Variational Integrators and Generating Functions for Stochastic Hamiltonian Systems

Zur Erlangung des akademischen Grades eines

DOKTORS DER NATURWISSENSCHAFTEN

von der Fakultät für Mathematik der Universität Karlsruhe (TH) genehmigte

DISSERTATION

von

Dipl.-Math. Lijin Wang

aus Tangshan, V.R. China

Tag der mündlichen Prüfung: 06. Juli 2007

Referent: Prof. Dr. Rudolf Scherer Korreferent: Prof. Dr. Jialin Hong

Foreword

The present doctoral thesis results from a cooperation between the Department of Mathematics of the University of Karlsruhe (TH), Germany, and the Institute of Computational Mathematics and Scientific/Engineering Computing, Chinese Academy of Sciences, Beijing, V.R. China.

The preparation of the thesis was organized in sandwich form: the author spends the first year in Beijing, the second year in Karlsruhe, the third year again in Beijing, and then three months for preparing the doctoral examination in Karlsruhe again.

The supervisors of the thesis with equal rights are Prof. Dr. Jialin Hong and Prof. Dr. Rudolf Scherer.

The project was supported by a 6-months scholarship of Kronmüller at the University of Karlsruhe.

Contents

In	troduction	1
1	Basic Knowledge 1.1 Stochastic Differential Equations	
2	2.1 Lagrangian and Hamiltonian Formalism	19 19 23 27
3	3.1 Definitions and Examples	31 31 35 40
4	8	45 45 50
5	5.1 Generating Functions \bar{S}^1 , \bar{S}^2 , and \bar{S}^3 with Noise	53 53 55 58 65
6		71 71 79
7	7.1 A Partitioned Runge-Kutta Method	91 93 94 95
8	Backward Error Analysis 8.1 Deterministic Modified Equations and Generating Functions	100

	8.4	Modified Equations for Methods with Two Noises	 				 . 112
9	Nur	merical Tests					123
	9.1	A Linear Stochastic Oscillator	 				. 123
	9.2	Kubo Oscillator	 				 . 126
	9.3	A Model of Synchrotron Oscillations	 				. 129
	9.4	A System with Two Additive Noises	 				 . 131
	9.5	Modified Equations	 				 133
Bi	bliog	graphy					141

Introduction

Stochastic differential equations describe dynamics of systems under random disturbances, which are universal in physical, biological, engineering, and social sciences. At the beginning they were proposed by physicists and mathematicians to construct trajectories of diffusion processes, and after further development, these equations have been applied to many other aspects, such as the famous Black-Scholes-Model in economics. With the fast infiltration of stochastic differential equations into a large variety of fields in sciences and technology, books and monographs on this topic have been published, such as Evans [6], Li [18], Mao [21], and Yeh [46].

A very important impetus of the development of stochastic differential equations is the study of Brownian motion (Section 1.1). In 1650, the phenomenon of Brownian motion was mentioned by Leeuwenhoek (1632-1723). Later, in 1827, R. Brown (1773-1858) observed the motion of pollen suspended in water, which is highly irregular and has no tangent at any point, and furthermore, the motions of two distinct particles seem to be independent ([6]). Deeper study on this phenomenon reveals that it is not caused by biological reasons, but the bombardment of the water molecules.

In 1905, the Brownian motion was studied by A. Einstein (1879-1955) by observing motions of ink particles ([6]): Consider a long, thin tube filled with clear water and inject at time t=0 a unit amount of ink into the water at the point x=0. Suppose that f(x,t) denotes the amount of ink particles at time t and position x, which reflects the probability density of Brownian motion of ink particles. It is found that f(x,t) satisfies a diffusion equation, and its solution indicates that the Brownian motion is a Gaussian process.

Further, it is found that the sample paths of Brownian motions are continuous but nowhere differentiable, with Markov and martingale property. The equation that describes the velocity of Brownian particles, the Langevin's equation (equation (1.1.2)) contains the term of white noise.

Based on the study of stochastic integrals and Itô's formula, theories of stochastic differential equations, such as existence and uniqueness of solutions, properties of solutions, and methods of solving some kinds of linear equations, etc., have been established (see e.g. [6] and [21]). In general, however, stochastic differential equations are difficult to solve, although solutions are ensured to exist under certain conditions. This leads to the development of numerical integration methods of them, for which there has been an accelerating interest during the past decades. More and more works are devoted to this topic, e.g. Higham [13], Klöden [16], Klöden & Platen [17], and Milstein [25].

In [16], a brief overview of numerical methods for stochastic differential equations is given. The Wagner-Platen expansion plays an important role in the construction of

stochastic numerical schemes, as the Taylor expansion does in the deterministic cases. Integrands in the integral expression of solution of a stochastic differential equation are expanded successively according to the stochastic chain rule, the Itô's formula, as illustrated in (1.2.14)-(1.2.16). Schemes are constructed by discarding remainder terms in the expansion. Difficulties hereby consist of simulation of higher order derivatives, as well as multiple stochastic integrals. Suitable treatment of derivatives such as using difference quotients instead of derivatives in the scheme leads to Runge-Kutta type methods, e.g. the Platen scheme in Section 1.2.

Different from the concept of consistency and convergence of a numerical method in deterministic case, they are both defined in strong and weak sense in stochastic context, according to whether the closeness is valid path-wise or in certain mean sense (see Definitions 1.7-1.11). Stochastic numerical stability is defined and introduced in Definition 1.12. In the book of Klöden and Platen ([17]), a systematic presentation about issues concerning different aspects of numerical integration of stochastic differential equations is given, including strong and weak approximation. Milstein paid more attention in his monograph [25] to different techniques of constructing and analyzing a numerical method, such as analysis of mean-square order, simulation of multiple stochastic integrals, and so on. An important and concise introduction to algorithms of stochastic numerical simulation, including simulation of Brownian motion etc., is given by Higham [13].

Definition and study of deterministic Hamiltonian systems can be found in Arnold [1] and Hairer, Lubich & Wanner [12]. Symplectic numerical integration methods that preserve symplecticity of the Hamiltonian systems are developed (Feng [7], [8], Feng, Wu, Qin & Wang [9], Ruth [39], de Vogelaere [43]). Based on the requirement of preserving symplectic structure, stochastic Hamiltonian systems are defined (Bismut [2], Milstein, Repin & Tretyakov [26], [28]), where the drift and diffusion coefficients are product of an anti-symmetric matrix and the gradient of the Hamiltonians H and H_i (i = 1, 2, ..., r), respectively (Definition 3.1). In the same articles ([26], [28]), as well as in [27] and [29], numerical methods that satisfy the discrete symplectic structure conservation law are constructed, whereby symplectic methods for deterministic Hamiltonian systems are adapted to stochastic context according to the consistency and realizability requirements. This results in some stochastic symplectic Runge-Kutta type methods (Section 3.2 and Chapter 7).

For deterministic Hamiltonian systems, the generating function theory is important (Feng et al. [9]), which gives a systematic method of constructing symplectic schemes. Three kinds of generating functions are deduced to satisfy three Hamilton-Jacobi partial differential equations, respectively. Approximations of solutions of the Hamilton-Jacobi equations are studied, which gives in practice the possibility to the establishment of symplectic schemes (Section 2.3). Another important technique frames symplectic schemes through variational approach, i.e., the variational integrators. It is based on the Hamilton's principle, and generates symplectic methods by discrete Lagrangian and Legendre's transform (Section 2.2). The well-known partitioned Runge-Kutta methods, Gauss collocation methods, and Lobatto IIIA-IIIB pairs etc. can be structured by variational integrators ([12], Marsden & West [24]).

"In 1966, Nelson gave a stochastic view of quantum mechanics, which is now called stochastic quantization procedure or Nelson's stochastic mechanics (Nelson [35], [36]). Since his creative work, there have been attempts to endow Nelson's stochastic mechanics with

a dynamical framework in the Lagrangian formalism (Guerra & Morato [11], Nelson [37], Zambrini [47], [48]) and in the Hamiltonian formalism (Misawa [30], Zambrini [47], [48]). In each of these works Nelson's original mechanics is developed as stochastic Newtonian mechanics, on the model of classical mechanics." (see Misawa [32]). Hamiltonian formalism for Nelson's stochastic mechanics is developed (Zambrini [47]), based on variational principle. Hamiltonian mechanics for diffusion processes is formulated, which is different from that of Zambrini and based on the 'stochastic Hamilton-Jacobi equation (Nelson [37])' (see Misawa [30]). Canonical transformations in stochastic mechanics are given (Misawa [31]). A series of articles applying Lagrangian variational principle to analysis of quantum mechanics are written (Davies [5], Loffredo & Morato [19]), whereby the stochastic action integral and Lagrangian are treated in certain mean sense.

The deterministic generating function and variational integrator theories stimulate our attempts to develop stochastic generating functions and variational integrators, which are not studied yet. We start from searching for the stochastic Hamilton's principle and the Hamilton-Jacobi theory, since their deterministic parallel is the base for deterministic generating functions and variational integrators. The theories developed by Nelson et al. ([35]-[37]) give an important hint. In order to get mean-square methods, we apply mechanics for nonconservative systems ([1], Frederico & Torres [10], Marsden & Ratiu [23], Morita & Ohtsuka [34], Recati [38], Tveter [42]), with the consideration that the 'random force', the white noise, is a certain 'nonconservative force'.

Mainly, we use the Lagrange equations of motion for nonconservative systems (4.1.5)which contain the nonconservative force, and the generalized action integral (4.1.1) which is an integral of the difference of Lagrangian function and the work done by the nonconservative force. Based on these and the Hamilton's principle which states that the equation (4.1.5) extremizes (4.1.1), we propose the generalized Hamilton's principle and action integral with noises. Further, the stochastic variational integrators are established (Chapter 4). The action integral with noises generates a symplectic mapping, which gives rise to generating functions of the first, second and third kind through coordinates transformation. The Hamilton-Jacobi partial differential equations with noises are derived, whereby forms of stochastic partial differential equations give inspirations (Carmona & Rozovskii [3], Prato & Tubaro [4]). Numerical methods are achieved by an approximation of solution of the Hamilton-Jacobi equations with noises, which is a truncated series in powers of the Brownian motion W(t) and time t. The mean-square order of the methods can be controlled by truncating this series to proper term (Chapter 5 and 6). The Wagner-Platen expansion in Stratonovich sense, and the Stratonovich chain rule (Theorem 1.4) are vital for involved calculations. Numerical tests are performed for a linear stochastic oscillator, Kubo oscillator, a model of synchrotron oscillations, and a system with two additive noises (Chapter 9). In order to check validity of our theory, we derive generating functions for some symplectic methods given in literature (Chapter 7). Numerical tests and contents in Chapter 7 show that, the stochastic variational integrators and generating functions are two efficient approaches to construct stochastic symplectic methods.

The idea of preserving symplecticity proposed by Feng et al. is later developed to the theory of structure-preserving algorithms, which aims to construct numerical methods that can preserve properties of the original systems, and is now a fast developing branch of numerical analysis. "On the other hand, it is well-known that the theory of conserved quantities (the first integrals) of dynamical systems is one of the most important subjects, because such quantities are fundamental characters of dynamical systems described

by differential equations. Moreover, in the field of numerical analysis for deterministic dynamical systems described by ordinary differential equations, it is also recognized that the studies on the numerical preservation of the conserved quantities for dynamical systems are very important in performing reliable numerical calculations to the systems. Hence, it seems quite natural to investigate stochastic numerical schemes which leave the conserved quantities of stochastic systems numerically invariant." (see Misawa [33]). The invariance of asymptotic laws of methods for linear stochastic systems (Schurz [40]), and an energy conservative stochastic difference scheme for a one-dimensional stochastic Hamiltonian system (Misawa [33]) are discussed. Compared to the accuracy and stability analysis of stochastic numerical methods, however, the study on structure preservation properties of stochastic numerical methods is rare.

At the beginning of our research, we consider a linear stochastic oscillator (3.1.7)-(3.1.8). A stochastic midpoint rule is proposed, which is symplectic. Its ability of preserving linear growth property of the second moment of the solution, as well as oscillation property of the solution is checked (Hong, Scherer & Wang [14]). Further, some stochastic predictor-corrector methods for the linear stochastic oscillator (3.1.7)-(3.1.8) are given, and their structure-preserving properties are studied (Hong, Scherer & Wang [15], see Section 3.3). In Chapter 5 and 6, we construct some symplectic methods for different stochastic Hamiltonian systems. Their behaviors in preserving conserved quantities and properties of original systems are observed through numerical tests in Chapter 9.

Backward error analysis is applied in numerical integration of deterministic ordinary differential equations. Instead of the local and global errors, backward error analysis studies difference between the vector fields of the original system and its modified equation, which has the discrete points produced by the numerical method as its exact solution points. Observing the exact flow of the modified equation gives insight into the qualitative properties of the numerical methods ([12]). Construction of modified equation of a numerical method is vital for backward error analysis. It is verified that the modified equation of a symplectic method is a Hamiltonian system, which can be written by using generating functions of the numerical method ([12]). Inspired by these results, we propose in this dissertation stochastic modified equations for symplectic methods with noises, by applying their generating functions with noises. We prove that the modified equation of a stochastic symplectic method is a stochastic Hamiltonian system, which can be determined by generating functions of the method (Chapter 8). Numerical tests show good coincidence between the trajectories of the numerical methods and their stochastic modified equations (Chapter 9). This gives help to the study of qualitative and long time behavior of stochastic symplectic methods.

Contents of this dissertation are organized in the following way:

Chapter 1 is an introduction to stochastic differential equations and an overview of their numerical approximations. Chapter 2 gives basic knowledge of deterministic Hamiltonian systems, and the theory of deterministic variational integrators and generating functions. Definition and properties of stochastic Hamiltonian systems, as well as some results on numerical integration methods of them are presented in Chapter 3. Chapter 4 gives representation of stochastic action integral, based on which the Lagrangian formalism of stochastic Hamiltonian systems is derived, and the stochastic Hamilton's principle is obtained. As a result, stochastic variational integrators that create symplectic numerical integration methods are constructed. On the basis of the stochastic action integral, as

well as coordinates transformations, three kinds of generating functions containing one noise for producing stochastic symplectic mappings are given in Chapter 5. Meanwhile, three kinds of stochastic Hamilton-Jacobi partial differential equations satisfied by the three kinds of generating functions are derived. An approach to approximate solutions of the stochastic Hamilton-Jacobi partial differential equations is given. Symplectic numerical methods for some stochastic Hamiltonian systems are constructed on the basis of the stochastic generating function theory, whereby mean-square order of the methods can be theoretically sufficiently high. The results in Chapter 5 for systems with one noise are generalized to that for systems with two noises in Chapter 6, which contain stochastic Hamilton-Jacobi partial differential equations with two noises, as well as approximations of their solutions which are generating functions for stochastic symplectic schemes with two noises. Cases of more noises can be treated similarly. In Chapter 7, generating functions are found for some stochastic symplectic methods given in literature, according to the stochastic generating function theory in Chapter 5 and 6. A symplectic Runge-Kutta method for systems with additive noises is generalized to systems with any type of noises, for which three kinds of generating functions are derived. Chapter 8 contributes to stochastic backward error analysis, where an approach of constructing modified equations for stochastic symplectic schemes is given, which applies stochastic generating functions. The obtained modified equations are proved to be stochastic Hamiltonian systems. Modified equations for some symplectic methods proposed in previous chapters are established. The numerical methods produced by variational integrators and generating functions for discretizing a linear stochastic oscillator, the Kubo oscillator, a model of synchrotron oscillations and a system with two additive noises are tested through numerical experiments. Chapter 9 illustrates the numerical results, which show efficiency of the methods in simulating the original systems with preservation of some important structures of the original systems. Good coincidence between trajectories of numerical methods and their modified equations gives another support to validity of the stochastic generating function theory proposed in this thesis.

I would like to express my deepest gratitude to my supervisors, Prof. Dr. Rudolf Scherer (University of Karlsruhe) and Prof. Dr. Jialin Hong (Chinese Academy of Sciences) for leading me into this interesting and vivid field of study, their constant support and inspiration, their patience, and their professional guidance and supervision, without which the accomplishment of this dissertation would have been impossible.

My thankfulness is also given to the Department of Mathematics at the University of Karlsruhe (TH), and to the Institute of Computational Mathematics and Scientific/Engineering Computing, Chinese Academy of Sciences, for accepting me as a PhD student in their cooperation project, for the excellent study and working environment, facilities and resources, especially the Kronmüller Scholarship provided by the Department of Mathematics in Karlsruhe.

I also want to thank the staff of the two institutions for giving me uncountable help in my study and life, and my fellow students for their valuable discussions and friendship.

Last, but never the least, I thank my family, since without their support I would not be able to accomplish this thesis. Thank you very much!

Chapter 1

Basic Knowledge

Basic definitions related to stochastic differential equations (SDEs), such as Wiener process, stochastic integrals, and Itô's formula are given in this chapter. A brief overview of the numerical methods for SDEs, especially the Wagner-Platen expansion is made. Concepts of convergence, consistence, and stability of a numerical method for SDEs are introduced.

1.1 Stochastic Differential Equations

In modern control theory, stochastic differential equations play an important role, because they can successfully model systems with random perturbations.

Recall that a d-dimensional ordinary differential equation (ODE) system has the following form

$$\dot{X}(t) = f(X(t), t), \qquad X(0) = X_0,$$
 (1.1.1)

where X is a d-dimensional vector and $f: \mathbb{R}^d \times [0, +\infty] \mapsto \mathbb{R}^d$ a \mathbb{R}^d -valued function. Stochastic differential equations arise when an ordinary differential equation is forced by an irregular stochastic process such as Gaussian white noise $\xi(t)$, the name of which comes from the fact that its average power is uniformly distributed in frequency, which is a characteristic of white light ([17]). For example, Langevin wrote the following equation for the acceleration of a particle of Brownian motion, resulting from the molecular bombardment of the particle suspended on a water surface,

$$\dot{X}(t) = aX(t) + b\xi(t), \tag{1.1.2}$$

with a < 0, b > 0, and X(t) being the velocity of the particle. This is the sum of a retarding frictional force depending on the velocity and the molecular forces represented by a white noise process $\xi(t)$. -a and b are called drift coefficient and diffusion coefficient respectively.

A mathematical description of Brownian motion was proposed by Wiener ([6],[17]), therefore, Brownian motion is also called standard Wiener process, namely, a Gaussian process denoted with W(t), $t \ge 0$, and characterized by the following properties:

- 1. W(0) = 0 with probability 1.
- 2. For any partition $0 = t_0 < t_1 < t_2 < \cdots$, the increments $W(t_{i+1}) W(t_i)$ and $W(t_{i+1}) W(t_i)$ are independent for all $i \neq j$.

3. $\mathbb{E}(W(t)) = 0$ and Var(W(t) - W(s)) = t - s for all $0 \le s \le t$, where \mathbb{E} and Var denote the expectation and variance respectively.

An important character of the standard Wiener process is that its sample paths are nowhere differential almost surely ([6],[17]). However, the white noises are usually regarded as the derivative of standard Wiener process, i.e., $\xi(t) = \dot{W}(t)$, which suggests that the white noise process is an unusual process. In fact, it can not be realized physically, but can be approximated to any accuracy by conventional stochastic process with broad banded spectra such as the following process

$$X^{h}(t) = \frac{W(t+h) - W(t)}{h},$$
(1.1.3)

where W(t), $t \ge 0$ is a standard Wiener process ([17]).

