\pm^{\delta,j} = X_k^j \pm \sqrt{h_k} b^\delta(X_k^j),$$

and for every \(k\) and \(j\), \(\Delta W_k^j = (\xi_0, \ldots, \xi_0) \top\), \(\Delta W_k^j = (\xi_1, \ldots, \xi_0) \top\) are vectors of i.i.d approximations of \(\int_{t_k}^{t_{k+1}} dW_s = W_{t_{k+1}} - W_t\) and \(\Xi_{\delta} \approx \int_{t_k}^{t_{k+1}} W_s^\delta dW_s^\delta\), as in Section 3.1. Remember that \(b^\delta\) denotes the \(\delta\)th column of \(b\).

The principle is the same for the \textit{ode23-Euler}, \textit{ode23s-Euler}, \textit{ode23-wpp} and \textit{ode23s-wpp} schemes: simply use the corresponding \texttt{MATLAB} routine instead of \texttt{ode45} to solve \((3.21)\). Similarly, the Euler or wpp methods can be replaced by other stochastic methods. Simply add the corresponding stochastic terms that were not already approximated by \(\tilde{X}_{k+1}\). Among the choices tested for \texttt{S2} were the Milstein method, the order 1.5 strong Taylor method (if used on the \(\alpha, \beta\)-SDE, the scheme for commutative noise of the second kind was used, see \[57\]) in both Itô and Stratonovich form.
3.3. Split-step methods

Figure 3.18.: \( \hat{X} \)- and \( \hat{Z} \)-observable simulations for the \( \alpha, \beta \)-SDE using the ode45-order 1.5 strong Taylor, ode45-wpp and ode45-Milstein split-step methods with \( h = 5 \cdot 10^{-4} \) and 1000 sample paths. Notice that the last two methods yield very similar-looking results.

When applied to the \( \alpha, \beta \)-SDE, the split-step methods ode45-Euler, ode45-Milstein and ode45-wpp all returned similar results (using the same simulated Brownian motion increments), see Figure 3.18. Notice that establishing which method works best based on Figures 3.18-3.19 is not that obvious, since although the ode45-order 1.5 strong Taylor method clearly performs better than ode45-Milstein in Figure 3.19, it does not do as well in Figure 3.18. One would expect the ode45-order 1.5 strong Taylor method to be the best combination among the presented methods, since it has the highest (strong) order, yet the extra terms added in the stochastic step do not seem to be enough to prevent the divergence of the simulated solution.

Of course, other deterministic methods can be used instead of the adaptive MATLAB routines ode45, ode23s and ode23s. Among others, the adaptive fifth order Runge-Kutta solver controlrk5.m presented in [70] (which was built upon the adaptive algorithm of [83]) was compared with ode45 on various ODEs with known exact solution. Since the performances of ode45 and controlrk5 were comparable for the tested ODEs (those presented in Chapter 7 of [70]), ode45 was used in most computations due to the fact that it is slightly more user-friendly.

In the case of the \( \alpha, \beta \)-SDE, all results obtained were similar to those presented in Figures 3.18-3.19, i.e. displaying the same behaviour as the methods of Sections 3.1-3.2 starting at \( \alpha_0 = \beta_0 = 0 \) the estimates were only reliable up to \( t \approx 0.3 \) and then diverged.
3. Numerical schemes and experiments

![Graph](image)

**Figure 3.19.** \( \hat{Y} \)- and \( \hat{Z} \)-observable simulations for the \( \alpha, \beta \)-SDE using the ode45-order 1.5 strong Taylor and ode45-Milstein split-step methods with \( h = 5 \cdot 10^{-4} \) and 8000 sample paths.

Hence, the higher order in the deterministic step did not seem to be worth the additional computational cost in this context.

When applied to the modified \( \alpha \)-SDE with \( \zeta = \frac{1}{2} \), the ode45-wpp method had the advantage over the linear splitting method that the simulated paths did not diverge, hence eliminating the need of path rejection (and the loss of accuracy in the simulation of \( E[|\alpha_t|^2] \)). The resulting approximations of \( E[|\alpha_r|] \) and \( E[|\alpha_i|] \) were comparable to those obtained with the linear splitting with path rejection (see Figures 3.20-3.21), yet the approximation of \( E[|\alpha_t|^2] \) was far better than when using the linear splitting method with path rejection (see Figure 3.22).

The main drawback of the ode45-wpp scheme when applied to the modified \( \alpha \)-SDE was its huge computational cost. In the simulations leading to Figures 3.20-3.22 the steps computed with the ode45 routine (with both absolute and relative tolerances set to \( 10^{-5} \)) needed so much effort that the overall split-step method took roughly 300 times as much time than the linear splitting method. Whether the improved results justify the extra effort is hence debatable. One can argue that the extra work being caused by the adaptive refinement of the step for the ODE method might not help much when solving unstable SDEs like the \( \alpha \)- and \( \alpha, \beta \)-SDEs, but would make sense when used on a less unstable problem as a first try method, since the method is very easy to implement and will take care of the amount of work it considers necessary.
3.3. Split-step methods

A possible advantage of the split-step methods is that one can combine a robust implicit ODE solver with an explicit stochastic solver, avoiding the randomness for the internal computations (damped Newton, regula falsi, etc.) involved in the time stepping procedure of the implicit scheme. Hence, if the implicit method is able to guarantee the convergence to a solution $\tilde{X}_{k+1}$ of (3.19) for every $X_k$, every step of the method can be computed. This is something that should be tested.

Figure 3.20.: Simulations of $\mathbb{E}[\alpha_r]$ and $\mathbb{E}[\alpha_i]$ (with and without path rejection) for the $\alpha$-SDE (2.135) with $\zeta = \frac{1}{2}$ using the linear splitting with $h = \frac{2\pi}{3} \cdot 10^{-4}$ and 1000 sample paths. Compare with Figure 3.21. See Figure 3.22 for the corresponding mean $|\alpha|^2$. 

$\begin{align*}
\text{Re} \quad \text{Im} \\
\alpha \quad \alpha \quad \alpha \\
\text{expected} \quad \alpha \text{ linsplit} \quad \alpha \text{ linsplit, TOL=50} \end{align*}$

$\begin{align*}
\text{expected} \quad \alpha \text{ linsplit} \quad \alpha \text{ linsplit, TOL=50} \end{align*}$
3. Numerical schemes and experiments

ode45-wpp split-step solution of the SDE $d\alpha = -i(|\alpha|^2 + 1/2)\alpha \, dt + \sqrt{-i}/2 \alpha \, dW_t$

Figure 3.21.: Simulations of $E[\alpha_r]$ and $E[\alpha_i]$ for the $\alpha$-SDE (2.135) with $\zeta = \frac{1}{2}$ with the ode45-wpp method with $h = \frac{2\pi}{3} \cdot 10^{-4}$ and 1000 sample paths. Compare with the linear splitting results from Figure 3.20. See Figure 3.22 for the corresponding mean $|\alpha|^2$.

Expected vs mean of $|\alpha|^2$ for $d\alpha = -i(|\alpha|^2 + 1/2)\alpha \, dt + \sqrt{-i}/2 \alpha \, dW_t$

Figure 3.22.: Simulations of $E[|\alpha|^2]$ for the $\alpha$-SDE (2.135) with $\zeta = \frac{1}{2}$ with the ode45-wpp and the linear splitting methods (with and without path rejection) with $h = \frac{2\pi}{3} \cdot 10^{-4}$ and 1000 sample paths. See Figures 3.20,3.21 for the corresponding mean $\alpha_r, \alpha_i$. 

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3.4. Fixed $n$ method

In Chapter 2, it was shown that the variable $n = \alpha \beta =: n_r + i n_i$ plays an important role in the stability of the $\alpha, \beta$-SDE

$$d\alpha = -i(n + \frac{1}{2})\alpha dt + \frac{1-i}{\sqrt{2}}\alpha dW^1_t,$$  \hspace{1cm} (3.26)

$$d\beta = -i(\pi + \frac{1}{2})\beta dt + \frac{1-i}{\sqrt{2}}\beta dW^2_t,$$  \hspace{1cm} (3.27)

and that the solution of the $n$-SDE satisfies $\mathbb{E}[n_t] = n_0$. Note that if $n$ were constant between $t$ and $t+h$, the SDE (3.26)-(3.27) would be linear and its solution at time $t+h$ would be (see Section 1.2.2)

$$\alpha_{t+h} = \exp \left( n_i h - in_r h + \frac{1-i}{\sqrt{2}}(W^1_{t+h} - W^1_t) \right) \alpha_t,$$  \hspace{1cm} (3.28)

$$\beta_{t+h} = \exp \left( -n_i h - in_r h + \frac{1-i}{\sqrt{2}}(W^2_{t+h} - W^2_t) \right) \beta_t.$$  \hspace{1cm} (3.29)

One can thus discretize the time axis (e.g. considering times $t_j = j \cdot h$, $j = 0, \ldots, M$) and at each time step, fix $n$ and solve (3.26)-(3.27) ‘exactly’ through (3.28)-(3.29). Note that, using (3.28)-(3.29), one has

$$n_{t+h} = \alpha_{t+h} \beta_{t+h} = \exp \left( \frac{1-i}{\sqrt{2}}(W^1_{t+h} - W^1_t) + \frac{1+i}{\sqrt{2}}(W^2_{t+h} - W^2_t) \right) n_t,$$  \hspace{1cm} (3.30)

thus returning the exact representation of $n_t$ known from (2.107). For practical purposes, rewrite (3.26)-(3.27) as a linear real system for $X = (\alpha, \alpha_r, \alpha_i, \beta, \beta_r, \beta_i)^\top \in \mathbb{R}^4$:

$$dX = AX dt + B_1 X dW^1_t + B_2 X dW^2_t,$$  \hspace{1cm} (3.31)

where

$$A = \begin{pmatrix} n_i & n_r + \frac{1}{2} & 0 & 0 \\ -(n_r + \frac{1}{2}) & n_i & 0 & 0 \\ 0 & 0 & -n_i & n_r + \frac{1}{2} \\ 0 & 0 & -(n_r + \frac{1}{2}) & -n_i \end{pmatrix}, \hspace{1cm} B_1 = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 & 0 \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix},$$

$$B_2 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \end{pmatrix}.$$  

Since $A$, $B_1$ and $B_2$ commute, it follows from Remark 1.2.11 that the solution of (3.31), starting from $X_t$ at time $t$, is

$$X_{t+h} = \exp \left( \left[A - \frac{1}{2}(B_1^2 + B_2^2) \right] h + B_1(W^1_{t+h} - W^1_t) + B_2(W^2_{t+h} - W^2_t) \right) X_t,$$  \hspace{1cm} (3.32)

$$=: M_E.$$
where the matrix $M_E$ is

$$M_E = \begin{pmatrix}
e^{a_1} \cos(b_1) & e^{a_1} \sin(b_1) & 0 & 0 \\
-e^{a_1} \sin(b_1) & e^{a_1} \cos(b_1) & 0 & 0 \\
0 & 0 & e^{a_2} \cos(b_2) & e^{a_2} \sin(b_2) \\
0 & 0 & -e^{a_2} \sin(b_2) & e^{a_2} \cos(b_2)
\end{pmatrix}$$

and (3.33)

$$a_1 = n_i h + \frac{1}{\sqrt{2}}(W_{t+h} - W_t), \quad a_2 = -n_i h + \frac{1}{\sqrt{2}}(W_{t+h}^2 - W_t^2),$$

(3.34)

$$b_\ell = n_r h + \frac{1}{\sqrt{2}}(W_{t+h}^\ell - W_t^\ell), \quad \ell = 1, 2.$$  (3.35)

Figure 3.23.: Simulations of $\langle \hat{Y} \rangle$ and $\langle \hat{Z} \rangle$ for the $\alpha, \beta$-SDE using the fixed $n$ method for various $h$ and 2000 sample paths.

The procedure for obtaining approximations $X_{k}^{j}$ to $X_{k} \cdot h$ using (3.32)-(3.35) for $j = 1, \ldots, N$ and $k = 1, \ldots, M$ will be called the fixed $n$ method. In the simulations leading to Figures 3.23-3.28, the increments $W_{t+h}^\ell - W_t^\ell$ were approximated by $N(0,h)$-distributed pseudorandom numbers.

Unsurprisingly, the simulated mean values of $\alpha$ and $\beta$ (given through the $\langle \hat{Y} \rangle$ and $\langle \hat{Z} \rangle$) start to diverge around $t \approx 0.3$ (for $\alpha_0 = \beta_0 = 3$) when using the fixed $n$ method directly (see Figures 3.23, 3.24). However, the corresponding simulated $n$-values do not diverge at first, as predicted in (3.30). Indeed, although their mean tends to drift away from the expected $E[n_t] = n_0$ over time (see Figures 3.25-3.26), the simulated paths $n^j$ remain several orders of magnitude smaller than the corresponding $\alpha^j$ and $\beta^j$.

As with the splitting methods seen earlier in this chapter, reducing the step size $h$ below $10^{-3}$ does not lead to better results in the simulation of $\alpha$ and $\beta$ (see Figure 3.23). As can
3.4. Fixed n method

Figure 3.24.: Simulations of $\langle \hat{Y} \rangle$ and $\langle \hat{Z} \rangle$ for the $\alpha, \beta$-SDE using the fixed $n$ method with $h = 10^{-3}$ and various numbers of sample paths.

be seen in Figure [3.24] increasing the number of the simulated paths does not improve the results for $\langle \hat{Y} \rangle$ and $\langle \hat{Z} \rangle$ either (the chance that one path will diverge increases with the size of the sample). Yet the quality of the mean value simulations of $n$ improves (i.e. the mean value of the sample gets closer to $n_0$) as the sample size grows (see Figure [3.26]), which underlines the greater numerical stability of $n$ compared to $\alpha$ and $\beta$. However, appearances can be deceptive, since even the $n$-simulation will not survive having an $\alpha^j$ or $\beta^j$ reaching the numerical infinity, as will happen over longer time intervals (this will start occurring around $t \approx 2$). Of course, one could again use path rejection to get rid of such paths, but that would not change the fact that the method does not give good results for the $\alpha, \beta$-SDE even while $E[n_t]$ is conserved empirically.

Note that the exact solution of the $n$-SDE is known and given by (2.107). This information can be used for example to compare at time $t$ the probability $P(n^*_t > n^*_0)$ with the proportion of the simulated samples satisfying $n^*_t > n^*_0$, where $n^*_t := \text{Re}(n_t)$. From the results of the simulations shown in Figures [3.23]-[3.28], one can see that better results in the approximation of $E[n_t]$ and $P(n^*_t > n^*_0)$ do not imply better results in the $\alpha$ and $\beta$ simulation. Although the case with step size $h = 10^{-3}$ and $2 \cdot 10^5$ sample paths yields by far the best statistics for $n$, its $\langle \hat{Y} \rangle$-approximation is worse than for the case with only 2000 paths.

Since one knows from both Section 2.2.2 and (3.28)-(3.29) that $n_i \neq 0$ implies an exponential growth in size of either $\alpha$ or $\beta$, a variant of the fixed $n$ method where $n$ is forced to be real is presented below.
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Figure 3.25.: Mean value of $n$ for the $\alpha, \beta$-SDE using the fixed $n$ method for various $h$ and 2000 sample paths.

Figure 3.26.: Mean value of $n$ for the $\alpha, \beta$-SDE using the fixed $n$ method with $h = 10^{-3}$ and various numbers of sample paths.
3.4. Fixed n method

Figure 3.27.: Percentage of simulated paths where $n_r > n_0^r$ when using the fixed $n$ method on the $\alpha, \beta$-SDE for various $h$ and 2000 sample paths.

Figure 3.28.: Percentage of simulated paths where $n_r > n_0^r$ when using the fixed $n$ method on the $\alpha, \beta$-SDE with $h = 10^{-3}$ and various numbers of sample paths.
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3.4.1. Real $n$ case

Consider the following fixed $n \in \mathbb{R}$ algorithm:

**Algorithm 3.4.1.** Given: $X_0$, $M$, $T = M \cdot h$

for $k = 1 : M$

\[ t = (k - 1) \cdot h \]

\[ n_r = n_r(X_{k-1}) = X_{k-1}^1 X_{k-1}^3 + X_{k-1}^2 X_{k-1}^4 \]

\[ n_i = 0 \]

\[ M^{(k)}_E = M^{(k)}_E(n_r, n_i, h, W_{t+h}^1, W_{t+h}^2 - W_t^2) \text{ (as in (3.33))} \]

\[ X_k = M^{(k)}_E X_{k-1} \]

end

**Remark 3.4.2** (Identical Brownian motions). Forcing the condition $n_i = 0$ in each step of the algorithm might seem to be too strong a constraint, therefore a variant was also implemented where

\[ W_t^1 \equiv W_t^2, \quad \forall t \in [0, T], \text{ and } \]

\[ \alpha_0 = \beta_0 \quad \text{(3.37)} \]

hold. It can be shown that (3.36)-(3.37) automatically imply that, using exact arithmetic, $n_i = X_1^2 X_1^3 - X_1^1 X_1^4 = 0$ holds for $X_1 = M^{(1)}_E X_0$, as well as $\alpha_1 = \beta_1$ (i.e. $X_1^1 = X_1^3$, $X_1^2 = X_1^4$). This obviously holds recursively for $X_k$, $k = 1, \ldots, M$. However, setting $W_t^1 \equiv W_t^2$ and $\alpha_0 = \beta_0$ also implies (using exact arithmetic) that, at time $t$, one will have $n_r^t = e^{\sqrt{2}W_t^1 n_r^0}$. Thus, using Lemma 1.1.7 one will expect

\[ \mathbb{E}[n_r^t] = e^{t n_r^0} \quad \text{(3.38)} \]

when (3.36)-(3.37) hold. This is of course very different from the result $\mathbb{E}[n_r] = n_0$ derived in Section 2.3, therefore the bad numerical results corresponding to $W_t^1 \equiv W_t^2$ in Figure 3.29 are to be expected. The simulations depicted in Figure 3.30 confirm that $n_i$ is zero for all paths even without forcing it and that $\langle n^j \rangle_j$ behaves as expected from (3.38). The fact that $n_r > n_r^0$ holds for roughly 50% of the paths (see Figure 3.32 and Figure 3.35) is hardly surprising when remembering that $n_r^t = e^{\sqrt{2}W_t^1 n_r^0}$ and that $W_t^1 \sim N(0, t)$ is symmetric around zero.

In the Figures 3.30,3.31 and 3.34 the plotted $\langle n_i \rangle$ is the mean of the simulated $\alpha_i \beta_r - \alpha_r \beta_i$. This value is never used in the simulations, since $n_i$ is always set to zero when using the fixed $n \in \mathbb{R}$ method.

Keeping $W_t^1$ and $W_t^2$ independent of each other yields better numerical approximations for $\alpha$ and $\beta$ than those obtained under the conditions (3.36)-(3.37), yet they are still far from satisfying. As in the case of the general fixed $n$ method, the Algorithm 3.4.1 with independent Brownian motions respects the proportion of paths for which $n_r^t > n_r^0$ holds which would be expected from (2.107), see Figure 3.32 and Figure 3.35.
3.4. Fixed n method

The results obtained with the fixed (and real) n method (in the independent Brownian motion case) when considering a longer time interval showed that the apparent conservation of the mean of $n$ seen in Figures 3.30-3.31 is not a lasting phenomenon (see Figure 3.34). Not surprisingly, the whole simulation becomes unstable when the mean of $n$ is too far from $n_0$, as can be seen in Figure 3.33. Again, this is not simply a question of computational effort. The various simulations done with different step sizes and number of simulated paths all showed a similar behaviour.

It is interesting to notice how similar the case $W^1_t \neq W^2_t$ in Figure 3.29 is to the results shown in Figure 3.11 for the case where $\mu = 1$ (‘hermitian $P$’-case in [31]) in the $\phi, \psi, \tilde{\theta}$-SDE (2.1)-(2.3).

Overall, the fixed $n$ method is not satisfactory. Setting $n_t$ to zero might prevent the simulation from diverging, yet the results are still unreliable. Despite the good statistics up to $t \approx 2$ (for $\alpha_0 = \beta_0 = 0$) for $n$ w.r.t. its mean and $P(n^r_t > n^r_0)$, this is not enough to simulate $\alpha$ and $\beta$ accurately. In the next section, a method conserving $n_0$ as the mean value of $n_t$ by forcing $\alpha \beta = n_0$ for all paths will be presented.
3. Numerical schemes and experiments

Figure 3.30.: Mean value of $n$ for the $\alpha, \beta$-SDE using the fixed and real $n$ method (for both $W_1^t \equiv W_2^t$ and $W_1^t \neq W_2^t$), $h = 10^{-4}$, $10^4$ sample paths. The plot for $\langle n_i \rangle$ shows the mean value of $\alpha_i \beta_r - \alpha_r \beta_i$, since $n_i$ is always set to zero.

Figure 3.31.: Zooms into Figure 3.30.
3.4. Fixed $n$ method

Figure 3.32.: Percentage of simulated paths where $n_r > n^*_r$ when using the fixed and real $n$ method on the $\alpha, \beta$-SDE (for both $W^1_t \equiv W^2_t$ and $W^1_t \neq W^2_t$), $h = 10^{-4}$, $10^4$ sample paths.

Figure 3.33.: Simulations of $\langle \hat{Y} \rangle$ and $\langle \hat{Z} \rangle$ for the $\alpha, \beta$-SDE using the fixed and real $n$ method (for both $W^1_t \equiv W^2_t$ and $W^1_t \neq W^2_t$), $h = 2\pi \cdot 10^{-4}$, $10^4$ sample paths.
3. Numerical schemes and experiments

Figure 3.34.: Mean value of \( n \) for the \( \alpha, \beta \)-SDE using the fixed and real \( n \) method (for both \( W_t^1 \equiv W_t^2 \) and \( W_t^1 \neq W_t^2 \)), \( h = 2\pi \cdot 10^{-4} \), 10^4 sample paths. The plot for \( \langle n_i \rangle \) shows the mean value of \( \alpha_i \beta_n - \alpha_n \beta_i \), since \( n_i \) is always set to zero.

Figure 3.35.: Percentage of simulated paths where \( n_r > n_0 \) when using the fixed and real \( n \) method on the \( \alpha, \beta \)-SDE (for both \( W_t^1 \equiv W_t^2 \) and \( W_t^1 \neq W_t^2 \)), \( h = 2\pi \cdot 10^{-4} \), 10^4 sample paths.
3.5. Pathwise projection onto the \( \{ n = n_0 \} \)-manifold

In Section 2.2.2 and Section 2.3, it was shown that the quantity \( n = \alpha \beta \) plays a central role in the stability of the \( \alpha, \beta \)-SDE. Remember that the exact solution of the \( n \)-SDE is

\[
 n_t = e^{\xi_1 t + i \xi_2 t} n_0, \tag{3.39}
\]

where \( \xi_1, \xi_2 \) are independent Brownian motions in \( \mathbb{R} \) and that

\[
 E[n_t] = n_0, \quad \forall t \in \mathbb{R}_+. \tag{3.40}
\]

In this section, a method is presented which, after every time step, projects each simulated path of the numerical solution of the \( \alpha, \beta \)-SDE onto a manifold where \( n = n_0 \) holds. This is of course a much stronger condition than merely requiring that the average of \( n \) over the paths is \( n_0 \), yet keeping \( n = n_0 \) at each step avoids both the possibility of having the simulation diverge due too large \( n \)-values and the situation where \( n_i \neq 0 \) (assuming \( \alpha_0 = \beta_0 \)). The method will be derived for the more general case where \( n_0 \in \mathbb{C} \) despite the fact that one is more interested in \( n_0 \in \mathbb{R} \).