Now write the Langevin's equation (1.1.2) in the usual form of a stochastic differential equation

$$dX(t) = aX(t)dt + bdW(t) (1.1.4)$$

with regarding $\xi(t)dt = dW(t)$ which is a consequence of the relation between white noise and standard Wiener process. The equivalent integral form of (1.1.4) is

$$X(t) = X(0) + \int_0^t aX(s)ds + \int_0^t bdW(s)$$
 (1.1.5)

More general, the drift and diffusion coefficients a and b of a stochastic differential equation can be functions of X(t) and t. A d-dimensional stochastic differential equation (SDE) system is usually expressed as

$$dX(t) = a(X(t), t)dt + b(X(t), t)dW(t), (1.1.6)$$

where $a: \mathbb{R}^d \times [0, +\infty] \mapsto \mathbb{R}^d$ is a d-dimensional vector and $b: \mathbb{R}^d \times [0, +\infty] \mapsto \mathbb{R}^{d \times r}$ a $d \times r$ -matrix. W(t) is a r-dimensional Wiener process, the components of which are pairwise independent standard Wiener processes.

Componentwise, the SDE system (1.1.6) are also written as

$$dX_i(t) = a_i(X(t), t)dt + \sum_{k=1}^r b_{ik}(X(t), t)dW_k(t), \quad i = 1, \dots, d,$$
(1.1.7)

or equivalently

$$X_i(t) = X_i(0) + \int_0^t a_i(X(s), s)ds + \sum_{k=1}^r \int_0^t b_{ik}(X(s), s)dW_k(s), \quad i = 1, \dots, d. \quad (1.1.8)$$

(1.1.7) or (1.1.8) is called a stochastic differential equation system with r noises. Since $t \mapsto W_k(\omega, t)$ is of infinite variation for almost every $\omega \in \Omega$, $\{\Omega, \mathcal{A}, P\}$ being the probability space, the stochastic integral

$$\int_0^t b_{ik}(X(s), s) dW_k(s)$$

can not be understood as an ordinary integral. It is defined for $b_{ik} \in \mathcal{L}_t^2$ as the mean square limit of the sums ([17])

$$S_n(\omega) = \sum_{j=0}^{n-1} b_{ik}(X(\xi_j^{(n)}, \omega), \xi_j^{(n)}) \left\{ W_k(\omega, t_{j+1}^{(n)}) - W_k(\omega, t_j^{(n)}) \right\}$$
(1.1.9)

with $\xi_j^{(n)} \in [t_j^{(n)}, t_{j+1}^{(n)}]$ for partitions $0 = t_0^{(n)} < t_1^{(n)} < t_2^{(n)} < \dots < t_n^{(n)} = t$ for which

$$\delta^{(n)} = \max_{0 \le j \le n-1} (t_{j+1}^{(n)} - t_j^{(n)}) \to 0 \quad \text{as} \quad n \to \infty.$$
 (1.1.10)

 \mathcal{L}_t^2 here is the linear space which consists of functions $f:\Omega\times[0,t]\mapsto\mathbb{R}$ satisfying

- 1. f is jointly $\mathcal{A} \times \mathcal{L}$ -measurable;
- 2. $\int_0^t \mathbb{E}(f(\cdot,s)^2)ds < \infty;$
- 3. $\mathbb{E}(f(\cdot,s)^2) < \infty$ for each $0 \le s \le t$;
- 4. $f(\cdot, s)$ is \mathcal{A}_s -measurable for each $0 \le s \le t$,

with \mathcal{L} being the σ -algebra of Lebesgue subsets on [0,t]. With the mean-square norm

$$\| f \|_{2,t} := \left(\int_0^t \mathbb{E}(f(\cdot, s)^2) ds \right)^{1/2},$$
 (1.1.11)

 \mathcal{L}_t^2 is a Banach space, if functions differing on sets of zero measure are identified ([17]). The mean square limit of the sum $S_n(\omega)$ in (1.1.9) depends on the choice of the point $\xi_j^{(n)}$ in the interval $[t_j^{(n)}, t_{j+1}^{(n)}]$, which distinguishes a stochastic integral from a classic Riemann Integral.

For example, if $\xi_j^{(n)}$ are chosen to be

$$\xi_j^{(n)} = (1 - \lambda)t_j^{(n)} + \lambda t_j^{(n)}, \qquad 0 \le \lambda \le 1, \tag{1.1.12}$$

and denote the resulted integrals with

$$(\lambda) \int_0^T f(\omega, t) dW(\omega, t),$$

for the integrand $f(\omega,t)=W(\omega,t)$ one has ([6],[17],[21])

$$(\lambda) \int_{0}^{T} W(\omega, t) dW(\omega, t) = \frac{1}{2} W(\omega, T)^{2} + (\lambda - \frac{1}{2}) T, \tag{1.1.13}$$

the value of which depends on λ .

Arbitrary choice of evaluation points $\xi_j^{(n)}$, however, is of little theoretical or practical interest. The most widely used two cases are $\xi_j^{(n)} = t_j^{(n)}$ and $\xi_j^{(n)} = \frac{t_j^{(n)} + t_{j+1}^{(n)}}{2}$, i.e., $\lambda = 0$ and $\lambda = \frac{1}{2}$, which results in the so-called Itô integral and Stratonovich integral respectively.

Definition 1.1. For partitions $0 = t_0^{(n)} < t_1^{(n)} < t_2^{(n)} < \dots < t_n^{(n)} = T$ on [0,T], the Itô integral $\int_0^T f(\omega,t) dW(\omega,t)$ for an integrand $f \in \mathcal{L}_T^2$ is defined as the mean-square limit of the sums

$$S_n(\omega) = \sum_{j=0}^{n-1} f(\omega, t_j^{(n)}) \left\{ W(\omega, t_{j+1}^{(n)}) - W(\omega, t_j^{(n)}) \right\}.$$
 (1.1.14)

The Stratonovich integral $\int_0^T f(\omega, t) \circ dW(\omega, t)$ is equal to the mean-square limit of the sums

$$S_n(\omega) = \sum_{j=0}^{n-1} f(\omega, \frac{t_j^{(n)} + t_j^{(n+1)}}{2}) \left\{ W(\omega, t_j^{(n+1)}) - W(\omega, t_j^{(n)}) \right\}.$$
 (1.1.15)

Here we use the convention of expressing Stratonovich integral with a small circle \circ before dW. The stochastic differential equation (1.1.6) is said to be of Itô sense, if the stochastic integrals appearing in its integral form (1.1.8) are Itô integrals. For a stochastic differential equation in the sense of Stratonovich we write

$$dX(t) = a(X(t), t)dt + b(X(t), t) \circ dW(t), \tag{1.1.16}$$

which means that the stochastic integrals involved are Stratonovich integrals. From Definition 1.1 of the two kinds of integrals, it is derived by simple calculation that they are related in an interesting manner ([6]).

Proposition 1.2. ([17],[21],[25]) The d-dimensional stochastic differential equation in the sense of Stratonovich

$$dX(t) = a(X(t), t)dt + \sum_{k=1}^{r} b_k(X(t), t) \circ dW_k(t)$$
(1.1.17)

with a and b_k being smooth \mathbb{R}^d -valued functions, is equivalent to the d-dimensional Itô stochastic differential equation

$$dX(t) = \left(a(X(t), t) + \frac{1}{2} \sum_{k=1}^{r} \frac{\partial b_k}{\partial x} (X(t), t) b_k(X(t), t)\right) dt + \sum_{k=1}^{r} b_k(X(t), t) dW_k(t).$$
(1.1.18)

Its proof is based on the Taylor expansion of $b_{kl}(X(\frac{t_j+t_{j+1}}{2}), \frac{t_j+t_{j+1}}{2})$ at the point t_j in the sum $S_n(\omega)$ defined in (1.1.15) but for function b_{kl} instead of $f, l = 1, \dots, d$. For details it is referred to [6].

In stochastic calculus, there is a very important formula which functions as the stochastic counterpart of the deterministic chain rule for derivative of composite functions. That is the following Itô's formula in Theorem 1.3. Similar to the definition of \mathcal{L}_T^2 , we denote with \mathcal{L}_T^1 the linear space of real-valued functions $f(t,\omega)$ satisfying $\int_0^T \mathbb{E}(|f(\cdot,t)|)dt < \infty$ and $\mathbb{E}(|f(\cdot,t)|) < \infty$ for each $0 \le t \le T$. In the theorem below we assume that the

stochastic differential equation is of one dimension.

Theorem 1.3 (Itô's formula). ([6],[17],[21]) Suppose

$$dX(t) = a(X(t), t)dt + b(X(t), t)dW(t), (1.1.19)$$

for $a \in \mathcal{L}_T^1$ and $b \in \mathcal{L}_T^2$. Assume $u : \mathbb{R} \times [0,T] \mapsto \mathbb{R}$ is continuous and that $\frac{\partial u}{\partial t}$, $\frac{\partial u}{\partial x}$, and $\frac{\partial^2 u}{\partial x^2}$ exist and are continuous. Set

$$U(t) := u(X(t), t).$$

Then it holds

$$dU(t) = \frac{\partial u}{\partial t}dt + \frac{\partial u}{\partial x}dX(t) + \frac{1}{2}\frac{\partial^2 u}{\partial x^2}b^2dt$$

$$= \left(\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x}a + \frac{1}{2}\frac{\partial^2 u}{\partial x^2}b^2\right)dt + \frac{\partial u}{\partial x}bdW(t), \qquad (1.1.20)$$

with equality interpreted in the mean-square sense.

It can be seen that an extra term $\frac{1}{2} \frac{\partial^2 u}{\partial x^2} b^2 dt$ appears, which is not present in the classic chain rule. In [17], Kloeden and Platen give the following simple explanation for it. Use the Taylor expansion for u, we have

$$\Delta U(t) = u(X(t) + \Delta X, t + \Delta t) - u(X(t), t)$$

$$= \left(\frac{\partial u}{\partial t} \Delta t + \frac{\partial u}{\partial x} \Delta X\right)$$

$$+ \frac{1}{2} \left(\frac{\partial^2 u}{\partial t^2} (\Delta t)^2 + 2 \frac{\partial^2 u}{\partial t \partial x} \Delta t \Delta X + \frac{\partial^2 u}{\partial x^2} (\Delta X)^2\right)$$

$$+ \cdots \qquad (1.1.21)$$

According to the equation (1.1.19), $(\Delta X)^2$ contains the term $(\Delta W)^2$, which gives the term Δt due to the fact that $\mathbb{E}(\Delta W^2) = \Delta t$. Thus follows the Itô's formula.

Generalized Itô's formula with dimension d is derived in the same way, based on Taylor expansion of functions with more independent variables. In the case of r noises, its derivation is more complicated. Details can be found in [6].

The Itô's formula (1.1.20) explains why there is an additional term $-\frac{1}{2}T$ in (1.1.13) for $\lambda = 0$. For $\lambda = \frac{1}{2}$ in (1.1.13), the extra term $(\lambda - \frac{1}{2})T$ vanishes, i.e., the classic chain rule holds. This illustrate an important advantage of the choice of $\lambda = \frac{1}{2}$, i.e., the Stratonovich integral, as stated in the following theorem. Here we assume that X is d-dimensional vector, and W is r-dimensional Wiener process. a and b are accordingly defined, as in (1.1.6).

Theorem 1.4 (Stratonovich chain rule). ([6]) Suppose

$$dX = a(X(t), t)dt + b(X(t), t) \circ dW(t)$$
(1.1.22)

and $u: \mathbb{R}^d \times [0,T] \mapsto \mathbb{R}$ is continuous. Define

$$U(t) := u(X(t), t).$$

Then

$$dU(t) = \frac{\partial u}{\partial t}dt + \sum_{i=1}^{d} \frac{\partial u}{\partial x_i} \circ dX_i$$

$$= \left(\frac{\partial u}{\partial t} + \sum_{i=1}^{d} \frac{\partial u}{\partial x_i} a_i\right) dt + \sum_{i=1}^{d} \sum_{k=1}^{r} \frac{\partial u}{\partial x_i} b_{ik} \circ dW_k(t). \tag{1.1.23}$$

Thus the classic chain rule holds for Stratonovich stochastic differentials $b(X(t), t) \circ dW(t)$, which is the major reason for its use. We give a proof for the simple case d = 1 and r = 1, which applies the relation between Itô and Stratonovich integrals, as well as the Itô's formula.

Proof. From $dX(t) = a(X(t),t)dt + b(X(t),t) \circ dW(t)$, applying formula (1.1.18), it is obtained that

$$dX(t) = \left(a + \frac{1}{2}\frac{\partial b}{\partial x}b\right)dt + bdW(t). \tag{1.1.24}$$

Now use the Itô's formula (1.1.20), we get

$$dU(t) = \left(\frac{\partial u}{\partial t} + \frac{1}{2}\frac{\partial^2 u}{\partial x^2}b^2\right)dt + \frac{\partial u}{\partial x}dX$$

$$= \left(\frac{\partial u}{\partial t} + \frac{1}{2}\frac{\partial^2 u}{\partial x^2}b^2 + \frac{\partial u}{\partial x}a + \frac{1}{2}\frac{\partial u}{\partial x}\frac{\partial b}{\partial x}b\right)dt + \frac{\partial u}{\partial x}bdW. \tag{1.1.25}$$

Proposition 1.2 implies

$$\frac{\partial u}{\partial x}bdW(t) = -\frac{1}{2}\left(\frac{\partial^2 u}{\partial x^2}b^2 + \frac{\partial u}{\partial x}\frac{\partial b}{\partial x}b\right)dt + \frac{\partial u}{\partial x}b \circ dW(t). \tag{1.1.26}$$

Substitute (1.1.26) into (1.1.25) we get

$$dU(t) = \left(\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x}a\right)dt + \frac{\partial u}{\partial x}b \circ dW(t). \tag{1.1.27}$$

For the Itô SDE system (1.1.6) with $0 \le t \le T$ and initial value $X(0) = X_0$ which is either a constant or a random variable, under Lipschitz and linear growth condition with respect to x of the drift and diffusion coefficients a(X(t),t) and b(X(t),t), with X_0 satisfying $\mathbb{E}(|X_0|^2) < \infty$ and being independent of the 'future', $\mathcal{W}^+(0) := \sigma(W(s)|0 \le s)$ of the Wiener process after time t = 0, there exists a unique solution $X \in \mathcal{L}_T^2$ of this system. One of the most important properties of the solutions of stochastic differential equations is that they are usually Markov processes.

Definition 1.5. ([6]) The d-dimensional stochastic differential equation with r noises

$$dX(t) = a(X(t), t)dt + b(X(t), t)dW(t)$$

is linear if the the coefficients a and b have the form

$$a(x,t) = c(t) + D(t)x,$$

for $c: [0,T] \mapsto \mathbb{R}^d$, $D: [0,T] \mapsto \mathbb{R}^{d \times d}$, and

$$b(x,t) = E(t) + F(t)x$$

for $E: [0,T] \mapsto \mathbb{R}^{d \times r}$, $F: [0,T] \mapsto L(\mathbb{R}^d, \mathbb{R}^{d \times r})$, the space of bounded linear mappings from \mathbb{R}^d to $\mathbb{R}^{d \times r}$.

Definition 1.6. ([6]) A linear SDE is called homogeneous if $c \equiv E \equiv 0$ for $0 \le t \le T$. It is called linear in the narrow sense if $F \equiv 0$.

For the linear equations in narrow sense, if EdW is written as $E\xi dt$ with ξ being the white noise, and regard $E\xi$ as an inhomogeneous term of the ODE

$$\dot{X}(t) = c(t) + D(t)X(t) + E(t)\xi, \tag{1.1.28}$$

the solution can be found by using the variation of constants method of solving an inhomogeneous linear ODE, which is

$$X(t) = \Phi(t) \left(X_0 + \int_0^t \Phi(s)^{-1} (c(s)ds + E(s)dW) \right), \tag{1.1.29}$$

where $\Phi(t)$ is the fundamental matrix of the ODE system

$$\dot{\Phi}(t) = D(t)\Phi, \qquad \Phi(0) = I. \tag{1.1.30}$$

However, if $F \neq 0$, the method of ODE system fails to function due to the extra term in Itô's formula.

In fact, it is generally very difficult to find explicitly the solution of a SDE system, except for some special cases such as the example above, as well as scalar linear equations ([6],[17]). This gives rise to the numerical methods of solving the stochastic differential equation systems.

1.2 Stochastic Approximation

A brief overview of the main issues concerning the stochastic time discrete approximation of a SDE is given in this section.

As the first example, we introduce one of the simplest numerical method of approximating the solution of the scalar Itô stochastic differential equation

$$dX(t) = a(X(t), t)dt + b(X(t), t)dW(t), X(0) = X_0 (1.2.1)$$

with $t \in [0, T]$, the Euler-Maruyama method

$$X_{n+1} = X_n + a(X_n, t_n)\Delta_n + b(X_n, t_n)\Delta W_n,$$
(1.2.2)

for the partition $0 = t_0 < t_1 < \dots < t_N = T$ of the time interval [0, T], and $\Delta_n = t_{n+1} - t_n$, $\Delta W_n = W(t_{n+1}) - W(t_n)$, for which the initial value of iteration is X_0 .

In stochastic context, two basic kinds of tasks are connected with the simulation of solutions of SDE, one is simulating the paths of the solutions, the other is approximating

expectations of functionals of the solution such as its probability distribution and its moments. Consequently arise two types of criteria of judging the error behavior of the simulations, namely the strong and weak convergence criteria.

Definition 1.7. ([16],[17]) A general time discrete approximation \bar{X} with maximum step size h is called to converge strongly to X if

$$\lim_{h \to 0} \mathbb{E}(|X(T) - \bar{X}_N|) = 0, \tag{1.2.3}$$

where \bar{X}_N is the value of approximation \bar{X} at time $T = t_N$.

For comparison of efficiency of different strong numerical approximations, the order of strong convergence is defined as follows.

Definition 1.8. ([16],[17]) A time discrete approximation \bar{X} is said to converge strongly with order $\gamma > 0$ at time T, if there exists a constant C > 0 which is independent of h, and a $h_0 > 0$ such that

$$\mathbb{E}(|X(T) - \bar{X}_N|) \le Ch^{\gamma} \tag{1.2.4}$$

for all $h \in (0, h_0)$.

On can see from the discussion above that, as the diffusion coefficient b vanishes, and the initial value X_0 of the SDE (1.2.1) is a constant, the two definitions 1.7 and 1.8 reduce to deterministic convergence criteria for ODE.

The strong convergence requires a closeness of each sample path of the theoretical and numerical solutions, as indicated by its definition. In many practical situations, however, it is only required that the probability distributions of X and its numerical approximation \bar{X} to be sufficiently close. For this less demanding task of stochastic approximation, the concept of weak convergence is introduced.

Definition 1.9. ([16],[17]) A time discrete approximation \bar{Y} with maximum step size h is said to converge weakly with order $\beta > 0$ to X at time T as $h \to 0$, if for each polynomial g, there exists a constant C > 0 which is independent of h, and a finite $h_0 > 0$ such that

$$\mid \mathbb{E}(g(X(T)) - \mathbb{E}(g(\bar{Y}_N)) \mid \leq Ch^{\beta}$$
(1.2.5)

for each $h \in (0, h_0)$.