The procedure was inspired by [59], although the projection will be done differently here. In the setting of the \( \alpha, \beta \)-SDE in its real form (2.21)-(2.24), consider the manifold

\[
 \Sigma_0 = \{ x \in \mathbb{R}^4 \mid \zeta(x) = 0 \},
\]

where \( x = (\alpha_r, \alpha_i, \beta_r, \beta_i)^\top \), \( \zeta \in C^1(\mathbb{R}^4, \mathbb{R}^2) \) with \( \zeta(x) = 0 \) when \( n(x) = n_0 \). For \( \zeta = (\zeta_1, \zeta_2)^\top \) given by

\[
 \zeta_1(x) = (n_r - \text{Re} n_0), \tag{3.41}
\]

\[
 \zeta_2(x) = (n_i - \text{Im} n_0), \tag{3.42}
\]

it holds that

\[
 \nabla \zeta_1(x) = (\beta_r, \beta_i, \alpha_r, \alpha_i)^\top, \tag{3.43}
\]

\[
 \nabla \zeta_2(x) = (-\beta_i, \beta_r, \alpha_i, -\alpha_r)^\top, \tag{3.44}
\]

\[
 (\nabla \zeta_1)^\top \nabla \zeta_2 = 0. \tag{3.45}
\]

Note that \( \zeta, \zeta_1, \zeta_2 \) have nothing to do with the free parameter \( \zeta \) in the modified \( \alpha \)-SDE (2.135).

Let \( x_0^0 \in \Sigma_0 \). Using some numerical SDE scheme for (2.21)-(2.24) with starting value \( x_0^0 \) at \( t_0 \), one simulates one path to obtain the estimate \( x_1^1 \in \mathbb{R}^4 \). In general, \( x_1^1 \in \Sigma_0 \) will not hold. Therefore, one searches for the projection of \( x_1^1 \) to \( z \in \Sigma_0 \) in the following sense:

\[
 z \in \Sigma_0, \quad z + \gamma_1 \nabla \zeta_1(z) + \gamma_2 \nabla \zeta_2(z) = x_1^1. \tag{3.46}
\]
3. Numerical schemes and experiments

This means that \( z, \gamma_1 \) and \( \gamma_2 \) have to satisfy the following equations:

\[
\begin{align*}
\zeta, \gamma_1 z_3 + z_2 z_4 &= \text{Re} n_0, \quad (3.47) \\
z_2 z_3 - z_1 z_4 &= \text{Im} n_0. \quad (3.48)
\end{align*}
\]

\[\zeta + \gamma_1 \nabla \zeta_1 (z) + \gamma_2 \nabla \zeta_2 (z) = x^1: \]

\[
\begin{align*}
z_1 + \gamma_1 z_3 - \gamma_2 z_4 &= x_1^1, \quad (3.49) \\
z_2 + \gamma_1 z_4 + \gamma_2 z_3 &= x_2^1, \quad (3.50) \\
z_3 + \gamma_1 z_1 + \gamma_2 z_2 &= x_3^1, \quad (3.51) \\
z_4 + \gamma_1 z_2 - \gamma_2 z_1 &= x_4^1. \quad (3.52)
\end{align*}
\]

To solve (3.47)-(3.52), one can rewrite the system as a non-linear error equation

\[
f(w) - c = r, \quad (3.53)
\]

where

\[
w = \begin{pmatrix} z_1 \\ z_2 \\ z_3 \\ z_4 \\ \gamma_1 \\ \gamma_2 \end{pmatrix}, \quad f(w) = \begin{pmatrix} w_1 w_3 + w_2 w_4 \\ w_2 w_3 - w_1 w_4 \\ w_1 + w_3 w_5 - w_4 w_6 \\ w_2 + w_3 w_6 + w_4 w_5 \\ w_3 + w_1 w_5 + w_2 w_6 \\ w_4 - w_1 w_6 + w_2 w_5 \end{pmatrix}, \quad c = \begin{pmatrix} \text{Re} n_0 \\ \text{Im} n_0 \\ x_1^1 \\ x_2^1 \\ x_3^1 \\ x_4^1 \end{pmatrix}.
\]

(3.54)

It is now possible to solve (3.53) using the Gauss-Newton method with minimization (see [79]). The corresponding Jacobian is

\[
A = (a_{i,j}) = \left( \frac{\partial f_i}{\partial w_j} \right) = \begin{pmatrix}
w_3 & w_4 & w_1 & w_2 & 0 & 0 \\
w_4 & w_3 & w_2 & -w_1 & 0 & 0 \\
1 & 0 & w_5 & -w_6 & w_3 & -w_4 \\
0 & 1 & w_6 & w_5 & w_4 & w_3 \\
w_5 & w_6 & 1 & 0 & w_1 & w_2 \\
-w_6 & w_5 & 0 & 1 & w_2 & -w_1
\end{pmatrix}.
\]

(3.55)

**Algorithm 3.5.1** (Pathwise projection of \( x^1 \) on \( \{ n = n_0 \} \) using Gauss-Newton with minimization).

**Given:**

\[
w^{(0)} := (x_1^1, x_2^1, x_3^1, x_4^1, 0, 0)^\top,
\]

\[
c = (\text{Re} n_0, \text{Im} n_0, x_1^1, x_2^1, x_3^1, x_4^1)^\top
\]

RTOL (relative tolerance, e.g. \( 10^{-5} \)), ATOL (absolute tolerance, e.g. \( 10^{-8} \)),

TOLS (absolute tolerance for \( S \), e.g. \( 10^{-6} \)),

MAXIT (maximal number of iterations, e.g. 100),

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3.5. Pathwise projection onto the \( \{n = n_0\} \)-manifold

\[
\text{MAXMINIT} \quad \text{(maximal number of minimization iterations, e.g. 50)}.
\]

\textbf{for} \( k = 0 : \text{MAXIT} \)
\begin{align*}
\text{Compute } A^{(k)} &:= A(w^{(k)}), \quad f^{(k)} := f(w^{(k)}), \quad S^{(k)} := \|f^{(k)} - c\|_2^2. \\
\text{Compute } \zeta^{(k+1)} &\text{ as the least square solution to } \\
A^{(k)}\zeta^{(k+1)} - (c - f^{(k)}) &= \rho^{(k)},
\end{align*}

where \( \rho^{(k)} \) is the residual vector. \( 91 \%

\text{Minimization}
\[
t = 1, \quad x = w^{(k)} + t\zeta^{(k+1)}, \quad S_x = \|f(x) - c\|_2^2, \quad \text{miniter} = 0
\]
\textbf{while} \( S_x \geq S^{(k)} \&\& \text{miniter} < \text{MAXMINIT} \)
\begin{align*}
t &= t/2, \quad x = w^{(k)} + t\zeta^{(k+1)}, \quad S_x = \|f(x) - c\|_2^2, \quad \text{miniter} = \text{miniter} + 1
\end{align*}
\textbf{end}

\textbf{if} \( \text{miniter} == \text{MAXMINIT} \)
\begin{align*}
\text{error} \quad &\% \text{ No convergence of the minimization scheme} \\
\textbf{end}
\end{align*}

\[ w^{(k+1)} = x \]
\begin{align*}
\textbf{if} \quad &\|w^{(k+1)} - w^{(k)}\| \leq \|w^{(k+1)}\| \cdot \text{RTOL} + \text{ATOL} \\
\textbf{break} \quad &\% \text{convergence} \\
\textbf{end}
\end{align*}

\textbf{end}
The projected value is then \( x_{\text{proj}} = x \).

\textbf{Remark 3.5.2.} Note that the projection in Algorithm 3.5.1 is done pathwise and that \( x^0 \) can (and will for \( t > 0 \)) have different values for each path.

It is now easy to use Algorithm 3.5.1 to project each path of the numerical solution back onto the \( \Sigma_0 \)-manifold after each step. This will ensure that (3.40) is (very nearly) satisfied for the projected solution. Indeed, within a very small numerical error margin, the \textbf{much} stronger condition

\[
n(x_{\text{proj}}) = n_0
\]

is satisfied \textbf{for all paths}.

This prevents the \( \langle \hat{Y} \rangle \)- and \( \langle \hat{Z} \rangle \)-simulation from diverging, but it still does not yield a reliable approximation for the solution of (2.19)-(2.20), as it just returns an oscillatory solution (see Figure 3.36). The Figures 3.37-3.38 are shown for comparison of the \( n \)-distribution statistics for the ode45-strong order 1.5 Taylor split-step method used in Figure 3.36 with the fixed \( n \) method of Section 3.4. Further methods were tried which preserved some aspects of the distribution of \( n \), yet without success so far. Of course, more statistics than just the mean of \( n \) and the quantity \( P(n_r > n_r^0) \) should be considered.
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Figure 3.36.: Simulations of $\langle \hat{Y} \rangle$ and $\langle \hat{Z} \rangle$ for the $\alpha, \beta$-SDE using the ode45-strong order 1.5 Taylor split-step method, with and without projection on $\Sigma_0$, step size $h = 10^{-3}$ and $10^4$ sample paths.

Figure 3.37.: Mean value of $n$ for the $\alpha, \beta$-SDE using the ode45-strong order 1.5 Taylor split-step method, with and without projection on $\Sigma_0$, step size $h = 10^{-3}$ and $10^4$ sample paths.
3.5. Pathwise projection onto the \( \{ n = n_0 \} \)-manifold

Figure 3.38.: Percentage of simulated paths where \( n_r > n_r^0 \) when using the ode45-strong order 1.5 Taylor split-step method, without projection on \( \Sigma_0 \), step size \( h = 10^{-3} \) and \( 10^4 \) sample paths. When projecting on \( \Sigma_0 \), all paths satisfied \( |n_r - n_r^0| \leq 10^{-10} \).
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3.6. Regularization techniques

Another way of avoiding the diverging sample paths when solving the $\alpha, \beta$-SDE (2.19)-(2.20) numerically is to add a correction term to the drift of the SDE. Consider the regularized

\[
d\alpha = -i(n + \frac{1}{2})\alpha \, dt + \frac{1-i}{\sqrt{2}} \alpha \, dW_1^1 - \lambda C_\alpha(\alpha, \beta) \alpha \, dt,
\]

\[=: a_\alpha \, dt + b_\alpha \, dW_1^1 - \lambda C_\alpha(\alpha, \beta) \alpha \, dt,
\]

\[
d\beta = -i(n + \frac{1}{2})\beta \, dt + \frac{1-i}{\sqrt{2}} \beta \, dW_1^2 - \lambda C_\beta(\alpha, \beta) \beta \, dt,
\]

\[=: a_\beta \, dt + b_\beta \, dW_2^2 - \lambda C_\beta(\alpha, \beta) \beta \, dt,
\]

with $\lambda \in \mathbb{R}^+$, and possible choices for $C_\alpha$, $C_\beta$ being e.g. $C_\alpha = |\alpha|^m$, $C_\beta = |\beta|^m$, $m \in \mathbb{N}$, or $C_\alpha = C_\beta = |n|$. Also tried were $C_\alpha = |\alpha|^m |\beta|$, $C_\beta = |\alpha| |\beta|^m$, $m \in \mathbb{N}$, but without success.

The following modified midpoint rule was used to solve the regularized SDE (3.57)-(3.58).

**Algorithm 3.6.1 (Modified midpoint rule for one sample path).**

**Wanted:** Approximations $\alpha_k, \beta_k$ to $\alpha, \beta$ at times $t_k$, $k = 1, \ldots, M$.

**Given:**
- Initial values $\alpha_0, \beta_0$ at time $t_0$,
- stepsizes $h_k = t_k - t_{k-1}$, $k \geq 1$,
- approximate Brownian motion increments $\Delta W_1^1, \Delta W_2^2$ i.i.d. $N(0, h_k)$,
- RTOL (relative tolerance, e.g. $10^{-6}$), ATOL (absolute tolerance, e.g. $10^{-8}$),
- MAXIT (maximal number of iterations, e.g. 50).

Set $k = 0$.

1. Set $\text{iter} = 0$, $h = h_k$,

\[
\begin{align*}
\alpha_{k+1}^{\text{old}} &= \alpha_k + a_\alpha(\alpha_k, \beta_k) h + b_\alpha(\alpha_k, \beta_k) \Delta W_1^1 - \lambda C_\alpha(\alpha_k, \beta_k) \alpha_k h,
\beta_{k+1}^{\text{old}} &= \beta_k + a_\beta(\alpha_k, \beta_k) h + b_\beta(\alpha_k, \beta_k) \Delta W_2^2 - \lambda C_\beta(\alpha_k, \beta_k) \beta_k h.
\end{align*}
\]

2. Pick the solution $\alpha_{k+1}^{\text{new}}$ of the quadratic equation

\[
\alpha_{k+1}^{\text{new}} = \alpha_k - h \left( \frac{\alpha_k + \alpha_{k+1}^{\text{old}} \beta_k + \beta_{k+1}^{\text{old}}}{2} + \frac{1}{2} \right) \frac{\alpha_k + \alpha_{k+1}^{\text{new}}}{2}
\]

\[
+ \frac{1-i}{\sqrt{2}} \alpha_k \Delta W_1^1 - \lambda C_\alpha(\alpha_k, \beta_k) \alpha_{k+1}^{\text{new}} h
\]

which is closest to $\alpha_{k+1}^{\text{old}}$.

Set $\Delta_\alpha = \alpha_{k+1}^{\text{new}} - \alpha_{k+1}^{\text{old}}$, $\alpha_{k+1}^{\text{new}} = \alpha_{k+1}$. 

3.6. Regularization techniques

3. Pick the solution $\beta_{k+1}^{new}$ of the quadratic equation

$$\beta_{k+1}^{new} = \beta_k - i h \left( \frac{\alpha_k + \alpha_{old}^k}{2} + \frac{\beta_k + \beta_{old}^k}{2} + \frac{1}{2} \right) \frac{\beta_k + \beta_{old}^k}{2}$$

\[ + \frac{1 - i}{\sqrt{2}} \beta_k \Delta W_k^2 - \lambda C_\beta(\alpha_k, \beta_k) \beta_{k+1}^{new} h \]

which is closest to $\beta_{k+1}^{old}$.

Set $\Delta_\beta = \beta_{k+1}^{new} - \beta_{k+1}^{old}$, $\beta_{k+1}^{old} = \beta_{k+1}^{new}$, iter = iter + 1.

4. if $\sqrt{|\Delta\alpha|^2 + |\Delta\beta|^2} \geq ATOL + RTOL \cdot \sqrt{|\alpha_{old}^k|^2 + |\beta_{old}^k|^2}$

if iter < MAXIT
goto 2.
else
no convergence
end
else
$\alpha_{k+1} = \alpha_{k+1}^{old}$, $\beta_{k+1} = \beta_{k+1}^{old}$,
k = k + 1, repeat algorithm for next step.
end

Figure 3.39.: Midpoint rule for regularized $\alpha, \beta$-SDE for various $\lambda$’s (values in the legend), $C_\alpha = |\alpha|^2$, $C_\beta = |\beta|^2$, $h = 0.6 \cdot 10^{-4}$, 2000 sample paths.

Numerical experiments with various values of $\lambda$ show that even relatively small $\lambda$’s (say $\lambda \geq 10^{-4}$) prevent the solution from diverging towards infinity (remember that the
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Figure 3.40.: Midpoint rule for regularized $\alpha, \beta$-SDE for various $\lambda$'s (values in the legend), $C_\alpha = |\alpha|^2$, $C_\beta = |\beta|^2$, $h = \frac{\pi}{5} \cdot 10^{-3}$, 2000 sample paths.

$\alpha, \beta$-SDE corresponds to the choice $\mu = 0$ of the $\phi, \psi, \tilde{\theta}$-SDE, which is highly unstable numerically). The optimal $\lambda$-value seems to lie somewhere around $\lambda \approx 0.001$ when one wishes to negotiate the second curve of $\langle \hat{Y} \rangle$ and $\langle \hat{Z} \rangle$ well, yet the results are still far from satisfactory even then. Larger $\lambda$-values emphasize the 'shortcuts' taken by the numerical approximation to $\langle \hat{Y} \rangle$ and $\langle \hat{Z} \rangle$ in the curves, whereas smaller values still oscillate too much where the solution should stay around zero, see Figures 3.39-3.40. In each figure, the Brownian motion increments were the same for all values of $\lambda$.

One obvious flaw in the regularized SDE approach is that the added terms in (3.57)-(3.58) do not change the fact that the $\alpha = 0$ and $\beta = 0$ are attracting (see 2.2.5). In fact, the damping terms are forcing the paths of $\alpha$ and $\beta$ towards zero. Hence, although the numerical solution is prevented from diverging and looks reasonable in the time interval $[1, 5]$, the appearances are deceptive: the solution will miss any further turning points.

Linear damping was also tried for various $\lambda$ by setting $C_\alpha = C_\beta = 1$ in (3.57)-(3.58). However, linear damping alone is not enough to stabilise the SDE, as it cannot avoid the divergence of the paths while keeping the statistical error low. Large values of $\lambda$ are needed for the first (but then the solution only drifts towards zero), while small $\lambda$ values do not prevent the divergence of the solution for some paths, see Figure 3.41. Hence, what was described in [44] as the fourth signature of non-vanishing boundary conditions is missing, which could indicate that the instability is not necessarily caused by non-negligible boundary conditions. A deeper investigation of this phenomenon is needed, in particular using other methods than the midpoint rule from Algorithm 3.6.1.
3.7. Artificial boundary conditions

In Sections 3.4-3.6, some effort was spent to control the $\alpha, \beta$-SDE through the variable $n = \alpha \beta$. Another way to prevent the divergence of $\alpha$ and $\beta$ without having to reject samples is to use boundary conditions (BCs). Since one particularly wants to avoid $\alpha$ or $\beta$ reaching the critical points 0 and $\infty$, it makes sense to have both an upper and lower boundary on the magnitude of $\alpha$ and $\beta$. Several variants were tested with variable degrees of success. Some with soft boundaries (i.e. $\alpha, \beta$ were allowed to cross the boundaries, yet were forced back with more or less insistence depending on the variant), some with sticky boundaries (paths trying to cross them get stuck) and some with reflective boundaries (paths that hit them are sent back). The two boundary conditions which yielded the best results are presented in this section. Both constrain $\alpha$ and $\beta$ to the same annulus $A := \{ z \in \mathbb{C}; r_{\text{min}} \leq |z| \leq r_{\text{max}} \}$, where the lower and upper radii are given by

$$r_{\text{min}} := \lambda \cdot |\alpha_0|, \quad r_{\text{max}} := \frac{|\alpha_0|}{\lambda^2}$$

for some $\lambda < 1$. When combined with a numerical integrator for the $\alpha, \beta$-SDE, each boundary condition is used in the following way. Start with the non-random initial condition $\alpha_0 = \beta_0$ (i.e. all the paths start at the same point). At time step $k \geq 0$, for each path $j = 1, \ldots, N$, the BC is applied on $\alpha_k^j$ and $\beta_k^j$ separately to obtain new values $\tilde{\alpha}_k^j$ and $\tilde{\beta}_k^j$. The $\tilde{\alpha}_k^j$ and $\tilde{\beta}_k^j$ are then used instead of $\alpha_k^j$ and $\beta_k^j$ in the computation leading

Figure 3.41.: Midpoint rule for linearly damped $\alpha, \beta$-SDE for various $\lambda$’s (values in the legend), $C_\alpha = C_\beta = 1$, $h = 10^{-4}$, 2000 sample paths.
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to the next approximations $\alpha_{k+1}^j$ and $\beta_{k+1}^j$ with the SDE integrator. Set $k = k + 1$ and repeat.

Algorithm 3.7.1 (Toroid boundary condition).

Given: a value $z \in \mathbb{C}$.

Wanted: a value $\tilde{z} \in A$.

if $|z| \leq r_{\text{max}}$
  if $|z| \geq r_{\text{min}}$
    $\tilde{z} = z$
  else
    $\tilde{z} = \frac{r_{\text{max}}}{r_{\text{min}}}z = \lambda^{-3}z$
  end
else
  $\tilde{z} = \frac{r_{\text{min}}}{r_{\text{max}}}z = \lambda^{3}z$
end

Algorithm 3.7.2 (Annulus boundary condition).

Given: a value $z \in \mathbb{C}$.

Wanted: a value $\tilde{z} \in A$.

if $|z| \leq r_{\text{max}}$
  if $|z| \geq r_{\text{min}}$
    $\tilde{z} = z$
  else
    $\tilde{z} = \left(2 \frac{r_{\text{min}}}{|z|} - 1 \right)z$
  end
else
  $\tilde{z} = \left(2 \frac{r_{\text{max}}}{|z|} - 1 \right)z$
end

The simulations leading to Figures 3.42-3.44 were computed using the modified midpoint rule of Algorithm 3.6.1 without damping, i.e. setting $C_{\alpha} = C_{\beta} = 0$ in (3.57)-(3.58). In order to distinguish it from the regularized algorithm presented in Section 3.6, the method used here for the $\alpha, \beta$-SDE (2.19)-(2.20) will be denoted as the decoupled semi-implicit method.

Remark 3.7.3. The toroid BC has soft boundaries: when using the toroid BC on an $z$ satisfying $|z| > r_{\text{max}}$, the returned value $\tilde{z}$ will be shrunk by a factor of $\lambda^3$ compared to $|z|$ and still larger than $r_{\text{min}}$, but $\tilde{z} \notin A$ if $|z| > \lambda^{-3}r_{\text{max}}$. Similarly, $|z| < r_{\text{min}}$ implies that $|\tilde{z}| = \lambda^{-3}|z| < r_{\text{max}}$, but not necessarily that $|\tilde{z}| \geq r_{\text{min}}$. However, if $\lambda$ is chosen adequately, the values returned by the BC will stay small enough that for $\alpha_{k}^j$ (or $\beta_{k}^j$) in $A$, the probability that $|\alpha_{k+1}^j| > \lambda^{-3}r_{\text{max}}$ will be negligible. Based on the error from the simulations using the decoupled semi-implicit method, the optimal $\lambda$ for the toroid BC is $\lambda = 0.48$. 

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3.7. Artificial boundary conditions

Figure 3.42.: $\langle \alpha \rangle$ vs $E[\alpha]$ for the decoupled semi-implicit method for the $\alpha, \beta$-SDE using annulus vs toroid BC with their optimal $\lambda$, $h = 10^{-3}$, $2^{16}$ sample paths. The values for $\beta$ are similar.

Remark 3.7.4. The external boundary of the annulus BC is also a soft boundary: when using the annulus BC on an $z$ satisfying $|z| > r_{\text{max}}$, the returned value $\tilde{z} = \left( \frac{2 r_{\text{max}}}{|z|} - 1 \right) z$ will only be on $A$ if $r_{\text{max}} < |z| < (2 - \lambda^{3}) r_{\text{max}}$ or $(2 + \lambda^{3}) r_{\text{max}} < |z| < 3 r_{\text{max}}$, but the condition only makes sense as long as $|z| > 2 r_{\text{max}}$, as larger $|z|$ will cause $\tilde{z}$ to be on the other side of the origin (which would yield bad dynamics, as experienced for the reflective boundary conditions). But as in the toroid BC case, by choosing $\lambda$ appropriately (e.g. $\lambda = 0.64$, which minimizes the error of simulations for various $\lambda$ with the decoupled semi-implicit method), the values returned by the BC will stay small enough that for $\alpha_{k}^{j}$ (or $\beta_{k}^{j}$) in $A$, the probability that $|\alpha_{k+1}^{j}| > 2 r_{\text{max}}$ is so small that this possibility can be ignored. This is confirmed by the simulation results.