The assignment of g to polynomials is stimulated by the requirement of the practice of approximating different moments of the solution X, since polynomials involve all powers needed. In fact, the functional class of g can be even larger ([17]). In case $b \equiv 0$, X_0 being constant, and $g(x) \equiv x$, the definition above reduces to the deterministic convergence criterion of ODE.

Another strong convergence criterion is the mean-square convergence, which is widely used in literature on stochastic approximation, such as in Milstein's monography [25]. It is defined in similar way as Definition 1.7 and 1.8, but with a little modification.

Definition 1.10 (Mean-Square Convergence Order). A time discrete approximation \bar{X} with maximum step size h is said to converge strongly with mean-square order γ

to X at time T as $h \to 0$, if there exists a constant C > 0 which is independent of h, and a $h_0 > 0$ such that

$$\left(\mathbb{E}(X(T) - \bar{X}_N)^2\right)^{\frac{1}{2}} \le Ch^{\gamma} \tag{1.2.6}$$

for all $h \in (0, h_0)$.

It is verified that the Euler-Maruyama method (1.2.2) has mean-square order $\gamma = \frac{1}{2}$ and weak order $\beta = 1$, which are quite low. ([16],[17],[25],[28]).

We note that the Euler-Maruyama method (1.2.2) is a natural generalization of the classic Euler method for ODE to numerical integration of SDE. This generalization is valid, because the increment functions of the Euler-Maruyama scheme a and b take values at the left endpoint of the small interval $[t_n, t_{n+1}]$, which is consistent with the definition of the Itô's integral. Not every classic numerical method can be adapted for solving stochastic differential equations, because they are usually inconsistent with Itô calculus. The consistency requirement in numerical approximation of SDE coincides in idea with ODE, but differs in expressions from ODE by involving expectations, since random elements exist. Moreover, two kinds of consistency are concerned in stochastic context, namely strong and weak consistency corresponding to strong and weak convergence respectively.

Definition 1.11. ([17]) A discrete time approximation \bar{X} of the solution X of equation (1.2.1) corresponding to a time discritization $\{t_n : n = 0, 1, ...\}$ with maximum step size h is said to be strongly consistent, if there exists a nonnegative function c = c(h) with

$$\lim_{h \to 0} c(h) = 0 \tag{1.2.7}$$

such that

$$\mathbb{E}\left(\left|\mathbb{E}\left(\frac{\bar{X}_{n+1} - \bar{X}_n}{\Delta_n} \mid \mathcal{A}_{t_n}\right) - a(\bar{X}_n, t_n)\right|^2\right) \le c(h)$$
(1.2.8)

and

$$\mathbb{E}\left(\frac{1}{\Delta_n}\left|\bar{X}_{n+1} - \bar{X}_n - \mathbb{E}(\bar{X}_{n+1} - \bar{X}_n|\mathcal{A}_{t_n}) - b(\bar{X}_n, t_n)\Delta W_n\right|^2\right) \le c(h) \tag{1.2.9}$$

for all fixed values $\bar{X}_n = x$ and $n = 0, 1, \ldots, where <math>\Delta_n = t_{n+1} - t_n$ and $\Delta W_n = W(t_{n+1}) - W(t_n)$.

(1.2.8) requires that the increment in the drift part of the approximation converges in mean-square sense to the drift coefficient a of the SDE, while (1.2.9) expresses that the increment in diffusion part of the approximation converges to the diffusion coefficient b of the solution in mean-square sense. Thus it can be seen as a generalization of the consistency condition in ODE, and reduces to that in absence of noise. Moreover, the definition of strong consistency indicates the path-wise closeness between the approximation and the solution. In fact, strong consistency implies strong convergence, as the relation between consistency and convergence in ODE.

Weak consistency is defined similarly but less demanding for the closeness of the diffusion parts of the approximation and solution. We omit the definition here. It is referred to [17] for more details. To obtain higher order methods for SDE, it may be a natural thought to adapt higher order methods of ODE to SDE. This is, however, often unsuccessful, because the adapted method may be either inconsistent or unable to improve the order. To illustrate the importance of consistency, we cite an example which is introduced by Kloeden in his article [16]. The deterministic Heun scheme adapted to Itô SDE (1.2.1) has the form

$$X_{n+1} = X_n + \frac{1}{2} \left[a(X_n, t_n) + a(X_n + a(X_n, t_n) \Delta_n + b(X_n, t_n) \Delta W_n, t_{n+1}) \right] \Delta_n$$

$$+ \frac{1}{2} \left[b(X_n, t_n) + b(X_n + a(X_n, t_n) \Delta_n + b(X_n, t_n) \Delta W_n, t_{n+1}) \right] \Delta W_n. \quad (1.2.10)$$

For the Itô SDE dX(t) = X(t)dW(t) it becomes

$$X_{n+1} = X_n + \frac{1}{2}X_n(2 + \Delta W_n)\Delta W_n.$$
 (1.2.11)

Thus

$$\mathbb{E}\left(\frac{X_{n+1} - X_n}{\Delta_n} \mid X_n = x\right) = \frac{x}{\Delta_n} (0 + \frac{1}{2}\Delta_n) = \frac{1}{2}x,\tag{1.2.12}$$

which should approximate the drift coefficient $a(x,t) \equiv 0$ but failed. Consequently the adapted Heun method does not converge to the solution X(t), neither strongly nor weakly.

When an adapted ODE method happens to be consistent with Itô's calculus, it can not have higher order of accuracy, because it contains only the increments Δ_n and ΔW_n , with the latter not involving any information of the Wiener process W(t) inside the subinterval $[t_n, t_{n+1}]$, but only information on the nodes of the time partition. In fact, using a theorem about order of convergence in Milstein's monograph [25], it is not difficult to verify that such adapted consistent methods can usually only have strong order $\frac{1}{2}$.

In [44], Wagner and Platen expand the solution X(t+h) of the Itô equation (1.1.6) at the point (t,x) in powers of h, and in integrals depending on $W_k(s) - W_k(t)$, $t \le s \le t + h$, $k = 1, \ldots, r$. Such integrals provide with more information of W(t) inside the subinterval of time discretization. This kind of expansion is called the Wagner-Platen expansion, which is the stochastic counterpart of Taylor expansion of ODE. In case that the diffusion coefficient $b(X(t),t) \equiv 0$, it comes down to the deterministic Taylor expansion. Theoretically it provides with the possibility of constructing numerical schemes for SDE with arbitrarily high order of accuracy, as the Taylor expansion does for ODE.

For convenience, we discuss the scalar Itô SDE (1.2.1). In the Itô's formula (1.1.20), denote the coefficient of dt with L^0u , and that of dW(t) with L^1u , i.e., the two operators L^0 and L^1 are defined as

$$L^{0} = \frac{\partial}{\partial t} + a \frac{\partial}{\partial x} + \frac{1}{2} b^{2} \frac{\partial^{2}}{\partial x^{2}}, \qquad L^{1} = b \frac{\partial}{\partial x}.$$
 (1.2.13)

In the equivalent integral form of SDE (1.2.1)

$$X(t+h) = X(t) + \int_{t}^{t+h} a(X(s), s)ds + \int_{t}^{t+h} b(X(s), s)dW(s), \tag{1.2.14}$$

apply Itô's formula to the functions a(X(s), s) and b(X(s), s) to obtain

$$X(t+h) = X(t) + \int_{t}^{t+h} \left[a(X(t),t) + \int_{t}^{s} L^{0}a(X(u),u)du + \int_{t}^{s} L^{1}a(X(u),u)dW(u) \right] ds$$

$$+ \int_{t}^{t+h} \left[b(X(t),t) + \int_{t}^{s} L^{0}b(X(u),u)du + \int_{t}^{s} L^{1}b(X(u),u)dW(u) \right] dW(s)$$

$$= X(t) + a(X(t),t)h + b(X(t),t)(W(t+h) - W(t)) + R_{1}, \qquad (1.2.15)$$

with the remainder

$$R_{1} = \int_{t}^{t+h} \int_{t}^{s} L^{0}a(X(u), u)duds + \int_{t}^{t+h} \int_{t}^{s} L^{1}a(X(u), u)dW(u)ds$$

$$+ \int_{t}^{t+h} \int_{t}^{s} L^{0}b(X(u), u)dudW(s) + \int_{t}^{t+h} \int_{t}^{s} L^{1}b(X(u), u)$$

$$dW(u)dW(s).$$
(1.2.16)

In (1.2.15), eliminate the remainder term R_1 and replace t and t + h by t_n and t_{n+1} respectively, we obtain the scheme

$$X_{n+1} = X_n + a(X_n, t_n)\Delta_n + b(X_n, t_n)\Delta W_n,$$

which is the Euler-Maruyama scheme.

Higher order schemes can be achieved by expanding the integrands in the remainder term at (X(t), t) using Itô's formula. For example, in the remainder R_1 , apply Itô's formula to the last integrand $L^1b(X(u), u)$ in (1.2.16), we get

$$X(t+h) = X(t) + a(X(t),t)h + b(X(t),t)(W(t+h) - W(h)) + L^{1}b(X(t),t) \int_{t}^{t+h} \int_{t}^{s} dW(u)dW(s) + R_{2},$$
 (1.2.17)

with the remainder

$$R_{2} = \int_{t}^{t+h} \int_{t}^{s} L^{0}a(X(u), u)duds + \int_{t}^{t+h} \int_{t}^{s} L^{1}a(X(u), u)dW(u)ds$$

$$+ \int_{t}^{t+h} \int_{t}^{s} L^{0}b(X(u), u)dudW(s) + \int_{t}^{t+h} \int_{t}^{s} \int_{t}^{u} L^{0}L^{1}b(X(v), v)dvdW(u)dW(s)$$

$$+ \int_{t}^{t+h} \int_{t}^{s} \int_{t}^{u} L^{1}L^{1}b(X(v), v)dW(v)dW(u)dW(s). \tag{1.2.18}$$

Based on (1.2.17), the following scheme is constructed:

$$X_{n+1} = X_n + a(X_n, t_n) \Delta_n + b(X_n, T_n) \Delta W_n + L^1 b(X_n, t_n) \int_{t_n}^{t_{n+1}} \int_{t_n}^{s} dW(u) dW(s),$$
(1.2.19)

which is called the Milstein scheme, and has strong order 1 and weak order 1 ([16]). Theoretically, the successive expansions can be performed unlimitedly, which give numerical methods of arbitrary high order. However, with the improvement of order of

expansion, stochastic integrals appear with more and more multiplicities, which causes great difficulties in implementation.

The simplest stochastic integral with single multiplicity $\int_{t_n}^{t_{n+1}} dW(s) = \Delta W_n$ can be modeled by $\sqrt{\Delta_n}\xi$, where $\xi \sim \mathcal{N}(0,1)$ is a random variable with standard normal distribution, since $\Delta W_n \sim \mathcal{N}(0,\Delta_n)$. Most digital computers include pseudo-random number generators which gives the possibility of realization of ξ , and thus the simulation of ΔW_n . In Milstein's book [25], modeling of Itô integrals is studied. It is pointed out that the modeling of multiple Itô integrals can be reduced to that of single integrals. Explicit techniques of simulation of single integrals such as $\int_{t_n}^{t_{n+1}} s dW(s)$ are analyzed.

Other types of schemes, for example the stochastic Runge-Kutta type methods which are derivative-free, can be constructed by making some modifications on the Wagner-Platen expansion. For example, replacing the derivative term $L^1b(X_n, t_n)$ in the Milstein scheme (1.2.19) by the forward difference

$$\frac{1}{\sqrt{\Delta_n}} \left[b(X_n + a(X_n, t_n)\Delta_n + b(X_n, t_n)\sqrt{\Delta_n}) - b(X_n, t_n) \right]$$

results in the Platen scheme, which is of Runge-Kutta type and has strong order 1. By doing modifications, consistency requirement should be paid attention to.

Another feature of an efficient numerical method is its stability. As in the situation of ODE, stability analysis of numerical methods for SDE is also required. The concept of stability also means that the error propagation of a scheme is under control, as in deterministic systems, but is defined with using the probability measure P.

Definition 1.12. ([17]) A time discrete approximation \bar{X} to the solution X of SDE (1.1.6) with maximum step size h is stochastically numerically stable, if for any finite interval $[t_0, T]$ there exists a constant $h_0 > 0$ such that for each $\epsilon > 0$ and each $h \in (0, h_0)$

$$\lim_{|X(t_0) - \bar{X}_0| \to 0} \sup_{t_0 \le t \le T} P(|X(T) - \bar{X}_N| \ge \epsilon) = 0, \tag{1.2.20}$$

where \bar{X}_0 is the value of the approximation \bar{X} at time t_0 , and \bar{X}_N the value of \bar{X} at time T.

Under the conditions of existence and uniqueness of solution of a SDE system, the applied Euler-Maruyama method is proved to be numerically stable ([17]). A-stability, test equations, region of absolute stability, stochastic stiff systems, and so on construct the stochastic analog of the deterministic analysis of stability. We omit the details here.

Chapter 2

Deterministic Hamiltonian Systems

In this chapter, some basic knowledge about deterministic Hamiltonian systems is stated, such as the derivation of its formalism from variational principle, Lagrangian formalism of a mechanical system, Legendre transformation, and its properties such as symplecticity. Symplectic numerical methods as well as some known results about symplectic integrators, especially the variational integrators and generating function theory for deterministic Hamiltonian systems are introduced, which provides with a resource of reference and comparison for stochastic Hamiltonian systems, and stimulates the study on analogous numerical integration methods for them, which are topics of following chapters.

2.1 Lagrangian and Hamiltonian Formalism

After Newton's second law which deals with motion of free mass points, Lagrange developed a new way to describe the motion of more complicated systems such as rigid bodies. Denote the position of a mechanical system with d degrees of freedom with $q = (q_1, \ldots, q_d)^T$. Suppose $T = T(q, \dot{q})$ and U = U(q) to be the kinetic and potential energy of the system respectively. The Lagrangian of the system is defined as

$$L = T - U. (2.1.1)$$

Then the position q of the system satisfies the following Lagrange equation

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}}\right) = \frac{\partial L}{\partial q} \tag{2.1.2}$$

Through the Legendre transform of introducing the conjugate momentum

$$p = \frac{\partial L^T}{\partial \dot{a}},\tag{2.1.3}$$

and define

$$H := p^{T} \dot{q} - L(q, \dot{q}) \tag{2.1.4}$$

to be the Hamiltonian of the system, Hamilton gave an equivalent expression of the Lagrange equation (2.1.2), which is symmetric in structure and called the Hamiltonian formalism of motion.

Theorem 2.1. ([12]) The Lagrange equation (2.1.2) is equivalent to the Hamiltonian system

$$\dot{p} = -\frac{\partial H}{\partial q}^{T}, \qquad (2.1.5)$$

$$\dot{q} = \frac{\partial H^T}{\partial p}. \tag{2.1.6}$$

Proof. The formulae (2.1.4) and (2.1.3) imply

$$\frac{\partial H}{\partial q} = p^{T} \frac{\partial \dot{q}}{\partial q} - \frac{\partial L}{\partial q} - \frac{\partial L}{\partial \dot{q}} \frac{\partial \dot{q}}{\partial q} = -\frac{\partial L}{\partial q},
\frac{\partial H}{\partial p} = \dot{q}^{T} + p^{T} \frac{\partial \dot{q}}{\partial p} - \frac{\partial L}{\partial \dot{q}} \frac{\partial \dot{q}}{\partial p} = \dot{q}^{T}.$$
(2.1.7)

Thus (2.1.5)-(2.1.6) is equivalent to
$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}} \right) = \frac{\partial L}{\partial q}$$
, which is (2.1.2).

In fact, the Lagrange equation of motion (2.1.2) describes in variational problem the q(t) which extremizes the functional

$$S(q) = \int_{t_0}^{t_1} L(q(t), \dot{q}(t))dt$$
 (2.1.8)

among all curves q(t) that connect two given points $q(t_0) = q_0$ and $q(t_1) = q_1$. The functional S(q) is also called the action integral, and the Lagrange equation (2.1.2) has the name, the Euler-lagrange equation for the functional S.

Theorem 2.2 (Hamilton's Principle). ([1],[12]) Lagrange equation of motions (2.1.2) of mechanical systems extremizes the action integral (2.1.8).

Proof. Considering a variation $q(t) + \varepsilon \delta q(t)$ with $\delta q(t_0) = \delta q(t_1) = 0$, and setting

$$\frac{d}{d\varepsilon}|_{\varepsilon=0} \mathcal{S}(q + \varepsilon \delta q) = 0 \tag{2.1.9}$$

leads to

$$\int_{t_0}^{t_1} \left(\frac{\partial L}{\partial q} \delta q + \frac{\partial L}{\partial \dot{q}} \delta \dot{q} \right) dt = \int_{t_0}^{t_1} \left(\frac{\partial L}{\partial q} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}} \right) \delta q dt = 0, \tag{2.1.10}$$

which implies the Lagrange equation (2.1.2).

The phase flow $\{p(t), q(t)\}$ of a Hamiltonian system (2.1.5)-(2.1.6) preserves the natural symplectic structure of the phase space of a mechanical problem, which is the characteristic property of a Hamiltonian system. To explain it, we first introduce the definition of a symplectic mapping.

Definition 2.3. ([12]) A differentiable map $g: U \mapsto \mathbb{R}^{2d}$ (where $U \subset \mathbb{R}^{2d}$ is an open set) is called symplectic if the Jacobian matrix g'(p,q) satisfies

$$g'(p,q)^T J g'(p,q) = J, \quad for \ all \ (p,q) \in U,$$
 (2.1.11)

where $J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}$ and I denotes the d-dimensional identity matrix.

Geometrically, this definition describes the invariance of oriented area under the mapping g on the manifold $\{p,q\}$. The oriented area generated by two vectors $\xi = \begin{pmatrix} \xi^p \\ \xi^q \end{pmatrix}$

and $\eta = \begin{pmatrix} \eta^p \\ \eta^q \end{pmatrix}$ is the oriented area of the parallelogram generated by them, and is actually a 2-form $\omega^2(\xi, \eta)$ on the manifold $\{p, q\}$, defined by

$$\omega^2(\xi,\eta) = \xi^T J\eta. \tag{2.1.12}$$

Definition 2.3 implies that

$$\omega^{2}(\xi, \eta) = \omega^{2}(g'(p, q)\xi, g'(p, q)\eta). \tag{2.1.13}$$

Since a differentiable mapping can be locally approximated by a linear mapping, i.e., its Jacobian matrix, the equation (2.1.13) is approximately equivalent to

$$\omega^{2}(\xi, \eta) = \omega^{2}(g(\xi), g(\eta)), \tag{2.1.14}$$

which gives the geometric significance of a symplectic mapping q.

The phase flow of the Hamiltonian system (2.1.5)-(2.1.6) is a one-parameter group of transformation of phase space

$$g^t: (p(0), q(0)) \mapsto (p(t), q(t)),$$
 (2.1.15)

which is the mapping that advances the solution from the initial time to time t, where p(t), q(t) is the solution of the Hamiltonian system (2.1.5)-(2.1.6).

Theorem 2.4 (Poincaré). ([12]) Let H(p,q) be a twice continuously differentiable function on $U \subset \mathbb{R}^{2d}$. Then, for each fixed t, the flow g^t is a symplectic transformation wherever it is defined.

The proof checks the symplecticity of the mapping g^t by applying Definition 2.3, and can be found in [12].