The results shown in Figures 3.42-3.44 are surprisingly good for both the toroid and annulus BC, compared to what one has seen so far. The annulus BC in particular gives stable numerical results that give reasonable approximations to the expected solution $E[\alpha]$ up to $t \approx 0.7$, which is twice as large a time as obtained with the methods from Sections 3.1-3.6 and is comparable with the results shown in Figures 3.20-3.21 using the linear splitting method and the ode45-wpp split-step scheme for the more stable $\alpha$-SDE.

However, as one can seen from the results obtained for approximations of higher moments, the damping of the numerical solution caused by the BCs disturbs the natural dy-
3. Numerical schemes and experiments

Figure 3.43: $\langle \alpha^2 \rangle$ vs $\mathbb{E}[\alpha^2]$ for the decoupled semi-implicit method for the $\alpha, \beta$-SDE using annulus vs toroid BC with their optimal $\lambda$, $h = 10^{-3}$, $2^{16}$ sample paths. The values for $\beta^2$ are similar.

Dynamics of the solution process, which makes the numerical approximation miss the next oscillations. This is in principle the same phenomenon seen when using path rejection, as the large samples occurring naturally in such a simulation will not be contributing to the mean solution as they should. Yet the fact that the control of the magnitude of the solution is done more subtly and on both growing and decreasing paths allows the approximations to be more reliable than the mean of the accepted paths. As always, more experiments are needed: using other methods, other SDEs, other BCs. For example, there is bound to be better choices of BCs for reflective or absorbing boundaries than those tested, but thought has to be given about how exactly to redistribute the paths crossing the boundaries. A correlation for the BC between $\alpha$ and $\beta$ is also conceivable in order to preserve the dynamics of $n$. 
3.8. Wick rotation

3.8.1. Heuristic motivation

Consider the general Itô SDE
\[ dX_t = a(X_t) \, dt + b(X_t) \, dW_t, \quad (3.59) \]
where \( X_t \in \mathbb{C}^d, W_t \in \mathbb{R}^m \). As seen often enough throughout this thesis, some SDEs can be hard to solve numerically when met head-on. Among the SDE properties one might wish to avoid, moments growing exponentially in time (as for the \( \alpha \)-SDE \( \alpha^3 \) or in the linear SDE of Section 3.8.3) is something that a transformation of time within the complex plane might fix. If a suitable function \( F \) can be found to fit the numerical solution data of the modified SDE well enough, an analytical continuation of \( F \) back into the original setting can give satisfying results. This idea was inspired by the so-called Wick rotation, in honour of Wick’s 1954 paper [92]. Variants of this technique have been in use in physics and finance in various contexts (see for example [24], [25], [53], [91]), but the author is as yet unaware of any attempt made to solve SDEs in the way explained below.

The approach will be motivated heuristically as follows: introduce the variable \( s \), where
\[ t = \Theta s, \quad \Theta \in \mathbb{C}. \quad (3.60) \]
### 3. Numerical schemes and experiments

Assume that there exists an exact solution of (3.59) which can be described by $X_t := f(t, W_t, X_0) \in \mathbb{C}^d$. This means (using Remark 1.2.5) that for $\ell = 1, \ldots, d$, it holds

$$dX_t^\ell = \left\{ \frac{\partial f^\ell}{\partial t} + \frac{1}{2} \sum_{j=1}^{m} \sum_{i,k=1}^{m} \delta_{ij} \delta_{kj} \frac{\partial^2 f^\ell}{\partial w^i \partial w^k} \right\} dt + \sum_{j=1}^{m} \delta_{kj} \frac{\partial f^\ell}{\partial w^k} dW_t^j$$

$$= \left\{ \frac{\partial f^\ell}{\partial t} + \frac{1}{2} \sum_{j=1}^{m} \frac{\partial^2 f^\ell}{(\partial w^j)^2} \right\} dt + \sum_{j=1}^{m} \frac{\partial f^\ell}{\partial w^j} dW_t^j$$

(3.59)

Considering for the moment the case $s \in \mathbb{R}$ (i.e. $t, \Theta \in \mathbb{R}$), one can define

$$Y_s := U(s, \widetilde{W}_s) = f(\Theta s, \sqrt{\Theta} \widetilde{W}_s, X_0), \quad (3.62)$$

where $\widetilde{W}_s$ is a real Brownian motion in the real variable $s$ and is independent of $W_t$. The replacement of $W_{\Theta s}$ (only defined for $\Theta s \in \mathbb{R}_+$) by $\sqrt{\Theta} \widetilde{W}_s$ (defined for $s \in \mathbb{R}_+$) is motivated by the fact that $W_{\mu t}$ has the same distribution as $\sqrt{\mu} W_r$ for $\mu, r \geq 0$. As above, one can then use the Itô rule to obtain an SDE for $Y_s$ (when $s \in \mathbb{R}_+$):

$$dY_s^\ell = \left\{ \frac{\partial U^\ell}{\partial s} + \frac{1}{2} \sum_{j=1}^{m} \sum_{i,k=1}^{m} \delta_{ij} \delta_{kj} \frac{\partial^2 U^\ell}{\partial w^i \partial w^k} \right\} ds + \sum_{j=1}^{m} \sum_{k=1}^{m} \delta_{kj} \frac{\partial U^\ell}{\partial w^k} d\widetilde{W}_s^j$$

$$= \left\{ \frac{\partial f^\ell}{\partial t}(\Theta s, \sqrt{\Theta} \widetilde{W}_s, X_0) \frac{\partial t}{\partial s} + \frac{1}{2} \sum_{j=1}^{m} \frac{\partial f^\ell}{\partial \widetilde{w}^j} \left( \sum_{n=1}^{m} \frac{\partial f^\ell}{\partial \widetilde{w}^n}(\Theta s, \sqrt{\Theta} \widetilde{W}_s, X_0) \frac{\partial \widetilde{w}^n}{\partial \widetilde{w}^j} \right) \right\} ds$$

$$+ \sum_{j=1}^{m} \sum_{n=1}^{m} \frac{\partial f^\ell}{\partial \widetilde{w}^n}(\Theta s, \sqrt{\Theta} \widetilde{W}_s, X_0) \frac{\partial \widetilde{w}^n}{\partial \widetilde{w}^j} d\widetilde{W}_s^j$$

$$= \Theta \left\{ \frac{\partial f^\ell}{\partial t}(\Theta s, \sqrt{\Theta} \widetilde{W}_s, X_0) + \frac{1}{2} \sum_{j=1}^{m} \frac{(\partial f^\ell}{(\partial \widetilde{w}^j)^2}(\Theta s, \sqrt{\Theta} \widetilde{W}_s, X_0) \right\} ds$$

$$+ \sqrt{\Theta} \sum_{j=1}^{m} \frac{\partial f^\ell}{\partial \widetilde{w}^j}(\Theta s, \sqrt{\Theta} \widetilde{W}_s, X_0) d\widetilde{W}_s^j, \ell = 1, \ldots, d.$$

Using (3.61) and (3.62), one obtains the SDE

$$dY_s = \Theta a(Y_s) ds + \sqrt{\Theta} b(Y_s) d\widetilde{W}_s, \quad (3.63)$$

which will be said to be the Wick-rotated SDE of the SDE (3.59) with angle $\arg(\Theta)$.
3.8. Wick rotation

The idea is to solve (3.63) for \( s \in \mathbb{R}_+ \), which will of course be significantly different from solving (3.59) for \( t \in \mathbb{R}_+ \) if \( \Theta \in \mathbb{C} \setminus \mathbb{R}_+ \), but by continuing \( Y_s \) analytically, it is possible in certain cases to obtain more stable results than when solving (3.59) directly.

In order to justify the interpretation of \( W_\Theta s \) as \( \sqrt{\Theta} \tilde{W}_s \) for complex \( \Theta \) and \( s \geq 0 \), consider the Wick-rotated version of the complex geometric Brownian motion case discussed in Section 1.2.2:

\[
dY_s = \Theta b Y_s ds + \sqrt{\Theta} \sigma Y_s d\tilde{W}_s. \tag{3.64}
\]

For \( s \in \mathbb{R} \), the exact solution of (3.64) is of course

\[
Y_s = e^{\Theta (b - \frac{\sigma^2}{2}) s + \sqrt{\Theta} \sigma \tilde{W}_s} X_0. \tag{3.65}
\]

If one defines \( \tilde{W}_s \) as \( e^{i\theta/2} \tilde{W}_r \), formula (3.65) can still be evaluated for \( s = re^{i\theta} \in \mathbb{C} \) \((r \geq 0, \theta \in ]-\pi, \pi[)\). If \( s = \Theta^{-1} t \) with \(|\Theta| = 1 \) and \( t \geq 0 \), this leads to

\[
Y_{\Theta^{-1}t} := \exp \left( b - \frac{\sigma^2}{2} t + \sqrt{\Theta} \sigma \tilde{W}_{\Theta^{-1}t} \right) X_0
\]

\[
= e^{(b - \frac{\sigma^2}{2}) t + \sigma \tilde{W}_t} X_0, \tag{3.66}
\]

which has the same distribution as the exact solution of (1.25).

The question is now how, from numerical data obtained when solving (3.63), a satisfying approximation to the solution of (3.59) can be found. Denote the \( j \)th path of the numerical solution of (3.59) at time \( t_k \) by \( \tilde{X}^j_k \) and the numerical solution of (3.63) at time \( s_k \) by \( \hat{Y}^j_k \). In the general case where only the discrete numerical solution paths \( \hat{Y}^j_k \) at time \( s_k \) are known for \( k = 0, \ldots, M, \ j = 1, \ldots, N \), there is of course no way of using the inverse substitution \( s = \Theta^{-1} t \) to obtain the corresponding \( \tilde{X}^j_k \)'s. What can be done however, provided the components \( Y_\delta^\delta \) are ‘nearly real’, \( \delta = 1, \ldots, d \) (i.e. \( |\text{Im}(\hat{Y}^\delta_k)_{ij}| < \varepsilon_1 \) for most \( k \) with \( \varepsilon_1 \) ‘small’, which will be the case in the SDEs discussed in this Section), is to do some componentwise least-square type data fitting of \( Y_\delta \).

For \( Y_\delta^\delta \), find an appropriate function \( F^\delta(s) \) such that the 2-norm of the residual vector \( r^\delta \) is minimal, where

\[
r^\delta_{k+1} = F^\delta(s_k) - \text{Re}(\hat{Y}^\delta_k)_{ij}, \quad k = 0, \ldots, M. \tag{3.67}
\]

Once \( F^\delta \) is determined, it is easy to evaluate \( F^\delta(\Theta^{-1} t) \) for any \( t \), delivering the sought-after approximation of \( \mathbb{E}[X_\delta^\delta] \).

It is clear to the author that this approach may seem dubious from a strict theoretical point of view, in particular in the case of SDEs where no existence or uniqueness can be proved. Yet it was felt that it was something worth trying and that good results might partly excuse the lack of a solid theory to back them up (or kindle enough interest to lead to its development).
3. Numerical schemes and experiments

3.8.2. Wick-rotated $\alpha,\beta$-SDE

Consider the $\alpha,\beta$-SDE given by (2.19)-(2.20). With the choice $t = -is$, the corresponding Wick-rotated SDE in $s \in \mathbb{R}^+$ is

\[
\begin{align*}
\mathrm{d}\tilde{\alpha}_s &= -\left(\tilde{n}_s + \frac{1}{2}\tilde{\alpha}_s\right) \mathrm{d}s - i\tilde{\alpha}_s \mathrm{d}\tilde{W}_s^1, \\
\mathrm{d}\tilde{\beta}_s &= -\left(\tilde{n}_s + \frac{1}{2}\tilde{\beta}_s\right) \mathrm{d}s - i\tilde{\beta}_s \mathrm{d}\tilde{W}_s^2,
\end{align*}
\]

(3.68)

(3.69)

where $\tilde{n}_s = \tilde{\alpha}_s\tilde{\beta}_s$. In the rest of this section, the tilde will be omitted in $\tilde{\alpha}_s, \tilde{\beta}_s$ and $\tilde{n}_s$ whenever the $s$ is mentioned clearly enough elsewhere (be it as a subscript or through a $\mathrm{d}s$ in an SDE). Remember that $\alpha_s$ and $\alpha_t$ are not the same for $s,t \in \mathbb{R}^+$.