The symplectic 2-form ω^2 on the manifold $\{p,q\}$ can be expressed as the wedge product of the two 1-forms dp and dq, i.e.,

$$\omega^2 = dp \wedge dq = \sum_{i=1}^d dp_i \wedge dq_i. \tag{2.1.16}$$

In the sequel, the symplecticity of a mapping $g:(p,q)\mapsto(\bar p,\bar q)$ can also be defined as preservation of the symplectic structure:

$$d\bar{p} \wedge d\bar{q} = dp \wedge dq. \tag{2.1.17}$$

In the following, we show the equivalence between this description of symplecticity and that in Definition 2.3.

Theorem 2.5. (2.1.17) is equivalent to Definition 2.3.

Proof. Suppose

$$\begin{pmatrix} \bar{p} \\ \bar{q} \end{pmatrix} = g(p,q) = \begin{pmatrix} g_1(p,q) \\ g_2(p,q) \end{pmatrix},$$

where $g_1:U\mapsto\mathbb{R}^d$ and $g_2:U\mapsto\mathbb{R}^d$ are d-dimensional functions. Thus (2.1.11) in Definition 2.3 is equivalent to three conditions

$$\frac{\partial g_1}{\partial p}^T \frac{\partial g_2}{\partial q} - \frac{\partial g_2}{\partial p}^T \frac{\partial g_1}{\partial q} = I, \qquad (2.1.18)$$

$$\frac{\partial g_1}{\partial p}^T \frac{\partial g_2}{\partial p} - \frac{\partial g_2}{\partial p}^T \frac{\partial g_1}{\partial p} = 0, \qquad (2.1.19)$$

$$\frac{\partial g_1}{\partial q}^T \frac{\partial g_2}{\partial q} - \frac{\partial g_2}{\partial q}^T \frac{\partial g_1}{\partial q} = 0, \qquad (2.1.20)$$

where I is $d \times d$ identity matrix, and 0 is $d \times d$ zero matrix. On the other hand,

$$d\bar{p} \wedge d\bar{q} = \sum_{i=1}^{d} d\bar{p}_{i} \wedge d\bar{q}_{i} = \sum_{i=1}^{d} d(g_{1_{i}}(p,q)) \wedge d(g_{2_{i}}(p,q))$$

$$= \sum_{i=1}^{d} \sum_{k < j} \left(\frac{\partial g_{1_{i}}}{\partial p_{k}} \frac{\partial g_{2_{i}}}{\partial p_{j}} - \frac{\partial g_{1_{i}}}{\partial p_{j}} \frac{\partial g_{2_{i}}}{\partial p_{k}} \right) dp_{k} \wedge dp_{j}$$

$$+ \sum_{i=1}^{d} \sum_{k, j} \left(\frac{\partial g_{1_{i}}}{\partial p_{k}} \frac{\partial g_{2_{i}}}{\partial q_{j}} - \frac{\partial g_{1_{i}}}{\partial q_{j}} \frac{\partial g_{2_{i}}}{\partial p_{k}} \right) dp_{k} \wedge dq_{j}$$

$$+ \sum_{i=1}^{d} \sum_{k < j} \left(\frac{\partial g_{1_{i}}}{\partial q_{k}} \frac{\partial g_{2_{i}}}{\partial q_{j}} - \frac{\partial g_{1_{i}}}{\partial q_{j}} \frac{\partial g_{2_{i}}}{\partial q_{k}} \right) dq_{k} \wedge dq_{j}. \tag{2.1.21}$$

Thus, $d\bar{p} \wedge d\bar{q} = dp \wedge dq$ is equivalent to

$$\sum_{i=1}^{d} \left(\frac{\partial g_{1_i}}{\partial p_k} \frac{\partial g_{2_i}}{\partial q_j} - \frac{\partial g_{1_i}}{\partial q_j} \frac{\partial g_{2_i}}{\partial p_k} \right) = \begin{cases} 1, & k = j \\ 0, & k \neq j \end{cases}, \tag{2.1.22}$$

$$\sum_{i=1}^{d} \left(\frac{\partial g_{1_i}}{\partial p_k} \frac{\partial g_{2_i}}{\partial p_j} - \frac{\partial g_{1_i}}{\partial p_j} \frac{\partial g_{2_i}}{\partial p_k} \right) = 0, \quad \forall \ k < j, \tag{2.1.23}$$

$$\sum_{i=1}^{d} \left(\frac{\partial g_{1_i}}{\partial q_k} \frac{\partial g_{2_i}}{\partial q_j} - \frac{\partial g_{1_i}}{\partial q_j} \frac{\partial g_{2_i}}{\partial q_k} \right) = 0, \quad \forall \ k < j.$$
 (2.1.24)

(2.1.22), (2.1.23), and (2.1.24) are equivalent to (2.1.18), (2.1.19), and (2.1.20) respectively. Thus follows the assertion. \Box

In the following we mainly use the characterization (2.1.17) of a symplectic mapping.

Given initial conditions of the Hamiltonian system (2.1.5)-(2.1.6)

$$p(0) = p_0, \quad q(0) = q_0,$$
 (2.1.25)

another formalism of Theorem 2.4 in terms of characterization (2.1.17) is stated in the following theorem.

Theorem 2.6. For the Hamiltonian system (2.1.5)-(2.1.6) with initial conditions (2.1.25), it holds

$$dp(t) \wedge dq(t) = dp_0 \wedge dq_0, \tag{2.1.26}$$

for all t > 0.

Another significant property of a Hamiltonian system is its conservation of the Hamiltonian H(p,q).

Theorem 2.7. The Hamiltonian H of the Hamiltonian system (2.1.5)-(2.1.6) with initial conditions (2.1.25) satisfies

$$H(p(t), q(t)) = H(p_0, q_0)$$
(2.1.27)

for all t > 0.

Proof. Consider the relations (2.1.5)-(2.1.6), we have

$$\frac{d}{dt}H(p(t), q(t)) = \frac{\partial H}{\partial p}\dot{p} + \frac{\partial H}{\partial q}\dot{q}$$

$$= -\frac{\partial H}{\partial p}\frac{\partial H}{\partial q}^{T} + \frac{\partial H}{\partial q}\frac{\partial H}{\partial p}^{T} = 0.$$
(2.1.28)

In mechanical problems, in case that the kinetic energy $T = \frac{1}{2}\dot{q}^T M(q)\dot{q}$ is quadratic, where M(q) is a positive definite matrix, we have by the Legendre transform that $p = M(q)\dot{q}$. Thus according to the definition of the Hamiltonian H (2.1.4),

$$H(p,q) = \frac{1}{2}\dot{q}^{T}M(q)\dot{q} + U(q) = T(q,\dot{q}) + U(q), \qquad (2.1.29)$$

which is the total energy of the mechanical system. Thus the invariance of the Hamiltonian implies the conservation of the total energy of the system.

2.2 Variational Integrators for Hamiltonian Systems

Since the phase flows of Hamiltonian systems preserves symplectic structure, one wants to construct numerical integration methods which inherit this property.

Definition 2.8. A numerical method $(p_n, q_n) \mapsto (p_{n+1}, q_{n+1})$ $(n \ge 1)$ for numerically integrating the Hamiltonian system (2.1.5)-(2.1.6) with initial conditions (2.1.25) is called a symplectic method, if it preserves the symplectic structure, i.e., if

$$dp_{n+1} \wedge dq_{n+1} = dp_n \wedge dq_n, \tag{2.2.1}$$

for all n > 1.

One of the simplest symplectic method for Hamiltonian systems is the symplectic Euler method:

$$p_{n+1} = p_n - h \frac{\partial H}{\partial q}^T(p_{n+1}, q_n), \qquad q_{n+1} = q_n + h \frac{\partial H}{\partial p}^T(p_{n+1}, q_n).$$
 (2.2.2)

Its symplecticity can be verified in a straightforward way. Differentiating the equations in (2.2.2) yields

$$(I + h \frac{\partial^2 H}{\partial q \partial p}^T) dp_{n+1} = dp_n - h \frac{\partial^2 H}{\partial q^2} dq_n, \qquad (2.2.3)$$

$$-h\frac{\partial^2 H}{\partial p^2}dp_{n+1} + dq_{n+1} = (I + h\frac{\partial^2 H}{\partial p\partial q}^T)dq_n, \qquad (2.2.4)$$

where all the functions are evaluated at (p_{n+1}, q_n) . Thus, the wedge product of the left side of the two equations should equal that of the right side, i.e.,

$$(I + h \frac{\partial^2 H}{\partial q \partial p}^T) dp_{n+1} \wedge dq_{n+1} = (I + h \frac{\partial^2 H}{\partial p \partial q}) dp_n \wedge dq_n, \qquad (2.2.5)$$

which gives

$$dp_{n+1} \wedge dq_{n+1} = dp_n \wedge dq_n, \tag{2.2.6}$$

since
$$\frac{\partial^2 H}{\partial q \partial p}^T = \frac{\partial^2 H}{\partial p \partial q}$$
.

An important class of symplectic numerical methods is the symplectic Runge-Kutta methods, which are widely used and take many special efficient methods into a unified system. The idea of a Runge-Kutta method is to replace higher order derivatives in a Taylor expansion by information of the increment function on intermediate points inside each subinterval of time discretization, by which higher order derivative-free methods are expected to be obtained. It is usually characterized by its stage s and its coefficients a_{ij} , b_j and c_j , i, j = 1, ..., s. For example, for the Hamiltonian system (2.1.5)-(2.1.6), a general s-stage Runge-Kutta method takes the form

$$p_{n+1} = p_n - h \sum_{i=1}^s b_i H_q^T(\mathcal{P}_{ni}, \mathcal{Q}_{ni}), \qquad \mathcal{P}_{ni} = p_n - h \sum_{j=1}^s a_{ij} H_q^T(\mathcal{P}_{nj}, \mathcal{Q}_{nj}), (2.2.7)$$

$$q_{n+1} = q_n + h \sum_{i=1}^s b_i H_p^T(\mathcal{P}_{ni}, \mathcal{Q}_{ni}), \qquad \mathcal{Q}_{ni} = q_n + h \sum_{j=1}^s a_{ij} H_p^T(\mathcal{P}_{nj}, \mathcal{Q}_{nj}).$$
 (2.2.8)

The following theorem gives the conditions under which a general s-stage Runge-Kutta method is a symplectic one.

Theorem 2.9. ([12]) If the coefficients of the Runge-Kutta method (2.2.7)-(2.2.8) satisfy

$$b_i a_{ij} + b_j a_{ji} = b_i b_j, (2.2.9)$$

for all i, j = 1, ..., s, then it is symplectic.

The proof of the theorem can be found in [12].

In fact, a large variety of symplectic methods, including the symplectic Runge-Kutta methods, can be constructed by generating functions or variational integrators.

Variational integrators for deterministic systems are based on the Lagrange's equation of motion (2.1.2)

$$\frac{\partial L}{\partial q} = \frac{d}{dt} \frac{\partial L}{\partial \dot{q}}$$

and the action integral (2.1.8)

$$\mathcal{S}(q) = \int_{t_0}^{t_1} L(q(t), \dot{q}(t)) dt.$$

Now consider the action integral S as a function of (q_0, q_1) , where $q_0 = q(t_0)$ and $q_1 = q(t_1)$. Find the partial derivatives of $S(q_0, q_1)$ with respect to q_0 and q_1 :

$$\frac{\partial S}{\partial q_0} = \int_{t_0}^{t_1} \left(\frac{\partial L}{\partial q} \frac{\partial q}{\partial q_0} + \frac{\partial L}{\partial \dot{q}} \frac{\partial \dot{q}}{\partial q_0} \right) dt$$

$$= \frac{\partial L}{\partial \dot{q}} \frac{\partial q}{\partial q_0} \Big|_{t_0}^{t_1} + \int_{t_0}^{t_1} \left(\frac{\partial L}{\partial q} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}} \right) \frac{\partial q}{\partial q_0} dt$$

$$= -\frac{\partial L}{\partial \dot{q}} (q_0, \dot{q}(t_0))$$

$$= -p_0^T \tag{2.2.10}$$

The last two equalities are consequences of the Lagrange equation (2.1.2) and the Legendre transform (2.1.3) respectively.

Similarly one gets

$$\frac{\partial \mathcal{S}}{\partial q_1} = p_1^T. \tag{2.2.11}$$

As a result it follows that

$$dS = \frac{\partial S}{\partial q_0} dq_0 + \frac{\partial S}{\partial q_1} dq_1 = -p_0^T dq_0 + p_1^T dq_1.$$
 (2.2.12)

Theorem 2.10. ([12]) A mapping $g:(p,q)\mapsto(P,Q)$ is symplectic if and only if there exists locally a function S(p,q) such that

$$P^T dQ - p^T dq = dS. (2.2.13)$$

This mean that $P^T dQ - p^T dq$ is a total differential.

Remark. The proof of this theorem can be found in [12]. It applies the Definition 2.3 of a symplectic mapping to show that, the Jacobian matrix

$$\left(\begin{array}{cc} P_p & P_q \\ Q_p & Q_q \end{array}\right)$$

of the mapping $(p,q) \mapsto (P,Q)$ defined by (2.2.13) satisfies

$$\begin{pmatrix} P_p & P_q \\ Q_p & Q_q \end{pmatrix}^T J \begin{pmatrix} P_p & P_q \\ Q_p & Q_q \end{pmatrix} = J. \tag{2.2.14}$$

(2.2.14) is equivalent to the three conditions

$$P_p^T Q_p = Q_p^T P_p, \quad P_p^T Q_q - I = Q_p^T P_q, \quad Q_q^T P_q = P_q^T Q_q.$$
 (2.2.15)

On the other hand, with $dQ = Q_p dp + Q_q dq$, and using an integrability lemma in [12], one knows that the left side of the equation (2.2.13) is integrable if and only if the matrix

$$\begin{pmatrix} Q_p^T P_p & Q_p^T P_q \\ Q_q^T P_p - I & Q_q^T P_q \end{pmatrix} + \sum_i P_i \frac{\partial^2 Q_i}{\partial (p, q)^2}$$
 (2.2.16)

is symmetric, which is equivalent to the symplectic conditions (2.2.15).

This theorem builds up the basis of the generating function theories, which we discuss later. S here is called the generating function of the symplectic mapping $(p,q) \mapsto (P,Q)$, which is derived from (2.2.13) as

$$P = \frac{\partial S}{\partial Q}^{T}(q, Q), \qquad p = -\frac{\partial S}{\partial q}^{T}(q, Q). \tag{2.2.17}$$

From Theorem 2.10 and (2.2.12) it follows that the mapping $(p_0, q_0) \mapsto (p_1, q_1)$ generated by the action integral S via the relation (2.2.12) is a symplectic mapping.

Based on this fact, it is possible to construct symplectic schemes via action integral S by the relation (2.2.12). Consider q_n and q_{n+1} of a one-step method as the two endpoints of the variational problem on the small interval $[t_n, t_{n+1}]$, where q_n and q_{n+1} are approximations of $q(t_n)$ and $q(t_{n+1})$ respectively, and write out the action integral on $[t_n, t_{n+1}]$ by applying the definition (2.1.8). Then use the relation (2.2.12) to find p_n and p_{n+1} . The mapping $(p_n, q_n) \mapsto (p_{n+1}, q_{n+1})$ is thus symplectic owing to Theorem 2.10. Explicitly, let the discrete Lagrangian be ([12])

$$L_h(q_n, q_{n+1}) \approx \int_{t_n}^{t_{n+1}} L(q(t), \dot{q}(t)) dt,$$
 (2.2.18)

which plays the role of the 'local' action integral. Given q_n and q_{n+1} , p_n and p_{n+1} can be derived through

$$p_n = -\frac{\partial L_h}{\partial q_n}^T (q_n, q_{n+1}), \qquad (2.2.19)$$

$$p_{n+1} = \frac{\partial L_h}{\partial q_{n+1}}^T (q_n, q_{n+1})$$
 (2.2.20)

according to the relations (2.2.10) and (2.2.11). The equation (2.2.19) is also called the discrete Legendre transformation ([12]).

It then follows the problem of finding L_h . In fact, L_h can be approximated by applying different quadrature formulae, such as the trapezoidal or the midpoint rule to (2.2.18).

In MacKay [20] and Wendlandt & Marsden [45], $\dot{q}(t)$ in (2.2.18) was approximated by $\frac{q_{n+1}-q_n}{t_{n+1}-t_n}$. It is discovered in [24] that higher order symplectic methods can be created by proper choice of quadrature formulae for approximating the discrete Lagrangian. For example, Gaussian quadrature gives the Gauss collocation method, and Lobatto quadrature gives the Lobatto IIIA-IIIB pair ([12],[24]). Particularly, the symplectic partitioned Runge-Kutta methods can be produced by using a special quadrature formula to (2.2.18) ([12]).

2.3 Generating Functions

The existence of generating functions for symplectic mappings is already shown in the section above, where the action integral S of the variational problem is a generating function, and q_n and q_{n+1} are first assumed to be given to find p_n and p_{n+1} . Note that this is only a formal assumption, since p_n and q_n are actually given. It can be seen as a local change of coordinates, which requires $\frac{\partial q_{n+1}}{\partial p_n}$ to be invertible to ensure that it is well-defined.

Similarly, one can also make other change of coordinates. For example, presuming (p_{n+1},q_n) or (p_n,q_{n+1}) or $(\frac{(p_{n+1}+p_n)}{2},\frac{(q_{n+1}+q_n)}{2})$ to be the coordinates is sometimes more convenient. There exist analog of Theorem 2.10, namely Theorem 2.11, which describes generating functions S^1 , S^2 , and S^3 corresponding to these three cases respectively.

Theorem 2.11. ([12]) Let $(p,q) \mapsto (P,Q)$ be a smooth transformation, close to the identity. It is symplectic if and only if one of the following conditions holds locally:

a)
$$Q^T dP + p^T dq = d(P^T q + S^1)$$
 for some function $S^1(P, q)$; (2.3.1)

b)
$$P^T dQ + q^T dp = d(p^T Q - S^2)$$
 for some function $S^2(p, Q)$; (2.3.2)

c)
$$(Q-q)^T d(P+p) - (P-p)^T d(Q+q) = 2dS^3$$

for some function
$$S^3(\frac{(P+p)}{2}, \frac{(Q+q)}{2})$$
. (2.3.3)

Remark. The proof is based on Theorem 2.10 and given in [12]. In fact, with choosing

$$S^{1} = P^{T}(Q - q) - S (2.3.4)$$

and considering $d(P^TQ) = P^TdQ + Q^TdP$, a) is equivalent to (2.2.13), and thus follows the assertion of the theorem. The cases b) and c) can be similarly derived for proper choice of S^2 and S^3 . In particular,

$$S^{3} = \frac{(P+p)^{T}(Q-q)}{2} - S \tag{2.3.5}$$

makes (2.3.3) equivalent to (2.2.13).

Comparing the coefficient functions of dP and dq in (2.3.1), we obtain the following scheme

$$p = P + \frac{\partial S^1}{\partial q}^T(P, q), \qquad Q = q + \frac{\partial S^1}{\partial P}^T(P, q),$$
 (2.3.6)

which is called the symplectic one-step method generated by the first kind of generating function $S^1(P,q)$. It is obvious that as $S^1=0$, it becomes the identity mapping, which is

expected, since the initial point of iteration coincides the initial conditions.