In particular, for $\alpha_0 = \beta_0$ and $s \in \mathbb{R}^+$, one can see from numerical simulations that $E[\Re(\alpha_s)] \approx E[\Re(\beta_s)]$ decrease exponentially while $E[\Im(\alpha_s)] \approx E[\Im(\beta_s)] \approx 0$ (for comparison, remember from Section 2.5.1 that $E[\alpha_t] = E[\beta_t]$ oscillates with a period of $4\pi$; see (3.71) for metrics for $\alpha_s, \beta_s$).

Hence, one would guess that

\[
F(s) = \sum_{i=0}^{L} c_i e^{-\lambda_i s}
\]

(3.70)

could be a reasonable approximation of both $E[\alpha_s]$ and $E[\beta_s]$ for the right $c_i, \lambda_i \geq 0$, $\forall t$. It will be seen (see Figures 3.46-3.53) that decent results are still possible even if $\langle \Re(\tilde{\alpha}_j) \rangle_j$ is negative but small for some $k$’s, where $\tilde{\alpha}_j$ denotes the $j$th sample path of the simulation of $\alpha_{s_k}$. If $L$ and the $\lambda_i$’s are given, the problem (3.67) is linear in $c$ and the $c_i$’s can be found using the non-negative linear least squares algorithm described in [58] (already implemented in MATLAB as `lsqnonneg`).

The number of coefficients $L+1$ in (3.70) was usually chosen between 20 and 50 (starting with a higher number and then lowering it for the next experiments when it was clear that the $c_i$’s for $i$ ‘big’ were so small they could be considered zero for all practical purposes).

When using this approach directly on data from simulations of (3.68)-(3.69), however, the results obtained were rather disappointing, as the numerical approximations $\langle \Re(\tilde{\alpha}_j) \rangle_j$ for $E[\alpha_{s_k}]$ (and similarly for $\beta$) tended to take a sharp unexpected shortcut compared to the expected solution (see Figure 3.45). This threw the $\lambda_i, c_i$ coefficients of $F(s)$ completely off track and hence $F(it)$ did not nearly look like $E[\alpha_t]$. The `lsqnonneg’-routine returned coefficients that minimized $\|r\|_2$ for its given input data yet failed to describe the solution accurately when back into the framework of the original time variable $t$.

This setback led to the crucial question of whether the `lsqnonneg’ routine would be able to find the right $c_i$’s if given the exact $\lambda_i$’s and the exact $E[\alpha_{s_k}]$-data. Remember that
3.8. Wick rotation

Figure 3.45.: $E[\alpha_s]$ vs the means $\langle \alpha_s \rangle$, $\langle \beta_s \rangle$ simulated with ode23s-wpp using a similar path rejection procedure as shown in Section 3.1.1 (paths where $\max(|\alpha_r|, |\alpha_i|, |\beta_r|, |\beta_i|) > 20$ were rejected; in this case only one out of 2000). Notice how the simulated mean values of $\alpha_r$ and $\beta_r$ are significantly above the expected value.

the moments of the solution to the $\alpha, \beta$-SDE are known (thanks to the metrics shown in Section 2.5.1). In particular, it holds for $s = it$ that

$$E[\alpha_s] = E[\beta_s] = \alpha_0 \exp \left( |\alpha_0|^2 \left( e^{-s} - 1 \right) - \frac{s}{2} \right)$$

$$= \alpha_0 e^{-|\alpha_0|^2} \sum_{\iota=0}^{\infty} \frac{|\alpha_0|^{2\iota} e^{-\left(\iota + \frac{1}{2}\right)s}}{\iota!} =: G(s), \quad (3.71)$$

which can be approximated by (3.70). With the choices $L = \infty$,

$$\lambda_\iota = \iota + \frac{1}{2}, \quad (3.72)$$

and $c_\iota = \alpha_0 e^{-|\alpha_0|^2} |\alpha_0|^{2\iota}/\iota!$, \quad (3.73)

(i.e. $c_\iota = \alpha_0 P(Z = \iota)$, where $Z \sim \text{Pois}(|\alpha_0|^2)$), it holds that $F(s) = G(s)$. Since for $\alpha_0 \in \mathbb{R}$ and $s \in \mathbb{R}_+$, it follows that $E[\text{Im} (\alpha_s)] = E[\text{Im} (\beta_s)] = 0$ and $E[\text{Re} (\alpha_s)] = E[\text{Re} (\beta_s)] = G(s)$, consider for now the simplified

**Problem 3.8.1.** Given the exact values $G(s_k)$ (where $G$ is defined by (3.71)), $k = 0, \ldots, M$ with $s_k = kh$ and $h = 4\pi/M$, one wishes to find the coefficients $c_\iota \geq 0$.
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such that the residual

\[ r = Az - d \]  \hspace{1cm} (3.74)

has minimal 2-norm, where \( d_{k+1} = G(s_k), \ z_{i+1} = c_i \) and \( a_{k+1,i+1} = e^{-(i+\frac{1}{2})s_k}, \ k = 0, \ldots, M, \ i = 0, \ldots, L. \)

Unfortunately, the coefficients computed when solving Problem 3.8.1 directly with the \texttt{lsqnonneg} routine did not nearly look like (3.73), although the residual corresponding to the obtained coefficients was still very small (\( \|r\|_2 \approx 2 \cdot 10^{-7} \)) for the ‘no condition’-case in Figures 3.46-3.53. However, the fact that a few isolated coefficients were big (compared to each other; the sum of the \( c_i \)'s was roughly \( \alpha_0 \)) while the rest was almost zero was worth noticing (see Figure 3.48), which led to the following idea.

This apparent lack of correlation between \( c_i \) and its \( c_{i+1} \) can be corrected when using the unimaginatively called \textit{no hole condition}. The principle is simple: add the following lines to the residual vector from (3.74)

\[ r_{M+1+\ell} := \epsilon_\ell \left( \frac{c_{\ell+1} + c_{\ell-1}}{2} - c_\ell \right), \quad \ell = 1, \ldots, L - 1. \] \hspace{1cm} (3.75)

Solving the augmented linear least square problem (3.74)-(3.75) yielded a set a coefficients and an exponential series expansion which were much closer to what was expected from (3.71)-(3.73), as can be seen in Figures 3.46-3.53. The no hole condition approach still yielded reasonable results when the right-hand side data vector was perturbed, e.g. by picking \( d = G(s) + \Omega \overline{W}_s \) as in Figures 3.46-3.53, where \( \Omega \in \mathbb{R} \) and \( \overline{W}_s \) is a simulation of a real Brownian motion path, meaning \( \overline{W}_{s_{k+1}} - \overline{W}_{s_k} \sim N(0, h) \).

**Remark 3.8.2.** As mentioned earlier, the technique used in this section is still in its initial phase and how to best find an approximation \( F \) for the numerical data is far from clear depending on the problem. Even in the cases discussed here, there are of course endless other possible choices for \( F \) involving various numbers of parameters, but one has to keep in mind that the corresponding data fitting has to remain doable.

The same principle applies to the choice of the weights \( \epsilon_1, \ldots, \epsilon_{L-1} \), which are in principle arbitrary. In the computations leading to Figures 3.46-3.53 they were all chosen to be 10, since this gave reasonable results, but the best choice varied with the number of points considered in the fitting (i.e. \( M + 1 \) if one uses the information known at each computed time step, but this does not have to be).

Emboldened by this minor success (which shows that perfect simulation data for the Wick-rotated \( \alpha_s, \beta_s \)-SDE (3.68)-(3.69) is not necessary to obtain reasonable results for the original \( \alpha_t, \beta_t \)-SDE), more time was spent investigating the behaviour of numerical solutions to \( \alpha_s, \beta_s \)-SDE. In particular, the weird shortcut taken systematically by the approximation of \( \mathbb{E} [\alpha_s] \) (shown in Figure 3.45 for the ode23s-wpp split-step method and displayed for all tested methods) was surprising. Interestingly, it turned out that setting
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Figure 3.46.: Shows $G(s)$ and the perturbed $\Gamma(s) := G(s) + \Omega \hat{W}_s$ against their $F(s)$-approximations with or without the no hole condition. The $F(s)$ obtained from the exact data $G(s_k)$ without the no hole condition is not shown, since it is indistinguishable from the exact $G(s)$ by eyeball, even in the zoom of Figure 3.47.

$n_s \equiv n_0$ in the Wick-rotated SDE improved the situation significantly (measured on how well $\langle \text{Re} (\hat{\alpha}_j) \rangle_j$ approximated $G(s_k)$). Remember from Section 2.3 that $E[n] \equiv n_0$. However, this should not be the case for $n_s = \alpha_s \beta_s$, as the expectation of both $\alpha_s$ and $\beta_s$ decreases exponentially. This is something that remains to be clarified. Nevertheless, consider the following modified SDE for $\alpha_s, \beta_s$:

$$d\alpha_s = -(n_0 + \frac{1}{2})\alpha_s \, ds - i\alpha_s \, d\hat{W}_s^{-1}, \quad (3.76)$$

$$d\beta_s = -(n_0 + \frac{1}{2})\beta_s \, ds - i\beta_s \, d\hat{W}_s^{-2}. \quad (3.77)$$

Solving (3.76)-(3.77) numerically and finding a corresponding $F(s)$ with \texttt{lsqnonneg} (still for $\lambda_i = i + \frac{1}{2}$, of course: one should not ask for too much...) using the no hole condition yields much better results (see Figures 3.54-3.56) than when solving the original $\alpha_s, \beta_s$-SDE given by (3.68)-(3.69). Again, without the no hole condition, the returned $F(s)$ is useless (see Figure 3.57).

Picking $\lambda_i = i + \frac{1}{2}$ in the case of the $\alpha, \beta$-SDE (2.19)-(2.20) might be seen as cheating, and in a sense, it is true. However, bear in mind that one of the goals here was to see whether the method described in this section would work at all, so the progress was made one step at the time. So far, all the other choices tested (e.g. $\lambda_i = \frac{i}{2}$) failed to give satisfying results. Yet in the linear SDE of Section 3.8.3 assumptions of the type
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\[
\lambda_i = \nu + i \mu \quad \text{yielded reasonable results despite the fact that none of the provided } \lambda_i \text{ matched the exact and value } \lambda = b. \quad \text{Hence all hope is not lost.}
\]

In the $\alpha, \beta$-SDE setting, the following open questions still remain:

- Why does setting $n_s \equiv n_0$ in the drift of (3.68)-(3.69) yield far better than simulating (3.68)-(3.69) directly?

- How can one determine reasonable $\lambda_i$’s (i.e. for which good approximations of $E[\alpha_s]$ can be obtained) without using the information from the metrics computed in Section 2.5.1?

- More generally, how can one pick $F(s)$ efficiently without knowledge about (moments of) the exact solution?

More discussion along these lines can be found at the end of the next subsection.

Figure 3.47.: Zooms into Figure 3.46
3.8. Wick rotation

Figure 3.48: $c_i$ coefficients for the exact $G(s_k)$-data, with and without the no hole condition.

Figure 3.49: $c_i$ coefficients for $\Gamma(s_k) = G(s_k) + \Omega W_{s_k}$-data, with and without the no hole condition.
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Figure 3.50.: Exact $E[\alpha_t]$ vs the $F(it)$ corresponding to the exact $G(s_k)$-data without the no hole condition. Compare with Figure 3.51.

Figure 3.51.: Exact $E[\alpha_t]$ vs the $F(it)$ corresponding to the exact $G(s_k)$-data using the no hole condition. Compare with Figure 3.50.
3.8. Wick rotation

Figure 3.52.: Exact $E[\alpha(t)]$ vs the $F(it)$ corresponding to the perturbed $\Gamma(s) = G(s) + \Omega \overline{W}_s$ without the no hole condition. Compare with Figure 3.53.

Figure 3.53.: Exact $E[\alpha(t)]$ vs the $F(it)$ corresponding to the perturbed $\Gamma(s) = G(s) + \Omega \overline{W}_s$ using the no hole condition. Compare with Figure 3.52.
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Figure 3.54: \( G(s) \) vs the means \( \langle \alpha_s \rangle, \langle \beta_s \rangle \) simulated from the modified (3.76)-(3.77) SDE with \texttt{ode23s-wpp} using path rejection (paths where the absolute value was larger than 20 were thrown out; in this case none was).

Figure 3.55: \( c_i \) coefficients for the \( \langle \text{Re} (\hat{\alpha}_k') \rangle \)-data simulated numerically using an \texttt{ode23s-wpp} split-step solver on the modified (3.76)-(3.77) SDE, with and without the no hole condition (\( \lambda_i = \epsilon + \frac{1}{2} \)).
3.8. Wick rotation

Figure 3.56.: Exact $\mathbb{E}[\alpha_t]$ vs the $F(it)$ corresponding to the $\langle \text{Re} (\hat{\alpha}_j^i) \rangle_j$-data simulated numerically using an ode23s-wpp split-step solver on the modified (3.76)-(3.77) SDE using the no hole condition and $\lambda_i = \frac{t}{2}$, $i = 0, \ldots, 50$. Compare with Figure 3.57.

Figure 3.57.: Exact $\mathbb{E}[\alpha_t]$ vs the $F(it)$ corresponding to the $\langle \text{Re} (\hat{\alpha}_j^i) \rangle_j$-data simulated numerically using an ode23s-wpp split-step solver on the modified (3.76)-(3.77) SDE without the no hole condition and $\lambda_i = \frac{t}{2}$, $i = 0, \ldots, 50$. Compare with Figure 3.56.
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3.8.3. Linear SDEs

Consider the scalar complex linear SDE with purely imaginary drift coefficient

\[ dX_t = -ibX_t \, dt + \sigma X_t \, dW_t, \tag{3.78} \]

where \( b \in \mathbb{R}, \sigma \in \mathbb{C} \) and \( W_t \) is a real Brownian motion. As seen in Subsection 1.2.2, its exact solution is

\[ X_t = e^{-(ib+\sigma^2/2)t} + \sigma W_t X_0. \]

From (1.27)-(1.30), one knows that

\[ E[X_t] = e^{-ibt} X_0, \quad E[|X_t|] = e^{\sigma^2/2 |X_0|}, \quad E[|X_t|^2] = e^{2\sigma^2 |X_0|^2}. \]

This exponentially growing behaviour of the magnitude will lead to a rapidly increasing numerical error if not controlled, see for example Figure 3.58 for the choice \( b = 2, \sigma = \sqrt{3i} \).

Now consider the choice

\[ t = -is \]

and its corresponding SDE in the variable \( s \)

\[ dY_s = -bY_s \, ds + \sqrt{-1} \sigma Y_s \, d\tilde{W}_s. \tag{3.79} \]

The exact solution for this case is

\[ Y_s = e^{(-b+\sigma^2/\pi)s+\sqrt{-1} \sigma \tilde{W}_s} X_0, \]

with

\[ E[Y_s] = e^{-bs} X_0, \quad E[|Y_s|] = e^{(-b+(\sigma_i-\sigma_r)^2/4)s} |X_0|, \quad E[|Y_s|^2] = e^{((\sigma_i^2-2b)s)} |X_0|^2, \]

i.e. the expected magnitude of \( Y_s \) is now decreasing exponentially (for \((\sigma_i - \sigma_r)^2 < 4b\)), meaning that (3.79) should be easier to control numerically.

The SDEs (3.78) and (3.79) are both linear, hence the splitting method described in Section 3.1 with the linear choice \( A(x) = Ax \) should be an effective way of solving them. Some numerical results using this method are presented in Figures 3.58-3.64. The simulation of the \( t \)-SDE (3.78) and its corresponding \( s \)-SDE (3.79) both used the same pseudorandom numbers increments. The mean of the numerical solution to (3.79), which was real in the case considered \((b = 2, \sigma = \sqrt{3i}, X_0 = 2\)), was then approximated by (3.70), where \( \lambda_i = \frac{1}{2} \) for Figures 3.58-3.61 and \( \lambda_i = \frac{1}{2} + \frac{1}{10} \) for Figures 3.62-3.64. Note that the numerical simulation of the \( t \)-SDE (3.78) is only shown for the purpose of comparison. The numerical extrapolated results \( F(it) \) are using the \( s \)-SDE data.
3.8. Wick rotation

Figure 3.58.: Numerical (linear splitting method) vs expected solution of (3.78) with $b = 2, \sigma = \sqrt{3}i$. The results obtained using lsqnonneg with and without the no hole condition (with $\epsilon_1 = \cdots = \epsilon_{49} = 1, \lambda_i = \frac{i}{2}, i = 0, \ldots, 50$) are shown for comparison. Note that the $F(it)$ without the no hole condition and the expected value of $X_t$ are almost identical.

Note that adding the no hole condition in the scalar complex linear SDE context worsens the numerical results significantly. This is due to the fact that the exact $F(s)$ would be $e^{-bs}X_0$ (since $E[Y_s] = e^{-bs}X_0$), hence there should only be one coefficient $\lambda = b$ and one $c = X_0$, an unlikely outcome when adding (3.75) to the mix. Without the no hole condition, one can expect that picking a set of $\lambda_i$ which contains $b$ will be optimal, yet other choices can still give reasonable results although $b \not\in \{\lambda_0, \ldots, \lambda_L\}$ (as in Figures 3.62-3.64).

Similar experiments done for $b \not\in \mathbb{Q}$ and $b \not\in \{\lambda_0, \ldots, \lambda_L\}$ for $\sqrt{-}\sigma \in \mathbb{R}$ and $\sqrt{-}\sigma \in \mathbb{C}\setminus\mathbb{R}$ yielded similar result as shown in Figures 3.62-3.64, despite the fact that $\langle \text{Re}(\hat{\alpha}_k^i) \rangle_j$ was negative (but still small, e.g. $|\langle \text{Re}(\hat{\alpha}_k^i) \rangle_j| < 0.05$ for the cases tested) for some $k$’s. The imaginary part of $\langle \hat{\alpha}_k^i \rangle_j$ was simply ignored by the fitting procedure, but it did not seem to matter too much ($|\text{Im}(\hat{\alpha}_k^{ij})| < 0.05$ held for the relevant simulations). Of course, picking a finer $\lambda_i$-grid helped improving the accuracy of the procedure (without the no hole condition), as it increased the chance of finding a pair $(\lambda_i, c_i)$ close to the exact $(b, X_0)$.

This result is encouraging, since in the context presented in this section, it is possible to perform the whole procedure (solving the Wick-rotated SDE numerically, fitting the data to a function $F(s)$ given by (3.70) and looking at the corresponding $F(it)$) without
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Solution to \( dY_s = -2 Y_s \, ds + \sqrt{3} Y_s \, dW_s \), \( M=50000, N=50000, \varepsilon =1 \)

Figure 3.59.: Mean of numerical (linear splitting method) vs expected solution of (3.79). The rotated SDE is real, hence \( \text{Im } (Y_s) \) is not plotted. Since the various plots are indistinguishable, see Figure 3.61 to compare the size of the errors.

any a priori knowledge about the exact solution of the SDE. The choice of an exponential series for \( F(s) \) as defined by (3.70) could be guessed by looking at the numerical solution of (3.79) and, if picking a refined enough grid for the \( \lambda_i \)'s, the \( c_i \) coefficients can be found using \texttt{lsqnonneg}. One question remaining would be whether to trust the results obtained with the no hole condition or those without. It is obvious that the no hole condition works best when a ‘smoother’ set of \( (\lambda_i, c_i) \) is expected (as for the \( \alpha, \beta \)-SDE), yet this kind of information might not be easy to know in advance.

To conclude, more investigation of the procedure is needed. Non-exponential choices of \( F(s) \) should be tried, other methods for solving the associated (nonlinear) least squares problems have to be thought of (a Gauss-Newton method might help, but not necessarily) and not least the theory about the validity of the passage from one SDE to its Wick-rotated counterpart and back has to be examined carefully.

In any case, the good results obtained for the linear SDE in this section demonstrate the potential of the method. In particular, being able to solve numerically the much more stable Wick-rotated \( \alpha_s, \beta_s \)-SDE (3.68)-(3.69) instead of the original \( \alpha_t, \beta_t \)-SDE can potentially lead to a huge improvement in the accuracy and stability.

In particular, the link between the solution processes of original and Wick-rotated SDE should be looked into. Systematic ways also have been devised to extract the numerical data from the simulations of Wick-rotated SDE and turn it into accurate approximation for the solution of (3.59). It is however to be expected that the theory behind the
3.8. Wick rotation

\[ c_j \text{ for the exponential expansion of the solution to } dY_s = -2Y_s ds + \sqrt{3} Y_s dW_s, \]
\[ M=50000, N=50000, Y_0 = 2, T=2\pi, \lambda_j = j/2. \]

Figure 3.60: \( c_i \) coefficients for simulated data from the linear SDE \( dY_s = -2Y_s ds + \sqrt{3} Y_s d\tilde{W}_s \) with initial value \( X_0 = 2 \), with and without the no hole condition and using \( \epsilon_1 = \cdots = \epsilon_{49} = 1, \lambda_i = \frac{i}{2} \).

method will be more intricate when dealing with nonlinear SDEs (problems with the existence, uniqueness and even equivalence of the solutions are likely), but for these SDEs, pitfalls are to be expected in the original setting as well anyway. There truly is no free lunch. Therefore, having more options at disposal is not something one should spurn, the ultimate always-converging multi-purpose SDE solver having yet to be found.
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Figure 3.61.: Magnitude of the error $|\langle \tilde{Y}_j \rangle_j - E[\tilde{Y}_j]|$, respectively $|\langle \tilde{X}_j \rangle_j - E[\tilde{X}_j]|$ for the simulations shown in Figures 3.58-3.60.

Figure 3.62.: Numerical (linear splitting method) vs expected solution of (3.78) with $b = 2, \sigma = \sqrt{3i}$. The results obtained using lsqnonneg with and without the no hole condition (with $\epsilon_1 = \cdots = \epsilon_{49} = 1, \lambda_i = \frac{i}{5} + \frac{1}{10}, i = 0, \ldots, 50$) are shown for comparison.
3.8. Wick rotation

\[ c_j \text{ for the exponential expansion of the solution to } dY_s = -2Y_s \, ds + \sqrt{3}Y_s \, dW_s, \]
\[ M=50000, \quad N=50000, \quad Y_0=2, \quad T=2\pi, \quad \lambda_j=1/10+j/5 \]

**Figure 3.63:** \( c_j \) coefficients for simulated data from the linear SDE \( dY_s = -2Y_s \, ds + \sqrt{3}Y_s \, dW_s \) with initial value \( X_0 = 2 \), with and without the no hole condition and using \( \epsilon_1 = \cdots = \epsilon_{49} = 1, \lambda_i = \frac{i}{5} + \frac{1}{10}. \)

**Figure 3.64:** Magnitude of the error \( |\langle \tilde{Y}^j_s \rangle - E[Y_s] | \), respectively \( |\langle \tilde{X}^j_t \rangle - E[X_t] | \) for the simulations shown in Figures 3.62, 3.63.
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3.9. Matlab Programs

A selection of the Matlab codes used in conjunction with the various methods described in this thesis is available online on
http://www.sam.math.ethz.ch/people/cperret
This should allow the interested reader to experiment with them directly. Note that the parfor command (parallel for-loop) was often used in lieu of the for loop since the samples paths were independent of each other in all the simulations.
4. Conclusions and outlook

Among the things seen in Chapter 2, the results that deserve the most attention here in the author’s opinion are in fact the more qualitative than quantitative arguments made in Section 2.2.2 and Section 2.4.1. In particular the Remarks 2.2.4-2.2.7 illustrate very well what one is up against when dealing with numerically unstable SDEs. The combination of unstable underlying ODE-type dynamics w.r.t. perturbations with the stochastic uncertainty linked to the simulation of the Brownian motions is bad enough. Add that $n_t$ is expected to diffuse throughout the complex space with its expected magnitude growing exponentially with time and the fact that specific regions of the $(\alpha, \beta)$ $\mathbb{C}^2$-plane are prone to cause paths to diverge (typically if $|\alpha|$ or $|\beta|$ are outside of some annulus $A := \{ z \in \mathbb{C}; r_{\min} \leq |z| \leq r_{\max} \}$, as indicated by Section 3.7), and the general feeling when solving the problem for a large number of paths is that the law of large numbers seems to be related to Murphy’s law. If it can go wrong and you repeat it enough, it usually will.