For $S^1(P,q) := hH(P,q)$ with h being the step size and H the Hamiltonian, (2.3.6) is just the symplectic Euler method, while the same approach applied to (2.3.2) leads to the adjoint of the symplectic Euler method.

Analogously, (2.3.3) yields the scheme

$$P = p - \partial_2^T S^3(\frac{(P+p)}{2}, \frac{(Q+q)}{2}),$$

$$Q = q + \partial_1^T S^3(\frac{(P+p)}{2}, \frac{(Q+q)}{2}).$$
(2.3.7)

For $S^3 = hH$, it is the implicit midpoint rule applied to the Hamiltonian system (2.1.5)-(2.1.6).

As revealed in Theorem 2.10, each symplectic mapping $(p,q) \mapsto (P,Q)$ corresponds to a generating function S according to the rule (2.2.17). Theorem 2.4 asserts that, the mapping along the flow of a Hamiltonian system $(p,q) \mapsto (P(t),Q(t))$ with p=P(0) and q=Q(0) is symplectic for any $t \geq 0$. Consequently, there should exist a generating function S(q,Q,t), which generates the exact flow $(p,q) \mapsto (P(t),Q(t))$ of the Hamiltonian system (2.1.5)-(2.1.6) with initial value (p,q), via

$$P(t) = \frac{\partial S}{\partial Q}^{T}(q, Q(t), t), \quad p = -\frac{\partial S}{\partial q}^{T}(q, Q(t), t). \tag{2.3.8}$$

Starting from this analysis, differentiating the second equation in (2.3.8), it is found that such S can be a solution of a partial differential equation.

Theorem 2.12. ([12]) If S(q, Q, t) is a smooth solution of

$$\frac{\partial S}{\partial t} + H(\frac{\partial S}{\partial Q}, Q) = 0, \qquad (2.3.9)$$

and if the matrix $(\frac{\partial^2 S}{\partial q_i \partial Q_j})$ is invertible, the mapping $(p,q) \mapsto (P(t),Q(t))$ defined by (2.3.8) is the exact flow of the Hamiltonian system (2.1.5)-(2.1.6) with initial value (p,q). Equation (2.3.9) is called the Hamilton-Jacobi partial differential equation.

The invertibility of the matrix $(\frac{\partial^2 S}{\partial q_i \partial Q_j})$ is required by the implicit function theorem of ensuring solvability of P(t) and Q(t) from equation (2.3.8), as well as calculations in the proof of the theorem. For details see [12].

The generating functions S^1 , S^2 , and S^3 also satisfy corresponding Hamilton-Jacobi partial differential equations, which can be derived from the relation between S and S^1 indicated in (2.3.4), and that between S and S^3 in (2.3.5).

Theorem 2.13. ([12]) If $S^1(P,q,t)$ is a solution of the partial differential equation

$$\frac{\partial S^1}{\partial t}(P,q,t) = H(P,q + \frac{\partial S^1}{\partial P}(P,q,t)), \qquad S^1(P,q,0) = 0, \tag{2.3.10}$$

then the mapping $(p,q) \mapsto (P(t),Q(t))$ defined by

$$p = P(t) + \frac{\partial S^1}{\partial q}^T (P(t), q, t), \qquad Q(t) = q + \frac{\partial S^1}{\partial P}^T (P(t), q, t)$$
 (2.3.11)

is the exact flow of the Hamiltonian system (2.1.5)-(2.1.6) with initial value (p,q).

Theorem 2.14. ([12]) Let $u = \frac{P+p}{2}$ and $v = \frac{Q+q}{2}$. Assume that $S^3(u,v,t)$ is a solution of

$$\frac{\partial S^3}{\partial t}(u,v,t) = H(u - \frac{1}{2}\frac{\partial S^3}{\partial v}(u,v,t), v + \frac{1}{2}\frac{\partial S^3}{\partial u}(u,v,t))$$
 (2.3.12)

with $S^3(u, v, 0) = 0$. Then the mapping $(p, q) \mapsto (P(t), Q(t))$ defined by

$$P(t) = p - \frac{\partial S^3}{\partial v}^T(u(t), v(t), t), \qquad Q(t) = q + \frac{\partial S^3}{\partial u}^T(u(t), v(t), t)$$
 (2.3.13)

is the exact flow of the Hamiltonian system (2.1.5)-(2.1.6) with initial value (p,q).

Based on the results above, generating functions for symplectic schemes can be found by solving corresponding Hamilton-Jacobi partial differential equations. Feng Kang et. al. proposed an approximate solution of the Hamilton-Jacobi equations ([8],[12]). For example, substituting the assumption

$$S^{1}(P,q,t) = tG_{1}(P,q) + t^{2}G_{2}(P,q) + t^{3}G_{3}(P,q) + \dots$$
(2.3.14)

into (2.3.10) and comparing like powers of t yields

$$G_{1}(P,q) = H(P,q),$$

$$G_{2}(P,q) = \frac{1}{2} \left(\frac{\partial H}{\partial P} \frac{\partial H}{\partial q}\right) (P,q),$$

$$G_{3}(P,q) = \frac{1}{6} \left(\frac{\partial^{2} H}{\partial P^{2}} \left(\frac{\partial H}{\partial q}\right)^{2} + \frac{\partial^{2} H}{\partial P \partial q} \frac{\partial H}{\partial P} \frac{\partial H}{\partial q} + \frac{\partial^{2} H}{\partial q^{2}} \left(\frac{\partial H}{\partial P}\right)^{2}\right) (P,q), \quad (2.3.15)$$

and so on. Let

$$S^1 \approx hG_1(P,q) + h^2G_2(P,q) + \dots + h^rG_r(P,q),$$
 (2.3.16)

then the symplectic numerical scheme generated by it according to (2.3.11) has order r of convergence, since the error is of order r + 1.

The same approach applied to S^3 results in

$$S^{3}(w,t) = tG_{1}(w) + t^{3}G_{3}(w) + \dots + t^{2r-1}G_{2r-1}(w) + \dots,$$
 (2.3.17)

where w = (u, v), and

$$G_1(w) = H(w),$$

 $G_3(w) = \frac{1}{24} \nabla^2 H(w) (J^{-1} \nabla H(w), J^{-1} \nabla H(w)),$ (2.3.18)

and so on. Let

$$S^{3}(w,h) \approx hG_{1}(w) + h^{3}G_{3}(w) + \dots + h^{2r-1}G_{2r-1}(w), \tag{2.3.19}$$

The symplectic numerical scheme generated by (2.3.13) has order 2r of convergence.

Chapter 3

Stochastic Hamiltonian Systems

A stochastic Hamiltonian system is a Hamiltonian system under certain kinds of random disturbances. Its definition, properties and some known numerical integration methods are introduced. Examples of stochastic Hamiltonian systems are given. For a linear stochastic oscillator, special numerical schemes are constructed and their abilities of preserving certain structures of the oscillator system are studied.

3.1 Definitions and Examples

Definition 3.1. ([2],[28],[29]) For the 2d-dimensional stochastic differential equation in Stratonovich sense

$$dp = f(t, p, q)dt + \sum_{k=1}^{r} \sigma_k(t, p, q) \circ dW_k(t), \quad p(t_0) = p_0,$$
 (3.1.1)

$$dq = g(t, p, q)dt + \sum_{k=1}^{r} \gamma_k(t, p, q) \circ dW_k(t), \quad q(t_0) = q_0,$$
 (3.1.2)

if there exist functions H(t, p, q) and $H_k(t, p, q)$ (k = 1, ..., r) such that

$$f(t, p, q) = -\frac{\partial H}{\partial q}(t, p, q)^T, \qquad \sigma_k(t, p, q) = -\frac{\partial H_k}{\partial q}(t, p, q)^T,$$
 (3.1.3)

$$g(t, p, q) = \frac{\partial H}{\partial p}(t, p, q)^T, \qquad \gamma_k(t, p, q) = \frac{\partial H_k}{\partial p}(t, p, q)^T,$$
 (3.1.4)

for k = 1, ..., r, then it is a stochastic Hamiltonian system.

This definition is based on the requirement of preservation of the symplectic structure $dp \wedge dq$ along the phase trajectory of the stochastic system (3.1.1)-(3.1.2). It is proved in [28] that

Theorem 3.2. ([2],[28],[29]) For the stochastic Hamiltonian system (3.1.1)-(3.1.2) with conditions (3.1.3)-(3.1.4), it holds

$$dp(t) \wedge dq(t) = dp_0 \wedge dq_0 \tag{3.1.5}$$

for all t > 0.

The proof mainly applies the formula of change of variables in differential forms. The demand of the system being in Stratonovich sense simplifies the stochastic differential calculations, since the Stratonovich equations preserve classic chain rule.

In fact, (3.1.5) is the intrinsic characteristic of a stochastic Hamiltonian system, and we have the following result.

Theorem 3.3. (3.1.5) is equivalent to

$$B^T J B = J$$
,

where

$$B := \frac{\partial(p(t), q(t))}{\partial(p_0, q_0)} = \begin{pmatrix} \frac{\partial p(t)}{\partial p_0} & \frac{\partial p(t)}{\partial q_0} \\ \frac{\partial q(t)}{\partial p_0} & \frac{\partial q(t)}{\partial q_0} \end{pmatrix}.$$

Proof. The proof follows the same way as that of Theorem 2.5.

Due to the external stochastic disturbances, the total energy of the stochastic Hamiltonian systems may not be preserved. In other words, the Hamiltonian H can vary, which is different from deterministic Hamiltonian systems.

Definition 3.4. ([6],[17],[21]) The stochastic differential equation (1.1.6) is called a stochastic differential equation with additive noises, if b(X(t),t) = b(t), i.e. b does not depend on X. Otherwise it is called a stochastic differential equation with multiplicative noises.

Theorem 3.5. For a stochastic differential equation with additive noises, its Itô form and Stratonovich form coincide.

Proof. b being independent of X implies that

$$\frac{\partial b_{ik}}{\partial r} = 0, \qquad i = 1, \dots, d, \ k = 1, \dots, r.$$

The relation between Itô and Stratonovich equations given in Proposition 1.2 thus gives the result of the theorem.

We give in the following several examples of stochastic Hamiltonian systems.

Example 3.1. A linear Stochastic Oscillator

A linear stochastic oscillator with additive noise can be written as

$$\ddot{x}(t) + x(t) = \sigma \dot{w}(t), \tag{3.1.6}$$

where $\sigma > 0$ is a constant. Introducing $y = \dot{x}$, and given initial value, it can be expressed as the two-dimensional stochastic differential equation

$$dy(t) = -x(t)dt + \sigma dW(t), \quad y(0) = y_0,$$
 (3.1.7)

$$dy(t) = -x(t)dt + \sigma dW(t), \quad y(0) = y_0,$$

$$dx(t) = y(t)dt, \qquad x(0) = x_0.$$
(3.1.7)

Since (3.1.7)-(3.1.8) is a stochastic system with additive noise, its Itô and Stratonovich form are identical. We consider it as an equation system in Stratonovich sense. For

$$H(y,x) = \frac{1}{2}(y^2 + x^2), \qquad H_1(y,x) = -\sigma x,$$
 (3.1.9)

(3.1.7)-(3.1.8) is a stochastic Hamiltonian system, since

$$-x = -\frac{\partial H}{\partial x}, \quad \sigma = -\frac{\partial H_1}{\partial x},$$
 (3.1.10)

$$y = \frac{\partial H}{\partial y}, \qquad 0 = \frac{\partial H_1}{\partial y}.$$
 (3.1.11)

More general, it is not difficult to see the fact stated in the following proposition.

Proposition 3.6. ([26]) A Hamiltonian system with additive noises is a stochastic Hamiltonian system.

Since the noise parts contain neither p nor q, but only functions of t, the corresponding H_k must exist.

Given initial value $y(0) = y_0 \in \mathbb{R}$, $x(0) = x_0 \in \mathbb{R}$, it is shown that this system has the unique solution ([22],[41])

$$y(t) = -x_0 \sin t + y_0 \cos t + \sigma \int_0^t \cos(t - s) dW(s), \qquad (3.1.12)$$

$$x(t) = x_0 \cos t + y_0 \sin t + \sigma \int_0^t \sin(t - s) dW(s).$$
 (3.1.13)

The solution (3.1.12)-(3.1.13) possesses the following two important properties.

Proposition 3.7. (Markus & Weerasinghe [22], Strømmen Melbø & Higham [41]) For the linear stochastic oscillator (3.1.7)-(3.1.8) with $y_0 = 0$, $x_0 = 1$, the second moment of the solution satisfies

$$\mathbb{E}(y(t)^2 + x(t)^2) = 1 + \sigma^2 t. \tag{3.1.14}$$

Proposition 3.8. ([22],[41]) For the linear stochastic oscillator (3.1.7)-(3.1.8) with $y_0 = 0$, $x_0 = 1$, almost surely, x(t) has infinitely many zeros, all simple, on each half line $[t_0, \infty)$ for every $t_0 \ge 0$.

Proposition 3.7 reveals the linear growth property of the second moment with respect to time t of the solution. Since $H = \frac{1}{2}(y^2 + x^2)$, we can see that

$$\mathbb{E}(H) = \frac{1}{2}(1 + \sigma^2 t),\tag{3.1.15}$$

which implies the linear growth of the Hamiltonian, i.e., the Hamiltonian is not conserved. Proposition 3.8 indicates the oscillation property of the solution.

Example 3.2. Kubo Oscillator

The Kubo oscillator has the form

$$dp = -aqdt - \sigma q \circ dW(t), \qquad p(0) = p_0, \tag{3.1.16}$$

$$dq = apdt + \sigma p \circ dW(t), \qquad q(0) = q_0, \qquad (3.1.17)$$

where a and σ are constants, and W(t) is a one-dimensional standard Wiener process.

$$H(p,q) = \frac{a}{2}(p^2 + q^2), \quad H_1(p,q) = \frac{\sigma}{2}(p^2 + q^2),$$
 (3.1.18)

then we have

$$-aq = -\frac{\partial H}{\partial q}, \qquad -\sigma q = -\frac{\partial H_1}{\partial q},$$
 (3.1.19)

$$ap = \frac{\partial H}{\partial p}, \qquad \sigma p = \frac{\partial H_1}{\partial p}, \qquad (3.1.20)$$

which implies that the Kubo oscillator (3.1.16)-(3.1.17) is a stochastic Hamiltonian system. Moreover, the quantity $p^2 + q^2$ is conservative for this system ([29]), i.e.,

$$p(t)^{2} + q(t)^{2} = p_{0}^{2} + q_{0}^{2}$$
(3.1.21)

for all $t \ge 0$. Thus the Hamiltonian H of the system is conserved, and the phase trajectory of (3.1.16)-(3.1.17) is the circle with center at the origin and radius $\sqrt{p_0^2 + q_0^2}$.

Example 3.3. A Model for Synchrotron Oscillations of Particles in Storage Rings

In [29], the following model of synchrotron oscillations of particles in storage rings influenced by external fluctuating electromagnetic fields was considered:

$$dp = -\omega^2 \sin(q) dt - \sigma_1 \cos(q) \circ dW_1 - \sigma_2 \sin(q) \circ dW_2, \quad p(0) = p_0, \quad (3.1.22)$$

$$dq = pdt, \quad q(0) = q_0, \quad (3.1.23)$$

where ω , σ_1 , and σ_2 are constants, and p and q are both of one dimension.

$$H = \frac{1}{2}p^2 - \omega^2 \cos(q), \quad H_1 = \sigma_1 \sin(q), \quad H_2 = -\sigma_2 \cos(q), \tag{3.1.24}$$

then it follows that

$$-\omega^2 \sin(q) = -\frac{\partial H}{\partial q}, \quad -\sigma_1 \cos(q) = -\frac{\partial H_1}{\partial q}, \quad -\sigma_2 \sin(q) = -\frac{\partial H_2}{\partial q}, \quad (3.1.25)$$

$$p = \frac{\partial H}{\partial p}, \qquad 0 = \frac{\partial H_1}{\partial p} = \frac{\partial H_2}{\partial p},$$
 (3.1.26)

which ensures that the model (3.1.22)-(3.1.23) is a stochastic Hamiltonian system with two noises.

Example 3.4. A System with Two Additive Noises

The following system with two additive noises was studied in [28]:

$$dq = pdt + \sigma \circ dW_1(t), \quad q(0) = q_0,$$
 (3.1.27)

$$dp = -qdt + \gamma \circ dW_2(t), \quad p(0) = p_0,$$
 (3.1.28)

where p and q are scalar, and σ and γ are constants. Let $X = \begin{pmatrix} q \\ p \end{pmatrix}$, the exact solution of the system (3.1.27)-(3.1.28) can be expressed as ([28])

$$X(t_{k+1}) = FX(t_k) + U_k, \quad X(0) = X_0,$$
 (3.1.29)

where k = 0, 1, ..., N - 1, $0 = t_0 < t_1 < ... < t_N = T$, $t_{k+1} - t_k = h$, $X_0 = \begin{pmatrix} q_0 \\ p_0 \end{pmatrix}$, and

$$F = \begin{pmatrix} \cos(h) & \sin(h) \\ -\sin(h) & \cos(h) \end{pmatrix}, \tag{3.1.30}$$

$$u_{k} = \begin{pmatrix} \sigma \int_{t_{k}}^{t_{k+1}} \cos(t_{k+1} - s) dW_{1}(s) + \gamma \int_{t_{k}}^{t_{k+1}} \sin(t_{k+1} - s) dW_{2}(s) \\ -\sigma \int_{t_{k}}^{t_{k+1}} \sin(t_{k+1} - s) dW_{1}(s) + \gamma \int_{t_{k}}^{t_{k+1}} \cos(t_{k+1} - s) dW_{2}(s) \end{pmatrix} . (3.1.31)$$

If we denote

$$H = \frac{1}{2}(p^2 + q^2), \quad H_1 = \sigma p, \quad H_2 = -\gamma q,$$
 (3.1.32)

then it holds

$$dp = -\frac{\partial H}{\partial q}dt - \frac{\partial H_1}{\partial q} \circ dW_1(t) - \frac{\partial H_2}{\partial q} \circ dW_2(t), \qquad (3.1.33)$$

$$dq = \frac{\partial H}{\partial p}dt + \frac{\partial H_1}{\partial p} \circ dW_1(t) + \frac{\partial H_2}{\partial p} \circ dW_2(t), \qquad (3.1.34)$$

which implies that the system (3.1.27)-(3.1.28) is a stochastic Hamiltonian system.

3.2 Stochastic Symplectic Integration

As the case for deterministic Hamiltonian system, numerical integration methods that preserve the symplectic structure of stochastic Hamiltonian systems are expected, the research of which is at the beginning of development.

Definition 3.9. ([26],[28],[29]) A one step numerical method $(p_n,q_n) \mapsto (p_{n+1},q_{n+1})$ for the stochastic Hamiltonian system (3.1.1)-(3.1.2) is a symplectic method if

$$dp_{n+1} \wedge dq_{n+1} = dp_n \wedge dq_n \tag{3.2.1}$$

for all n > 1.

Pioneering work for symplectic integration of stochastic Hamiltonian systems owe to [28] and [29] by Milstein et. al.. In the two articles, symplectic Runge-Kutta type methods are proposed for stochastic Hamiltonian systems with additive noises and multiplicative noises, respectively.