The problem is that a large sample is necessary to reduce the sampling error. If one wants any meaningful statistical approximation of a quantity like $n_t$, which can take values in a region growing exponentially fast, one should increase the size of the sample accordingly (strictly speaking, the region where $n_t$ can be is unbounded for any $t > 0$, but numerically, one can interpret any probabilities $P(|n_t| > L)$ smaller than machine precision as being zero for most practical purposes). This gives a strong indication that a stochastic time-stepping integrator with a finite (fixed) number of simulated sample paths might not be up to the task without some extra assumptions, e.g. some boundary conditions as in Section 3.7. Indeed, the results obtained using the annulus BC are the best for all the tested methods by far in terms of the time of departure.

Among the methods seen in Chapter 3, the splitting methods of Sections 3.1.1-3.2 are perfectly valid methods for more stable SDEs, although the drift and diffusion coefficient splitting method of Section 3.2 should be used with caution, due to the mentioned danger of using implicit stochastic terms.

The split-step methods have also shown some merit, and can easily be implemented for most problems, making them good multi-purpose methods for a first try, especially when using an adaptive time stepping scheme as the deterministic method. The drawback is the mentioned relative slowness of the algorithm when using ode45 for unstable SDEs like the $\alpha$- and $\alpha, \beta$-SDEs. But in those cases, any method not using boundary conditions did not return satisfying results anyway, even if allowed to spend the same time computing
larger samples. The efficiency of ODE implicit solvers with stochastic correction terms is something that remains to be investigated.

The methods developed in Sections 3.4-3.6 were frankly disappointing in terms of the quality of the computed approximations to $\alpha$, $\beta$, although the modifications made were clearly too crude for the methods to be expected to work (always an easy claim to make afterwards, true, as the same could have been said of the BC approach from Section 3.7 if it had not worked). Yet their use was more to help gaining a better understanding of the dynamics of the problem. The fact that the fixed $n$ method preserves the exact realization of the stochastic process $n_t$ at each step despite assuming falsely that it is a constant and treating the $\alpha, \beta$-SDE as linear came as a surprise. This method also illustrated that too much confidence in success should not be given based on a single metrics, as the results showed the right statistics for $n$ yet did not prevent both means of $\alpha$ and $\beta$ to diverge.

As already celebrated a few times above, the quality of the results obtained using the annulus and toroid boundary conditions came almost as a shock, since it remains the only method to have successfully beaten the typical time of departure $t \approx 0.3$ (which is varying but is persistently smaller than 0.35 for all other methods). Here too, there are still a lot of parameters and other methods and BCs to experiment with. A theoretical justification of why exactly those two BCs work well and not the others would also be interesting.

Despite the remaining theoretical uncertainties about the validity of the Wick rotation (especially if the SDE is nonlinear), encouraging results were obtained for linear SDEs. For the $\alpha, \beta$-SDE case, more effort has to be spent on ways to guess the approximation $F(s)$ of $E[\alpha_s]$ without using any knowledge of the exact solution. The reason why the numerical solution of the Wick-rotated $\alpha_s, \beta_s$-SDE decays too slowly should also be looked into. In fact, it might well be that the metrics used are not correct anymore in the rotated setting, since analytical continuation of moments of a highly unstable stochastic process might be asking for too much. The fact that setting $n_s$ to the counterintuitive $n_0$ gives a much better solution is probably more than mere coincidence.

Nevertheless, it has been shown that finding the coefficients corresponding to a perturbed $E[\alpha_s]$ is possible, which is what one will have to deal with once a suitable assumption for $F(s)$ can be found and the theoretical misgivings about the whole method have been surmounted. If ways to overcome the difficulties presented here and in Section 3.8.2 can be found, the potential gain in accuracy (when computing moments only) and stability can be huge.

Of course, not all the methods that were tested on the problems are included in this thesis. Worth mentioning is the symplectic method presented in [66], which was tested naively on the $\alpha, \beta$-SDE without any success. Yet a closer look at the methods presented in [62], [63], [65] and [66] and a less head-on approach on the $\alpha, \beta$-SDE might give better results. The variance reduction technique based on control variates was also experimented with, but the results were not particularly gratifying.
Conversely, many methods and techniques were thought of but never ended up being tested thoroughly. Among the candidates are

- stochastic Runge-Kutta methods (see [20], [18], [17], [90]),
- linear multi-steps methods for SDEs (see [16]),
- split-step methods with higher order stochastic methods (i.e. Strong Taylor 2.0 or weak order 4.0),
- higher order implicit methods (e.g. implicit order 1.5 strong Taylor method),
- a splitting method based on Gautschi’s method (see [42]) and Deuflhard’s method (see [32]),
- when solving the $\alpha, \beta$-SDE with Wick rotation: using Gauss-Newton to solve
  \[
  \sum_{i=0}^{L} c_i e^{-\lambda_i s_k} - \langle \hat{\gamma}^j_k \rangle_j = r_k
  \]
  in the least square sense for both $c_i$ and $\lambda_i$,
- methods for highly oscillatory ODEs (e.g. [72]), adapted to fit in the SDE setting.
4. Conclusions and outlook
Bibliography


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A. More Gaussian integrals

In Lemma 1.1.8, a useful Gaussian integral was introduced to simplify the computation of the moments of complex linear SDEs. Another complex Gaussian integral of interest is provided by the following Lemma.

**Lemma A.0.1.** For all $\alpha \in \mathbb{C} \setminus \{0\}$ with $\text{Re} (\alpha) \geq 0$, it holds:

$$
\int_{-\infty}^{\infty} e^{-\alpha z^2} \, dz = \sqrt{\pi/\alpha}.
$$

**Proof of Lemma A.0.1** Let $\alpha = |\alpha| e^{i\phi}$, where $\phi \in [0, \frac{\pi}{2}]$. It follows that

$$
\int_{-\infty}^{\infty} e^{-\alpha z^2} \, dz \quad \overset{y=\sqrt{\alpha}z}{=} \quad \frac{1}{\sqrt{\alpha}} \int_{-\infty}^{\infty} e^{-y^2} \, dy
$$

$$
= \frac{1}{\sqrt{\alpha}} \lim_{R \to \infty} \int_{-R e^{i\phi/2}}^{Re^{i\phi/2}} e^{-y^2} \, dy =: \frac{1}{\sqrt{\alpha}} \lim_{R \to \infty} \int_{\gamma_0} e^{-y^2} \, dy,
$$

where $R \in \mathbb{R}$ and $\gamma_0, \ldots, \gamma_3$ are the differentiable curves shown in Figure A and defined by

- $\gamma_0(t) = te^{i\phi}$, $t \in [-R, R]$,
- $\gamma_1(t) = Re^{i\left(\frac{\phi}{2} - t\right)}$, $t \in \left[0, \frac{\phi}{2}\right]$,
- $\gamma_2(t) = -t$, $t \in [-R, R]$,
- $\gamma_3(t) = Re^{i(t+\pi)} = -Re^{it}$, $t \in \left[0, \frac{\phi}{2}\right]$. 

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A. More Gaussian integrals

Figure A.1.: Differentiable curves $\gamma_0, \ldots, \gamma_3$.

The curve $\gamma := \bigcup_{j=0}^{3} \gamma_j$ is closed. Hence, with Remark 1.1.11,

$$0 = \int_{\gamma} e^{-y^2} \, dy = \sum_{j=0}^{3} \int_{\gamma_j} e^{-y^2} \, dy,$$

and therefore

$$\int_{-\infty}^{\infty} e^{-\alpha z^2} \, dz = \frac{1}{\sqrt{\alpha}} \lim_{R \to \infty} \int_{\gamma_0} e^{-y^2} \, dy = -\frac{1}{\sqrt{\alpha}} \lim_{R \to \infty} \sum_{j=1}^{3} \int_{\gamma_j} e^{-y^2} \, dy$$

$$= \frac{1}{\sqrt{\alpha}} \lim_{R \to \infty} \left( \int_{-R}^{R} e^{-y^2} \, dy - \int_{\gamma_1} e^{-y^2} \, dy - \int_{\gamma_3} e^{-y^2} \, dy \right).$$

Estimate

$$\left| \int_{\gamma_1} e^{-y^2} \, dy \right| = \left| -iR \int_{\phi}^{\phi/2} e^{-R^2 e^{i(\phi-2\pi)}} e^{i(u-1)} \, dt \right|$$

$$\leq R \int_{0}^{\phi/2} e^{-R^2 \cos(\phi-2\pi)} \, dt \leq R \int_{0}^{\phi/2} e^{-R^2 \cos(2\pi)} \, du,$$
as well as
\[
\left| \int_{\gamma_3} e^{-y^2} \, dy \right| = \left| -iR \int_0^\frac{\pi}{2} e^{-R^2 e^{2it}} \, dt \right| \leq R \int_0^\frac{\pi}{2} e^{-R^2 \cos(2t)} \, dt.
\]

Since \(e^{-R^2 \cos(2t)} > 0\) and \(\phi \leq \frac{\pi}{2}\), it holds that
\[
R \int_0^\frac{\pi}{2} e^{-R^2 \cos(2t)} \, dt \leq R \int_0^\frac{\pi}{2} e^{-R^2 \cos(2t)} \, dt = \frac{R}{2} \int_0^1 e^{-R^2 x} \frac{1}{\sqrt{1 - x^2}} \, dx
\]
\[
= \frac{R}{2} e^{-R^2} \arcsin(x) \bigg|_{x=0}^1 + \frac{R^3}{2} \int_0^1 e^{-R^2 x} \arcsin(x) \, dx \leq \frac{\pi}{2} x \text{ for } x \in [0, 1]
\]
\[
\leq \frac{\pi R}{4} e^{-R^2} + \frac{\pi R^3}{4} \int_0^1 e^{-R^2 x} \, dx
\]
\[
= \frac{\pi R}{4} e^{-R^2} + \frac{\pi R^3}{4} \left( -\frac{1}{R^2} e^{-R^2 x} \bigg|_{x=0}^1 + \frac{1}{R^2} \int_0^1 e^{-R^2 x} \, dx \right)
\]
\[
= \frac{\pi R}{4} e^{-R^2} \bigg|_{x=0}^1 = \frac{\pi}{4R} \left( 1 - e^{-R^2} \right),
\]
hence
\[
\lim_{R \to \infty} \int_{\gamma_3} e^{-y^2} \, dy = \lim_{R \to \infty} \int_{\gamma_3} e^{-y^2} \, dy = 0.
\]

Therefore,
\[
\int_{-\infty}^\infty e^{-\alpha z^2} \, dz = \frac{1}{\sqrt{\alpha}} \lim_{R \to \infty} \int_{-R}^R e^{-y^2} \, dy = \frac{1}{\sqrt{\alpha}} \int_{-\infty}^\infty e^{-y^2} \, dy = \sqrt{\frac{\pi}{\alpha}},
\]
since from the Gaussian probability distribution function one knows that
\[
\int_{-\infty}^\infty e^{-\frac{(y-\mu)^2}{2\sigma^2}} \, dy = \sqrt{2\pi \sigma^2}. \quad \square
\]
A. More Gaussian integrals
Curriculum Vitae

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