In [28] and its preprint [26], for the Hamiltonian systems with additive noises

$$dP = f(t, P, Q)dt + \sum_{k=1}^{r} \sigma_k(t)dW(t), \qquad P(t_0) = p,$$
 (3.2.2)

$$dQ = g(t, P, Q) + \sum_{k=1}^{r} \gamma_k(t) dW(t), \qquad Q(t_0) = q, \qquad (3.2.3)$$

with the Hamiltonian H satisfying

$$f = -\frac{\partial H^T}{\partial q}, \qquad g = \frac{\partial H^T}{\partial p},$$
 (3.2.4)

the following s-stage symplectic Runge-Kutta methods are given.

$$P = p + h \sum_{i=1}^{s} b_{i} f(t_{0} + c_{i}h, \mathcal{P}_{i}, \mathcal{Q}_{i}) + \eta,$$

$$\mathcal{P}_{i} = p + h \sum_{j=1}^{s} a_{ij} f(t_{0} + c_{j}h, \mathcal{P}_{j}, \mathcal{Q}_{j}) + \varphi_{i},$$

$$Q = q + h \sum_{i=1}^{s} b_{i} g(t_{0} + c_{i}h, \mathcal{P}_{i}, \mathcal{Q}_{i}) + \zeta,$$

$$\mathcal{Q}_{i} = q + h \sum_{i=1}^{s} a_{ij} g(t_{0} + c_{j}h, \mathcal{P}_{j}, \mathcal{Q}_{j}) + \psi_{i},$$
(3.2.5)

where φ_i , ψ_i , η , ζ do not depend on p and q, the parameters a_{ij} and b_i satisfy

$$b_i a_{ij} + b_j a_{ji} = b_i b_j, \quad i, j = 1, \dots, s.$$
 (3.2.7)

It can be seen that the symplectic conditions of the parameters (3.2.7) coincide with that of the deterministic Runge-Kutta methods (2.2.9). For $\varphi_i = \psi_i = \eta = \zeta = 0$, (3.2.5)-(3.2.6) reduce to the deterministic Runge-Kutta method (2.2.7)-(2.2.8).

Theorem 3.10. ([26]) The scheme (3.2.5)-(3.2.6) preserves symplectic structure, i.e., $dP \wedge dQ = dp \wedge dq$ under conditions (3.2.7).

Its proof follows from a straightforward calculation on wedge products.

Since symplectic methods are usually implicit, it is necessary to find complete implicit methods, which are implicit in both drift and diffusion parts for stochastic differential equations with multiplicative noises. Directly adapted implicit methods are often unapplicable. As an example, the following Itô scalar equation was considered in [29]:

$$dX = \sigma X dW(t), \tag{3.2.8}$$

the Euler-Maruyama method applied to (3.2.8) has the form

$$X_{n+1} = X_n + \sigma X_n \Delta W_n, \tag{3.2.9}$$

which is an explicit method. Now change its form to

$$X_{n+1} = X_n + \sigma X_{n+1} \Delta W_n + \sigma (X_n - X_{n+1}) \Delta W_n = X_n - \sigma^2 X_n (\Delta W_n)^2 + \sigma X_{n+1} \Delta W_n.$$
(3.2.10)

Modeling $(\Delta W_n)^2$ by the step size h owing to the fact $\mathbb{E}(\Delta W_n^2) = h$, it follows from (3.2.10) the directly adapted implicit method

$$\tilde{X}_{n+1} = X_n - \sigma^2 X_n h + \sigma \tilde{X}_{n+1} \Delta W_n,$$
 (3.2.11)

or equivalently,

$$\tilde{X}_{n+1} = \frac{X_n(1 - \sigma^2 h)}{1 - \sigma \Delta W_n}. (3.2.12)$$

The scheme (3.2.12) is unapplicable because the denominator $1 - \sigma \Delta W_n$ can vanish for any small h, due to the unboundedness of ΔW_n for any small h. Milstein et. al. proposed the method of truncating ΔW_n to make it bounded. Model ΔW_n by $\sqrt{h}\zeta_h$ instead of the original $\sqrt{h}\xi$ with $\xi \sim \mathcal{N}(0,1)$. ζ_h has the form

$$\zeta_h = \begin{cases}
\xi, & |\xi| \le A_h, \\
A_h, & \xi > A_h, \\
-A_h, & \xi < -A_h,
\end{cases}$$
(3.2.13)

where $A_h > 0$ can takes the value $\sqrt{2k|\ln h|}$ with $k \ge 1$ to ensure the mean-square convergence of the method (3.2.12) with order larger than or equal to $\frac{1}{2}$. The proof of this fact is based on the following two theorems.

Theorem 3.11. ([25]) Suppose the one-step approximation $\bar{X}_{t,x}(t+h)$ to X at time t+h starting from time t and value x satisfies

$$|\mathbb{E}(X_{t,x}(t+h) - \bar{X}_{t,x}(t+h))| \le K(1+|x|^2)^{\frac{1}{2}}h^{p_1},$$
 (3.2.14)

$$\left[\mathbb{E}|X_{t,x}(t+h) - \bar{X}_{t,x}(t+h)|^2 \right]^{\frac{1}{2}} \le K(1+|x|^2)^{\frac{1}{2}}h^{p_2}$$
 (3.2.15)

for arbitrary $t_0 \le t \le t_0 + T - h$ and some K > 0, and

$$p_2 \ge \frac{1}{2}, \qquad p_1 \ge p_2 + \frac{1}{2}.$$
 (3.2.16)

Let $\{t_k\}$ be the partition of the time interval $[t_0, t_0 + T]$ with $t_{k+1} - t_k = h = \frac{T}{N}$. Then for any N and k = 0, 1, ..., N it holds:

$$|\mathbb{E} | X_{t_0, X_0}(t_k) - \bar{X}_{t_0, X_0}(t_k) |^2 |^{\frac{1}{2}} \le K(1 + \mathbb{E}|X_0|^2)^{\frac{1}{2}} h^{p_2 - \frac{1}{2}},$$
 (3.2.17)

namely, the mean-square order of the method based on the one-step approximation $\bar{X}_{t,x}(t+h)$ is $p=p_2-\frac{1}{2}$.

For the Euler-Maruyama method (1.2.2), it can be verified that $p_1 = 2$, $p_2 = 1$ in general cases. For a system with additive noises, it holds $p_1 = 2$ and $p_2 = \frac{3}{2}$ ([26]).

Theorem 3.12. ([25],[26]) Let the one-step approximation $X_{t,x}(t+h)$ satisfy the conditions of Theorem 3.11. Suppose that the one-step approximation $X_{t,x}(t+h)$ satisfies

$$\left| \mathbb{E} \left(\tilde{X}_{t,x}(t+h) - \bar{X}_{t,x}(t+h) \right) \right| = O(h^{p_1}),$$
 (3.2.18)

$$\left(\mathbb{E} \mid \tilde{X}_{t,x}(t+h) - \bar{X}_{t,x}(t+h) \mid^{2}\right)^{\frac{1}{2}} = O(h^{p_{2}})$$
(3.2.19)

with the same p_1 and p_2 . Then the method based on the one-step approximation $\tilde{X}_{t,x}(t+h)$ has the same mean-square order of accuracy as that based on $\bar{X}_{t,x}(t+h)$, i.e., its order is

$$p = p_2 - \frac{1}{2}$$
.

Theorem 3.12 is a natural consequence of Theorem 3.11, which can be verified by using triangular inequality.

Compare the truncated implicit method

$$\bar{X}_{n+1} = \frac{X_n(1 - \sigma^2 h)}{1 - \sigma \zeta_h \sqrt{h}}$$
 (3.2.20)

with the Euler-Maruyama method (3.2.9), it is obtained that ([29])

$$\left| \mathbb{E}(\bar{X}_{n+1} - X_{n+1}) \right| \le O(h^2),$$
 (3.2.21)

$$\left(\mathbb{E}(\bar{X}_{n+1} - X_{n+1})^2\right)^{\frac{1}{2}} \le O(h), \tag{3.2.22}$$

which means that the method (3.2.20) is of the same mean-square order as the Euler-Maruyama method (3.2.9), namely with order $\frac{1}{2}$, according to Theorem 3.12. But (3.2.20) is an implicit method.

With truncation of ΔW_n for building implicit methods, a class of symplectic Runge-Kutta type schemes was constructed for the general Hamiltonian system (3.1.1)-(3.1.2) with multiplicative noises, which has the form ([29])

$$p_{n+1} = p_n + f(t_n + \beta h, \alpha P_{n+1} + (1 - \alpha)p_n, (1 - \alpha)q_{n+1} + \alpha q_n)h$$

$$+ \left(\frac{1}{2} - \alpha\right) \sum_{k=1}^r \sum_{j=1}^d \left(\frac{\partial \sigma_k}{\partial p^j} \sigma_k^j - \frac{\partial \sigma_k}{\partial q^j} \gamma_k^j\right) h + \sum_{k=1}^r \sigma_k \cdot (\zeta_{kh})_n \sqrt{h}, \quad (3.2.23)$$

$$q_{n+1} = q_n + g(t_n + \beta h, \alpha P_{n+1} + (1 - \alpha)p_n, (1 - \alpha)q_{n+1} + \alpha q_n)h$$

$$+ \left(\frac{1}{2} - \alpha\right) \sum_{k=1}^r \sum_{j=1}^d \left(\frac{\partial \gamma_k}{\partial p^j} \sigma_k^j - \frac{\partial \gamma_k}{\partial q^j} \gamma_k^j\right) h + \sum_{k=1}^r \gamma_k \cdot (\zeta_{kh})_n \sqrt{h}, \quad (3.2.24)$$

where σ_k , γ_k $(k=1,\ldots,r)$ and their derivatives are calculated at $(t_n+\beta h, \alpha p_{n+1}+(1-\alpha)p_n, (1-\alpha)q_{n+1}+\alpha q_n)$, and $\alpha, \beta \in [0,1]$. For $\alpha=\beta=\frac{1}{2}, (3.2.23)$ -(3.2.24) gives the midpoint rule

$$p_{n+1} = p_n + f(t_n + \frac{h}{2}, \frac{p_n + p_{n+1}}{2}, \frac{q_n + q_{n+1}}{2})h$$

$$+ \sum_{k=1}^r \sigma_k(t_n + \frac{h}{2}, \frac{p_n + p_{n+1}}{2}, \frac{q_n + q_{n+1}}{2})(\zeta_{kh})_n \sqrt{h}, \qquad (3.2.25)$$

$$q_{n+1} = q_n + g(t_n + \frac{h}{2}, \frac{p_n + p_{n+1}}{2}, \frac{q_n + q_{n+1}}{2})h$$

$$+ \sum_{k=1}^r \gamma_k(t_n + \frac{h}{2}, \frac{p_n + p_{n+1}}{2}, \frac{q_n + q_{n+1}}{2})(\zeta_{kh})_n \sqrt{h}. \qquad (3.2.26)$$

For stochastic Hamiltonian systems (3.1.1)-(3.1.2) with condition (3.1.3)-(3.1.4), if

$$H_k(p,q) = U_k(t,q) + V_k(t,p),$$
 (3.2.27)

with k = 1, ..., r, i.e., if H_k are separable, the methods (3.2.23)-(3.2.24) with $\alpha = 1$, $\beta = 0$ become

$$p_{n+1} = p_n + f(t_n, p_{n+1}, q_n)h$$

$$+ \frac{h}{2} \sum_{k=1}^r \sum_{j=1}^d \frac{\partial \sigma_k}{\partial q^j}(t_n, q_n) \cdot \gamma_k^j(t_n, p_{n+1}) + \sum_{k=1}^r \sigma_k(t_n, q_n) \Delta_n W_k, \qquad (3.2.28)$$

$$q_{n+1} = q_n + g(t_n, p_{n+1}, q_n)h$$

$$- \frac{h}{2} \sum_{k=1}^r \sum_{j=1}^d \frac{\partial \gamma_k}{\partial p^j}(t_n, p_{n+1}) \cdot \sigma_k^j(t_n, q_n) + \sum_{k=1}^r \gamma_k(t_n, p_{n+1}) \Delta_n W_k, \quad (3.2.29)$$

where $\Delta_n W_k = W_k(t_{n+1}) - W_k(t_n)$ (k = 1, ..., r). They are not truncated here, because this method is explicit in stochastic terms, in which case $\Delta_n W_k$ do not appear in denominator.

For the Kubo oscillator (3.1.16)-(3.1.17), it is given in (3.1.18) that

$$H_1(p,q) = \frac{\sigma}{2}(p^2 + q^2),$$

which is separable. Applying method (3.2.28)-(3.2.29) to the Kubo oscillator results in

$$p_{n+1} = p_n - aq_n h - \frac{\sigma^2}{2} p_{n+1} h - \sigma q_n \Delta W_n,$$
 (3.2.30)

$$q_{n+1} = q_n + ap_{n+1}h + \frac{\sigma^2}{2}q_nh + \sigma p_{n+1}\Delta W_n.$$
 (3.2.31)

The midpoint rule (3.2.25)-(3.2.26) gives for the Kubo oscillator the following midpoint scheme

$$p_{n+1} = p_n - a \frac{q_n + q_{n+1}}{2} h - \sigma \frac{q_n + q_{n+1}}{2} (\zeta_h)_n \sqrt{h}, \qquad (3.2.32)$$

$$q_{n+1} = q_n + a \frac{p_n + p_{n+1}}{2} h + \sigma \frac{p_n + p_{n+1}}{2} (\zeta_h)_n \sqrt{h}, \qquad (3.2.33)$$

the mean-square order of which is 1 ([29]).

It is shown in [29] that the midpoint rule (3.2.32)-(3.2.33) preserves the circular phase trajectory of the Kubo oscillator with high accuracy over long time interval, while the method (3.2.30)-(3.2.31) produces a ring-shape trajectory. The Euler-Maruyama method

$$p_{n+1} = p_n - aq_n h - \frac{\sigma^2}{2} p_n h - \sigma q_n \Delta W_n,$$
 (3.2.34)

$$q_{n+1} = q_n + ap_n h - \frac{\sigma^2}{2} q_n h + \sigma p_n \Delta W_n,$$
 (3.2.35)

which is not symplectic, gives a spiral trajectory. The advantage of symplectic methods in preserving conservative properties over long time interval is illustrated by this example.

3.3 A Linear Stochastic Oscillator

For the linear stochastic oscillator (3.1.7)-(3.1.8), some numerical methods are proposed in [41]. Their abilities of preserving linear growth property (3.1.14) of the second moment and oscillation property of the solution of the oscillator system on long time interval are checked. It is found that the forward Euler-Maruyama method

$$x_{n+1} = x_n + hy_n, (3.3.1)$$

$$y_{n+1} = y_n - hx_n + \sigma \Delta W_n, \tag{3.3.2}$$

where h > 0 is the step size, produces a second moment that increases exponentially with time, and the backward Euler-Maruyama method

$$x_{n+1} = x_n + hy_{n+1}, (3.3.3)$$

$$y_{n+1} = y_n - hx_{n+1} + \sigma \Delta W_n (3.3.4)$$

has second moment bounded above for all time. The partitioned Euler-Maruyama method

$$x_{n+1} = x_n + hy_n, (3.3.5)$$

$$y_{n+1} = y_n - hx_{n+1} + \sigma \Delta W_n, (3.3.6)$$

however, gives linear growth for all step sizes less than 2. Moreover, it inherits a precise analogue of the infinite oscillation property of the solution, which is stated in Proposition 3.8.

It is straightforward to verify that the partitioned Euler-Maruyama method is symplectic by checking the relation

$$dx_{n+1} \wedge dy_{n+1} = dx_n \wedge dy_n. \tag{3.3.7}$$

We apply the midpoint rule to the oscillator to obtain the midpoint scheme

$$x_{n+1} = x_n + h \frac{y_{n+1} + y_n}{2}, (3.3.8)$$

$$y_{n+1} = y_n - h \frac{x_{n+1} + x_n}{2} + \sigma \Delta W_n, \qquad (3.3.9)$$

which can also be written in the form

$$\begin{pmatrix} x_{n+1} \\ y_{n+1} \end{pmatrix} = A \begin{pmatrix} x_n \\ y_n \end{pmatrix} + r_n, \tag{3.3.10}$$

where

$$A = \begin{pmatrix} \frac{4-h^2}{4+h^2} & \frac{4h}{4+h^2} \\ \frac{-4h}{4+h^2} & \frac{4-h^2}{4+h^2} \end{pmatrix}, \quad r_n = \begin{pmatrix} \frac{2\sigma h}{4+h^2} \\ \frac{4\sigma}{4+h^2} \end{pmatrix} \Delta W_n.$$
 (3.3.11)

The sympleticity of the scheme is obvious since it is a special case of the midpoint rule (3.2.25)-(3.2.26). For its ability of preserving the properties of the oscillator system, we have the following results.

Theorem 3.13. ([14]) Given initial data $x_0 = 1$, $y_0 = 0$, the numerical solution arising from (3.3.8)-(3.3.9) satisfies

i)
$$\mathbb{E}(x_n^2 + y_n^2) = 1 + \frac{\sigma^2}{1 + (\frac{h}{2})^2} t_n$$
, and consequently (3.3.12)

ii)
$$\mathbb{E}(x_n^2 + y_n^2) \le 1 + \sigma^2 t_n - \frac{\sigma^2}{4} t_n h^2 + \frac{\sigma^2}{16} t_n h^4$$
, (3.3.13)

for every h > 0.

Proof. The proof follows directly from the relations (3.3.10)-(3.3.11).

It is shown by numerical tests that the midpoint rule is more stable in preserving the linear growth property over long time interval than the partitioned Euler-Maruyama method.

Theorem 3.14. ([14]) The numerical solution $\{x_n\}_{n\geq 0}$ arising from the midpoint scheme (3.3.8)-(3.3.9) for the oscillator system (3.1.7)-(3.1.8) with initial values $x_0 = 1$, $y_0 = 0$ will switch signs infinitely many times as $n \to \infty$, almost surely.

Proof. The proof of the theorem follows the same way as that of the partitioned Euler-Maruyama method given in [41], except for some technical details. It can be derived from the midpoint scheme (3.3.8)-(3.3.9) that

$$\begin{pmatrix} x_{n+1} \\ x_n \end{pmatrix} = B \begin{pmatrix} x_n \\ x_{n-1} \end{pmatrix} + \begin{pmatrix} \hat{r}_n \\ 0 \end{pmatrix}, \tag{3.3.14}$$

where

$$B = \begin{pmatrix} \frac{2(4-h^2)}{4+h^2} & -1\\ 1 & 0 \end{pmatrix}, \quad \hat{r}_n = \frac{2\sigma h}{4+h^2} (\Delta W_n + \Delta W_{n-1}). \tag{3.3.15}$$

Denote $B^j = \begin{pmatrix} a_j & b_j \\ c_j & d_j \end{pmatrix}$, it follows

$$x_{n+1} = b_n + a_n \frac{4 - h^2}{4 + h^2} + a_n \frac{2\sigma h}{4 + h^2} \Delta W_0 + \sum_{j=1}^n a_{n-j} \hat{r}_j.$$
 (3.3.16)

By some algebraic discussion it can be shown that

$$\left| b_n + a_n \frac{4 - h^2}{4 + h^2} \right| \le K, \quad |a_j| \le K, \quad |b_j| \le K$$
 (3.3.17)

for some K > 0, $j = 0, 1, 2, \ldots$ Let $S_n = a_n \frac{2\sigma h}{4+h^2} \Delta W_0 + \sum_{j=1}^n a_{n-j} \hat{r}_j$. Then it can be calculated that $S_n \sim \mathcal{N}(0, s_n^2)$ with $s_n^2 \to \infty$ as $n \to \infty$. The law of iterated logarithm indicates that for such a random variable sequence $\{S_n\}$,

The law of iterated logarithm indicates that for such a random variable sequence $\{S_n\}$, $\forall \varepsilon > 0$ and sufficiently large n, S_n will almost surely exceed the bounds $-(1-\varepsilon)(2s_n^2 \ln \ln s_n^2)^{\frac{1}{2}}$ and $(1-\varepsilon)(2s_n^2 \ln \ln s_n^2)^{\frac{1}{2}}$ infinitely often. (3.3.17) ensures that $\{x_n\}$ behaves in the same way.

Superiority of symplectic schemes in preserving structure of the underlying systems on long time interval than non-symplectic methods is reflected in the simulation of the linear stochastic oscillator. For general systems, symplectic schemes are usually implicit. In deterministic case, predictor-corrector methods are proposed to give explicit schemes with nearly preservation of symplecticity.

We apply the predictor-corrector methods with equidistant time discretization to the linear stochastic oscillator (3.1.7)-(3.1.8) to observe the effect of such methods in stochastic case. Denote the predictor-corrector method by $P(EC)^k$, where k indicates that the corrector is applied k times. We say shortly, e.g., $P(EC)^k$ method with partitioned Euler-Maruyama and midpoint rule, to mean that the first mentioned method is the predictor and the second one the corrector.

It is derived that $P(EC)^k$ method with partitioned Euler-Maruyama and midpoint rule applied to the linear stochastic oscillator (3.1.7)-(3.1.8) has the form ([15])

$$\begin{pmatrix} x_{n+1}^{(k)} \\ y_{n+1}^{(k)} \end{pmatrix} = \begin{pmatrix} a_k & b_k \\ c_k & d_k \end{pmatrix} \begin{pmatrix} x_n \\ y_n \end{pmatrix} + \begin{pmatrix} r_k \\ s_k \end{pmatrix} \Delta W_n, \tag{3.3.18}$$

where

$$a_k = \begin{cases} \frac{4-h^2}{4+h^2}(1-a_{[k]}) + a_{[k]} & k \text{ even,} \\ \frac{4-h^2}{4+h^2}(1-b_{[k]}) + (1-\frac{h^2}{2})b_{[k]} & k \text{ odd,} \end{cases}$$
(3.3.19)

$$b_k = \begin{cases} \frac{4h}{4+h^2}(1-a_{[k]}) + ha_{[k]} & k \text{ even,} \\ \frac{4h}{4+h^2}(1-b_{[k]}) + h(1-\frac{h^2}{2})b_{[k]} & k \text{ odd,} \end{cases}$$
(3.3.20)

$$c_k = \begin{cases} -\frac{4h}{4+h^2}(1-a_{[k]}) - ha_{[k]} & k \text{ even,} \\ -\frac{4h}{4+h^2}(1-b_{[k]}) - hb_{[k]} & k \text{ odd,} \end{cases}$$
(3.3.21)

$$d_k = \begin{cases} \frac{4-h^2}{4+h^2}(1-a_{[k]}) + (1-h^2)a_{[k]} & k \text{ even,} \\ \frac{4-h^2}{4+h^2}(1-b_{[k]}) + (1-\frac{h^2}{2})b_{[k]} & k \text{ odd,} \end{cases}$$
(3.3.22)

$$r_k = \begin{cases} \frac{2\sigma h}{4+h^2} (1 - a_{[k]}) & k \text{ even,} \\ \frac{2\sigma h}{4+h^2} (1 - b_{[k]}) + \frac{\sigma h}{2} b_{[k]} & k \text{ odd,} \end{cases}$$
(3.3.23)

$$s_k = \begin{cases} \frac{4h}{4+h^2}(1-a_{[k]}) + ha_{[k]} & k \text{ even,} \\ \frac{4h}{4+h^2}(1-b_{[k]}) + hb_{[k]} & k \text{ odd,} \end{cases}$$
(3.3.24)

with

$$a_{[k]} = (-1)^{\frac{k}{2}} (\frac{h^2}{4})^{\frac{k}{2}}, \quad b_{[k]} = (-1)^{\frac{k-1}{2}} (\frac{h^2}{4})^{\frac{k-1}{2}},$$
 (3.3.25)

h > 0 is the step size, and the upper index (k) indicates that the value is obtained from the k-th correction.

Theorem 3.15. ([15]) The $P(EC)^k$ method with partitioned Euler-Maruyama and midpoint rule (3.3.18) preserves symplecticity of the linear oscillator system (3.1.7)-(3.1.8) to the degree of having error $O(k^{k+4})$ as k is even, and error $O(k^{k+3})$ as k is odd.

Proof. See [15].
$$\Box$$

As $h \to 0$, or h < 1 and $k \to \infty$, the $P(EC)^k$ method (3.3.18) tends to preserve symplecticity exactly ([15]).

Denote $t_n = n \cdot h$, preservation of linear growth property (3.1.14) by applying the method (3.3.18) is proved.

Theorem 3.16. ([15]) Given initial data $x_0 = 1$, $y_0 = 0$, the numerical solution arising from the $P(EC)^k$ method with partitioned Euler-Maruyama and midpoint rule (3.3.18) for the stochastic oscillator (3.1.7)-(3.1.8) satisfies

$$\mathbb{E}((x_n^{(k)})^2 + (y_n^{(k)})^2) = 1 + \sigma^2 t_n - \sigma^2 t_n \frac{h^2}{4 + h^2} + t_n \cdot O(h^{k+1}). \tag{3.3.26}$$

Proof. The proof follows a direct calculation of $\mathbb{E}((x_n^{(k)})^2 + (y_n^{(k)})^2)$ basing on the scheme (3.3.18) and the relations (3.3.19)-(3.3.25). For details see [15]. \square Compare (3.3.26) with (3.3.13), it is found that as $h \to 0$ and k > 1, the leading error of the second moment of the numerical solution arising from the $P(EC)^k$ scheme tends to that from the midpoint rule.

The following theorem states the oscillation property of the numerical solution produced by the $P(EC)^k$ scheme (3.3.18) as k = 4l + 1 and k = 4l + 2 ($l \ge 0$).

Theorem 3.17. ([15]) The numerical solution $\{x_n^{(k)}\}_{n\geq 0}$ arising from the $P(EC)^k$ method with partitioned Euler-Maruyama and midpoint rule (3.3.18) for the oscillator system (3.1.7)-(3.1.8) with $x_0 = 1$, $y_0 = 0$ will switch signs infinitely many times as $n \to \infty$, almost surely, for k = 4l + 1 and k = 4l + 2 $(l \geq 0)$.

Proof. See [15].
$$\Box$$

Moreover, the mean-square order of convergence is checked for the method (3.3.18).

Theorem 3.18. ([15]) The $P(EC)^k$ method with partitioned Euler-Maruyama and midpoint rule (3.3.18) applied to the oscillator system (3.1.7)-(3.1.8) has mean-square order 1 for all $k \ge 1$.

Proof. The proof applies Theorem 3.12 to compare the method (3.3.18) with the Euler-Maruyama method, the mean-square order of which is known to be 1 for systems with additive noises. It is referred to [15] for more details.

Similar results about preservation of symplecticity, linear growth property of second moment, oscillation property of the solution of the oscillator system (3.1.7)-(3.1.8), and mean-square order of the $P(EC)^k$ method with forward Euler-Maruyama and midpoint rule are also given in [15].

Chapter 4

Variational Integrators with Noises

Up to now some symplectic numerical schemes have been discussed, most of which are of Runge-Kutta type and constructed mainly by properly adapting deterministic methods for stochastic Hamiltonian systems. We construct in this chapter variational integrators with noises which produce symplectic schemes based on a generalized action integral and generalized Hamilton's principle with noises, and can be seen as the stochastic analog of the deterministic variational integrators introduced in section 2.2.

4.1 Generalized Hamilton's Principle

The classic Hamilton's principle stated in Theorem 2.2 asserts that the Lagrange equation of motion (2.1.2) extremizes the action integral (2.1.8). The form of the action integral and that of the Lagrange equation in this principle, however, is only valid for conservative systems. In the presence of nonconservative forces, the formulation must be changed ([38],[42]).

Denote the nonconservative force with \mathbf{F} , the generalized action integral in presence of \mathbf{F} is ([34],[38])

$$\tilde{S} = \int_{t_0}^{t_1} (L - A)dt,$$
(4.1.1)

where L is the Lagrangian of the system under consideration, and A is the work done by the nonconservative force \mathbf{F} , and

$$A = -\mathbf{F} \cdot \mathbf{r},\tag{4.1.2}$$

where \mathbf{r} is the position vector with $\mathbf{r} = \mathbf{r}(q, t)$. Let δ denote a variation, then it holds ([34],[38])

$$\delta A = -\mathbf{F} \cdot \delta \mathbf{r} = -\mathbf{F} \cdot \frac{\partial \mathbf{r}}{\partial q} \delta q, \qquad (4.1.3)$$

since **F** is independent of q. Consequently, the variation of \tilde{S} is

$$\delta \tilde{S} = \int_{t_0}^{t_1} \left(\frac{\partial L}{\partial q} \delta q + \frac{\partial L}{\partial \dot{q}} \delta \dot{q} - \delta A \right) dt$$

$$= \left[\frac{\partial L}{\partial \dot{q}} \delta q \right]_{t_0}^{t_1} + \int_{t_0}^{t_1} \left[-\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}} \right) + \frac{\partial L}{\partial q} + \mathbf{F}^T \frac{\partial \mathbf{r}}{\partial q} \right] \delta q dt. \tag{4.1.4}$$

Since

$$\delta q(t_0) = \delta q(t_1) = 0,$$

it follows

$$\delta \tilde{S} = 0$$

$$\Leftrightarrow \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}} \right) = \frac{\partial L}{\partial q} + \mathbf{F}^T \frac{\partial \mathbf{r}}{\partial q}.$$
(4.1.5)

Equation (4.1.5) is the Lagrange equation of motion of nonconservative systems.

In the equation (4.1.5), the Lagrangian is considered as a function of (q, \dot{q}, t) . It is pointed out in [42] that the Lagrange equations of motion can also be formulated in the general variable set $\{p, q, \dot{p}, \dot{q}, t\}$, where the position vector \mathbf{r} may depend on p and q, i.e., $\mathbf{r} = \mathbf{r}(p, q, t)$. This is referred to as the redundancy property of the Lagrange equations of motion. In this case, the Lagrange equations of motion are

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}} \right) = \frac{\partial L}{\partial q} + \mathbf{F}^T \frac{\partial \mathbf{r}}{\partial q}, \tag{4.1.6}$$

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{p}} \right) = \frac{\partial L}{\partial p} + \mathbf{F}^T \frac{\partial \mathbf{r}}{\partial p}, \tag{4.1.7}$$

which may include linearly dependent equations due to the redundancy of the variable set $\{p, q, \dot{p}, \dot{q}, t\}$.

Based on the formulation (4.1.6)-(4.1.7), as well as a simple variational principle, it is derived in [42] that the general Hamilton's equation of motion in presence of nonconservative force \mathbf{F} is

$$\dot{p} = -\frac{\partial H}{\partial q}^{T} + \frac{\partial \mathbf{r}}{\partial q}^{T} \mathbf{F}, \tag{4.1.8}$$

$$\dot{q} = \frac{\partial H}{\partial p}^{T} - \frac{\partial \mathbf{r}}{\partial p}^{T} \mathbf{F}. \tag{4.1.9}$$

Consider a stochastic Hamiltonian system with one noise

$$dp = -\frac{\partial H}{\partial q}^{T} dt - \frac{\partial H_{1}}{\partial q}^{T} \circ dW(t), \qquad (4.1.10)$$

$$dq = \frac{\partial H}{\partial p}^{T} dt + \frac{\partial H_{1}}{\partial p}^{T} \circ dW(t). \tag{4.1.11}$$

As the Langevin's equation (1.1.2), we write

$$dW(t) = \xi(t)dt = \dot{W}dt \tag{4.1.12}$$

as explained in section 1.1. Thus the system (4.1.10)-(4.1.11) can be rewritten in the form

$$\dot{p} = -\frac{\partial H}{\partial q}^{T} - \frac{\partial H_{1}}{\partial q}^{T} \dot{W}, \qquad (4.1.13)$$

$$\dot{q} = \frac{\partial H}{\partial p}^{T} + \frac{\partial H_{1}}{\partial p}^{T} \dot{W}. \tag{4.1.14}$$

In Example 3.1, it is given that the Hamiltonian H for the linear stochastic oscillator (3.1.7)-(3.1.8) is not conserved, as stated in (3.1.15) that

$$\mathbb{E}(H) = \frac{1}{2}(1 + \sigma^2 t).$$

This indicates that a stochastic Hamiltonian system is not a Hamiltonian systems in classic sense which preserves H, but in certain generalized sense. In other words, it may be disturbed by certain nonconservative force. Other than classic nonconservative force \mathbf{F} which dissipates energy, this force may also add energy to the system, as shown by the linear growth of H with time t in (3.1.15). Here we call it a random force. A natural association for it is the white noise $\xi(t)$, since it is the resource of the random disturbance of the system. Moreover, it does not depend on position q, which gives the possibility of its belonging to nonconservative forces.

In fact, compare (4.1.13)-(4.1.14) with (4.1.8)-(4.1.9), we find that the association between \mathbf{F} and \dot{W} is reasonable. And so is that between \mathbf{r} and $-H_1$. Under these considerations, stochastic Hamiltonian system is a special kind of nonconservative system, in which \dot{W} functions as the nonconservative force.

Thus, formally, the 'work' done by \dot{W} should be

$$\bar{A} = H_1 \dot{W} \tag{4.1.15}$$

according to (4.1.2). In the sequel, we may form the following action integral based on (4.1.1) for the stochastic Hamiltonian system (4.1.13)-(4.1.14):

$$\bar{S} = \int_{t_0}^{t_1} (L - \bar{A}) dt$$

$$= \int_{t_0}^{t_1} L dt - \int_{t_0}^{t_1} H_1 \circ dW, \qquad (4.1.16)$$

where in the last equation we use again the relation $\dot{W}dt = dW$.

For a general system with r noises (3.1.1)-(3.1.4), (4.1.15) need to be modified to

$$\bar{A} = \sum_{k=1}^{r} H_k \dot{W}_k, \tag{4.1.17}$$

which is the sum of the 'work' done by each \dot{W}_k . Consequently,

$$\bar{S} = \int_{t_0}^{t_1} (L - \bar{A}) dt$$

$$= \int_{t_0}^{t_1} L dt - \sum_{k=1}^{r} \int_{t_0}^{t_1} H_k \circ dW_k. \tag{4.1.18}$$

We call it the generalized action integral with noises.

According to (4.1.6)-(4.1.7), the Lagrange equations of motion for the stochastic Hamiltonian system (4.1.13)-(4.1.14) have the form

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}} \right) = \frac{\partial L}{\partial q} - \frac{\partial H_1}{\partial q} \dot{W}, \tag{4.1.19}$$

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{p}} \right) = \frac{\partial L}{\partial p} - \frac{\partial H_1}{\partial p} \dot{W}, \tag{4.1.20}$$

which we call the generalized Lagrange equations of motion with noise. In case of r noises, these equations are

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}} \right) = \frac{\partial L}{\partial q} - \sum_{k=1}^{r} \frac{\partial H_k}{\partial q} \dot{W}_k, \tag{4.1.21}$$

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{p}} \right) = \frac{\partial L}{\partial p} - \sum_{k=1}^{r} \frac{\partial H_k}{\partial p} \dot{W}_k, \tag{4.1.22}$$

Lemma 4.1. If

$$\int_{a}^{b} \sum_{i=1}^{n} F_i(t)g_i(t)dt = 0$$

is valid for any function $g_i(t)$, and $g_i(t)$ (i = 1, ..., n) are independent to each other, then it holds $F_i(t) = 0$ almost everywhere on [a, b] for $1 \le i \le n$.

Proof. We prove by induction on n. As n=1, we have $\int_a^b F_1(t)g_1(t)dt=0$. Since $g_1(t)$ can take any function, we let $g_1(t)=F_1(t)$. This leads to

$$\int_a^b F_1(t)^2 dt = 0,$$

which implies that $F_1(t) = 0$ almost everywhere on [a, b] since $F_1(t)^2 \ge 0$. Suppose the assertion holds for $i \le k$. As i = k + 1, we have

$$\int_{a}^{b} \sum_{i=1}^{k+1} F_i(t)g_i(t)dt = \int_{a}^{b} \left(\sum_{i=1}^{k} F_i(t)g_i(t) + F_{k+1}(t)g_{k+1}(t)\right)dt = 0.$$
 (4.1.23)

Let $g_i(t) = F_i(t)$ for $1 \le i \le k$ and $g_{i+1}(t) = F_{i+1}(t)$, it follows

$$\int_{a}^{b} \left(\sum_{i=1}^{k} F_{i}^{2} + F_{k+1}^{2}\right) dt = 0.$$
(4.1.24)

If we take $g_{i+1}(t) = 2F_{i+1}(t)$, it holds

$$\int_{a}^{b} \left(\sum_{i=1}^{k} F_{i}^{2} + 2F_{k+1}^{2}\right) dt = 0.$$
(4.1.25)

(4.1.24)-(4.1.25) implies

$$\sum_{i=1}^{k} F_i^2 + F_{k+1}^2 = 0 \quad \text{and} \quad \sum_{i=1}^{k} F_i^2 + 2F_{k+1}^2 = 0$$
 (4.1.26)

almost everywhere on [a,b], from which $F_{k+1}(t) = 0$ holds almost everywhere on [a,b]. By relation (4.1.23) and the induction hypothesis, we have $F_i(t) = 0$ almost everywhere on [a,b] for $1 \le i \le k$.

Theorem 4.2 (Generalized Hamilton's Principle with Noises). The generalized Lagrange equations of motion with noises (4.1.21)-(4.1.22) extremize the generalized action integral with noises (4.1.18).

Proof. The variation of \bar{S} in (4.1.18) is

$$\delta \bar{S} = \int_{t_0}^{t_1} \left(\frac{\partial L}{\partial p} \delta p + \frac{\partial L}{\partial q} \delta q + \frac{\partial L}{\partial \dot{p}} \delta \dot{p} + \frac{\partial L}{\partial \dot{q}} \delta \dot{q} \right) dt$$

$$- \sum_{k=1}^{r} \int_{t_0}^{t_1} \left(\frac{\partial H_k}{\partial p} \delta p + \frac{\partial H_k}{\partial q} \delta q \right) \dot{W}_k dt$$

$$= \left[\frac{\partial L}{\partial \dot{p}} \delta p \right]_{t_0}^{t_1} + \left[\frac{\partial L}{\partial \dot{q}} \delta q \right]_{t_0}^{t_1} + \int_{t_0}^{t_1} \left(\frac{\partial L}{\partial p} - \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{p}} \right) - \sum_{k=1}^{r} \frac{\partial H_k}{\partial p} \dot{W}_k \right) \delta p dt$$

$$+ \int_{t_0}^{t_1} \left(\frac{\partial L}{\partial q} - \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}} \right) - \sum_{k=1}^{r} \frac{\partial H_k}{\partial q} \dot{W}_k \right) \delta q dt. \tag{4.1.27}$$

Thus, $\delta \bar{S} = 0$ is equivalent to

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}} \right) = \frac{\partial L}{\partial q} - \sum_{k=1}^{r} \frac{\partial H_k}{\partial q} \dot{W}_k,$$

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{p}} \right) = \frac{\partial L}{\partial p} - \sum_{k=1}^{r} \frac{\partial H_k}{\partial p} \dot{W}_k,$$

due to $\delta q(t_0) = \delta q(t_1) = \delta p(t_0) = \delta p(t_1) = 0$ and Lemma 4.1.

Example 4.1. For the linear stochastic oscillator (3.1.7)-(3.1.8), we have

$$L(y, x, \dot{y}, \dot{x}, t) = \frac{1}{2}(y^2 - x^2), \tag{4.1.28}$$

which is obtained through the relation (2.1.4) between Lagrangian and Hamiltonian, and the Hamiltonian $H = \frac{1}{2}(y^2 + x^2)$ of the system. Here y and x are counterparts of p and q in (2.1.4) respectively. We show that the equations (3.1.7)-(3.1.8) of the oscillator are equivalent to the generalized Lagrange equations of motion with noise (4.1.19)-(4.1.20). In fact, we regard $L(y, x, \dot{y}, \dot{x}, t)$ as coming from a variable transformation on the Lagrangian $L(x, \dot{x}, t)$, i.e.,

$$L(y, x, \dot{y}, \dot{x}, t) = L(x(y, x, \dot{y}, \dot{x}, t), \dot{x}(y, x, \dot{y}, \dot{x}, t), t), \tag{4.1.29}$$

where

$$x(y, x, \dot{y}, \dot{x}, t) = -\dot{y} + \sigma \dot{W}, \quad \dot{x}(y, x, \dot{y}, \dot{x}, t) = y.$$
 (4.1.30)

Thus the equation (4.1.19) is equivalent to

$$\frac{d}{dt}\left(\frac{\partial L}{\partial y}\right) = \frac{\partial L}{\partial x} + \sigma \dot{W},\tag{4.1.31}$$

since $H_1 = -\sigma x$. Substitute (4.1.28) into (4.1.31), we obtain

$$\dot{y} = -x + \sigma \dot{W},\tag{4.1.32}$$

which is equivalent to equation (3.1.7).

The equation (4.1.20) is

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{y}}\right) = \frac{\partial L}{\partial y}.\tag{4.1.33}$$

Note that

$$\frac{\partial L}{\partial \dot{y}} = \frac{\partial L}{\partial x} \frac{\partial x}{\partial \dot{y}} = -\frac{\partial L}{\partial x},\tag{4.1.34}$$

which is a consequence of (4.1.30). Substitute (4.1.34) to (4.1.33), we obtain that (4.1.20) is equivalent to

$$\dot{x} = y, \tag{4.1.35}$$

which is the equation (3.1.8) and the second equation in (4.1.30).

4.2 Variational Integrators with Noises

Based on the formulation of the generalized action integral with noises (4.1.18), and the generalized lagrange equations of motion with noises (4.1.21)-(4.1.22), variational integrators with noises for creating symplectic schemes for stochastic Hamiltonian systems can be constructed analogously to the way for deterministic variational integrators.

Consider the generalized action integral \bar{S} in (4.1.18) as a function of the two endpoints q_0 and q_1 :

$$q_0 = q(t_0), \qquad q_1 = q(t_1),$$

and find the derivatives of \bar{S} with respect to q_0 and q_1 .

$$\frac{\partial \bar{S}}{\partial q_0} = \int_{t_0}^{t_1} \left(\frac{\partial L}{\partial q} \frac{\partial q}{\partial q_0} + \frac{\partial L}{\partial \dot{q}} \frac{\partial \dot{q}}{\partial q_0} + \frac{\partial L}{\partial p} \frac{\partial p}{\partial q_0} + \frac{\partial L}{\partial \dot{p}} \frac{\partial \dot{p}}{\partial q_0} \right) dt$$

$$- \sum_{k=1}^{r} \int_{t_0}^{t_1} \left(\frac{\partial H_k}{\partial q} \frac{\partial q}{\partial q_0} + \frac{\partial H_k}{\partial p} \frac{\partial p}{\partial q_0} \right) \circ dW_k$$

$$= \left[\frac{\partial L}{\partial \dot{q}} \frac{\partial q}{\partial q_0} \right]_{t_0}^{t_1} + \int_{t_0}^{t_1} \left(\frac{\partial L}{\partial q} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}} - \sum_{k=1}^{r} \frac{\partial H_k}{\partial q} \dot{W}_k \right) \frac{\partial q}{\partial q_0} dt$$

$$+ \left[\frac{\partial L}{\partial \dot{p}} \frac{\partial p}{\partial q_0} \right]_{t_0}^{t_1} + \int_{t_0}^{t_1} \left(\frac{\partial L}{\partial p} - \frac{d}{dt} \frac{\partial L}{\partial \dot{p}} - \sum_{k=1}^{r} \frac{\partial H_k}{\partial p} \dot{W}_k \right) \frac{\partial p}{\partial q_0} dt$$

$$= -p_0^T, \tag{4.2.1}$$

where the last equality follows from the equations (4.1.21)-(4.1.22), as well as the relation $p = \frac{\partial L}{\partial \dot{q}}$.

In the same way we get

$$\frac{\partial \bar{S}}{\partial q_1} = p_1^T. \tag{4.2.2}$$

Thus, it holds

$$d\bar{S} = -p_0^T dq_0 + p_1^T dq_1. \tag{4.2.3}$$

Note that, the differentials are calculated basing on stochastic differentials in Stratonovich sense. Therefore the classic chain rule is valid.

Theorem 4.3. Suppose that the Lagrangian L and the functions H_k (k = 1, ..., r) in the generalized action integral with noises (4.1.18) are sufficiently smooth with respect to p and q. Then the mapping $(p_0, q_0) \mapsto (p_1, q_1)$ defined by equation (4.2.3) is symplectic.

Proof. From (4.2.3) it follows that

$$dp_1 \wedge dq_1 = d\left(\frac{\partial \bar{S}}{\partial q_1}\right) \wedge dq_1 = \frac{\partial^2 \bar{S}}{\partial q_1 \partial q_0} dq_0 \wedge dq_1,$$
 (4.2.4)

$$dp_0 \wedge dq_0 = d\left(-\frac{\partial \bar{S}}{\partial q_0}\right) \wedge dq_0 = \frac{\partial^2 \bar{S}}{\partial q_0 \partial q_1} dq_0 \wedge dq_1.$$
 (4.2.5)

Smoothness of L and H_k in \bar{S} ensures that $\frac{\partial^2 \bar{S}}{\partial q_1 \partial q_0} = \frac{\partial^2 \bar{S}}{\partial q_0 \partial q_1}$, which implies

$$dp_1 \wedge dq_1 = dp_0 \wedge dq_0. \tag{4.2.6}$$

Consider the discretized time interval $[t_n, t_{n+1}]$ as the time interval of a variational problem with noises, the length of which is h for all $n \ge 0$, and suppose

$$q(t_n) \approx q_n, \qquad q(t_{n+1}) \approx q_{n+1}. \tag{4.2.7}$$

Approximate the corresponding action integral with noises on it with \bar{L}_h , which is the analog of the deterministic discrete Lagrangian (2.2.18), and has the form

$$\bar{L}_h(q_n, q_{n+1}) \approx \int_{t_n}^{t_{n+1}} L dt - \sum_{k=1}^r \int_{t_n}^{t_{n+1}} H_k \circ dW_k. \tag{4.2.8}$$

We call it the discrete Lagrangian with noises. Form the following scheme according to relations (4.2.1) and (4.2.2):

$$p_n = -\frac{\partial \bar{L}_h}{\partial x}^T (q_n, q_{n+1}), \quad p_{n+1} = \frac{\partial \bar{L}_h}{\partial y}^T (q_n, q_{n+1}), \tag{4.2.9}$$

where $p_n \approx p(t_n)$, $p_{n+1} \approx p(t_{n+1})$, and ∂x , ∂y refer to derivatives with respect to the first and second variable respectively. Follow the same way as the proof of Theorem 4.3, it can be shown that the mapping $(p_n, q_n) \mapsto (p_{n+1}, q_{n+1})$ defined by (4.2.9) is symplectic. \bar{L}_h in (4.2.9) can be approximated by numerical integration of the integrals in its defi-

 \bar{L}_h in (4.2.9) can be approximated by numerical integration of the integrals in its definition (4.2.8), which includes also stochastic integrals, the approximation of which can follow ways discussed in section 1.2.

The methods discussed above for creating the symplectic mappings $(p_n, q_n) \mapsto (p_{n+1}, q_{n+1})$ are called variational integrators with noises.

Example 4.2. (4.1.28) gives the Lagrangian of the linear stochastic oscillator (3.1.7)-(3.1.8)

$$L = \frac{1}{2}(y^2 - x^2) = \frac{1}{2}(\dot{x}^2 - x^2).$$

Moreover,

$$H_1 = -\sigma x$$
.

Thus, the discrete Lagrangian with noise is

$$\bar{L}_h \approx \int_{t_n}^{t_{n+1}} L dt - \int_{t_n}^{t_{n+1}} H_1 \circ dW(t)$$
 (4.2.10)

$$= \frac{1}{2} \int_{t_n}^{t_{n+1}} (\dot{x}(t)^2 - x(t)^2) dt + \sigma \int_{t_n}^{t_{n+1}} x(t) \circ dW(t)$$
 (4.2.11)

$$\approx \frac{1}{2} \left[\frac{(x_{n+1} - x_n)^2}{h^2} h - \left(\frac{x_{n+1} + x_n}{2} \right)^2 h \right] + \sigma \frac{x_{n+1} + x_n}{2} \Delta W_n \qquad (4.2.12)$$

$$= -\frac{h}{8}(x_{n+1} + x_n)^2 + \frac{(x_{n+1} - x_n)^2}{2h} + \frac{\sigma}{2}(x_{n+1} + x_n)\Delta W_n, \tag{4.2.13}$$

where $\dot{x}(t)$ in (4.2.11) is approximated by $\frac{x_{n+1}-x_n}{h}$, and midpoint rule has been applied to the integrals in (4.2.11). Note that such an approximation is consistent with the definition (1.1.15) of a stochastic integral in Stratonovich sense.

In the sequel, we can construct the following scheme according to (4.2.9):

$$y_n = -\frac{\partial \bar{L}_h}{\partial x_n}(x_n, x_{n+1}) = \frac{x_{n+1} - x_n}{h} + \frac{h}{4}(x_{n+1} + x_n) - \frac{\sigma}{2}\Delta W_n, \qquad (4.2.14)$$

$$y_{n+1} = \frac{\partial \bar{L}_h}{\partial x_{n+1}}(x_n, x_{n+1}) = -\frac{h}{4}(x_{n+1} + x_n) + \frac{x_{n+1} - x_n}{h} + \frac{\sigma}{2}\Delta W_n, \quad (4.2.15)$$

which is equivalent to

$$\begin{pmatrix} 1 + \frac{h^2}{4} & 0 \\ 1 - \frac{h^2}{4} & -h \end{pmatrix} \begin{pmatrix} x_{n+1} \\ y_{n+1} \end{pmatrix} = \begin{pmatrix} 1 - \frac{h^2}{4} & h \\ 1 + \frac{h^2}{4} & 0 \end{pmatrix} \begin{pmatrix} x_n \\ y_n \end{pmatrix} + \begin{pmatrix} \frac{\sigma h}{2} \\ -\frac{\sigma h}{2} \end{pmatrix} \Delta W_n. \tag{4.2.16}$$

Thus

$$\begin{pmatrix} x_{n+1} \\ y_{n+1} \end{pmatrix} = \begin{pmatrix} \frac{4-h^2}{4+h^2} & \frac{4h}{4+h^2} \\ -\frac{4h}{4+h^2} & \frac{4-h^2}{4+h^2} \end{pmatrix} \begin{pmatrix} x_n \\ y_n \end{pmatrix} + \begin{pmatrix} \frac{2\sigma h}{4+h^2} \\ \frac{4\sigma}{4+h^2} \end{pmatrix} \Delta W_n, \tag{4.2.17}$$

which is the midpoint rule (3.3.10)-(3.3.11) for the linear stochastic oscillator (3.1.7)-(3.1.8).

Chapter 5

Generating Functions with One Noise

The existence of generating functions producing symplectic schemes for stochastic Hamiltonian systems is shown by Theorem 4.3, where the generating function is the generalized action integral with noises \bar{S} , which creates symplectic scheme according to relations (4.2.1)-(4.2.2). In fact, there are other generating functions which are based on different coordinates, as in deterministic case. In this chapter, generating functions \bar{S}^1 , \bar{S}^2 , and \bar{S}^3 are deduced, which are analogs of the deterministic S^1 , S^2 , and S^3 , respectively, and the Hamilton-Jacobi equations with noise which the generating functions satisfy are derived. Based on approximation of the solution of the Hamilton-Jacobi equations with noise, symplectic schemes are created by generating functions with noise, and required mean-square order of convergence of the generated schemes can be achieved in a simple way. The case of one noise is discussed in this chapter, and cases of two noises are considered in the next chapter.

5.1 Generating Functions \bar{S}^1 , \bar{S}^2 , and \bar{S}^3 with Noise

It is asserted in Theorem 4.3 that, the following scheme

$$p = -\frac{\partial \bar{S}^T}{\partial a}, \qquad P = \frac{\partial \bar{S}^T}{\partial Q}$$
 (5.1.1)

generated by \bar{S} defines a symplectic mapping $(p,q)\mapsto (P,Q)$. We call it a symplectic scheme.

Now we look for the generating function $\bar{S}^1(P,q)$ which is based on coordinates (P,q) instead of (q,Q). This can be achieved by a series of equivalent transformations on the relation

$$d\bar{S} = -pdq + PdQ, (5.1.2)$$

which is identical with (5.1.1). We have the following result.

Theorem 5.1. (5.1.2) is equivalent to

$$Q^{T}dP + p^{T}dq = d(P^{T}q + \bar{S}^{1}), \tag{5.1.3}$$

where $\bar{S}^1(P,q)$ satisfies

$$\bar{S}^1 = P^T(Q - q) - \bar{S}. \tag{5.1.4}$$

Proof. Substituting (5.1.4) into (5.1.3) yields

$$d(P^{T}q + \bar{S}^{1}) = d(P^{T}Q - \bar{S}) \tag{5.1.5}$$

$$= P^{T}dQ + Q^{T}dP + p^{T}dq - P^{T}dQ (5.1.6)$$

$$= Q^T dP + p^T dq, (5.1.7)$$

where (5.1.6) is obtained by using the relation (5.1.2), as well as the Stratonovich chain rule

$$d(P^TQ) = P^T dQ + Q^T dP, (5.1.8)$$

since the differentials concerned in our discussion are of Stratonovich sense. \Box Thus, (5.1.3) is an equivalent version of (5.1.2), but with coordinates (P,q). Consequently, the scheme

$$p = P + \frac{\partial \bar{S}^{1}}{\partial q}^{T}(P, q), \qquad Q = q + \frac{\partial \bar{S}^{1}}{\partial P}^{T}(P, q),$$
 (5.1.9)

which is generated from (5.1.3) by comparing coefficients of dP and dq on both sides of the equality sign, is equivalent to (5.1.1), and therefore symplectic. We call \bar{S}^1 generating function with noise of the first kind.

Analogously, for generating functions based on coordinates (p,Q) and $(\frac{P+p}{2},\frac{Q+q}{2})$, we have the following results.

Theorem 5.2. (5.1.2) is equivalent to

$$P^{T}dQ + q^{T}dp = d(p^{T}Q - \bar{S}^{2}), (5.1.10)$$

where $\bar{S}^2(p,Q)$ satisfies

$$\bar{S}^2 = p^T (Q - q) - \bar{S}. \tag{5.1.11}$$

(5.1.10) implies that the symplectic scheme generated by \bar{S}^2 is

$$P = p - \frac{\partial \bar{S}^2}{\partial Q}^T(p, Q), \qquad q = Q - \frac{\partial \bar{S}^2}{\partial p}^T(p, Q). \tag{5.1.12}$$

Theorem 5.3. (5.1.2) is equivalent to

$$(Q-q)^{T}d(P+p) - (P-p)^{T}d(Q+q) = 2d\bar{S}^{3}, (5.1.13)$$

where $\bar{S}^3(\frac{P+p}{2},\frac{Q+q}{2})$ satisfies

$$\bar{S}^3 = \frac{1}{2}(P+p)^T(Q-q) - \bar{S}.$$
 (5.1.14)

According to (5.1.13), The symplectic scheme produced by \bar{S}^3 is

$$P = p - \partial_2^T \bar{S}^3(\frac{P+p}{2}, \frac{Q+q}{2}), \tag{5.1.15}$$

$$Q = q + \partial_1^T \bar{S}^3(\frac{P+p}{2}, \frac{Q+q}{2}), \tag{5.1.16}$$

where ∂_1 and ∂_2 refers to partial derivative with respect to $u = \frac{P+p}{2}$ and $v = \frac{Q+q}{2}$ respectively.

The proofs of Theorem 5.2 and 5.3 are similar to that of Theorem 5.1, which is established by a straightforward calculation with applying the Stratonovich chain rule given in Theorem 1.4.

We call \bar{S}^2 and \bar{S}^3 the generating functions with noise of the second and third kind respectively. As \bar{S} or \bar{S}^i (i=1,2,3) equal zero, the mapping $(p,q) \mapsto (P,Q)$ created by them becomes the identity mapping.

It can be seen that the relations between \bar{S} and the three kinds of generating functions \bar{S}^i (i=1,2,3), as well as the symplectic schemes generated by the generating functions with noise, have the same forms as that of the deterministic generating functions. This fact is mainly due to the Stratonovich chain rule, and the equation (5.1.2) for generalized action integral with noise.

5.2 Hamilton-Jacobi Equations with Noise

 $\bar{S}(q,Q)$ generates a symplectic mapping $(p,q)\mapsto (P,Q)$ via (5.1.1). Now let P(t),Q(t) move on the phase trajectory of the stochastic Hamiltonian system (4.1.13)-(4.1.14) starting from the point (p,q). We want to find a generating function with noise, $\bar{S}(q,Q(t),t)$, depending on t, which generates the phase trajectory \bar{g}^t of the stochastic Hamiltonian system, since it is known that the phase trajectory is a symplectic transformation for any $t\geq 0$. We find that the approach in [12] of deriving S(q,Q(t),t) for deterministic Hamiltonian systems can be adapted to that of the stochastic $\bar{S}(q,Q(t),t)$, as given below. (5.1.1) implies that $\bar{S}(q,Q(t),t)$ should satisfy

$$P(t) = \frac{\partial \bar{S}}{\partial Q}^{T}(q, Q(t), t), \qquad p = -\frac{\partial \bar{S}}{\partial q}^{T}(q, Q(t), t). \tag{5.2.1}$$

Differentiating the second equation with respect to t gives

$$0 = \frac{\partial^2 \bar{S}}{\partial q \partial t}(q, Q(t), t) + \dot{Q}(t)^T \frac{\partial^2 \bar{S}}{\partial q \partial Q}(q, Q(t), t)$$

$$= \frac{\partial^2 \bar{S}}{\partial q \partial t}(q, Q(t), t) + \frac{\partial}{\partial P}(H(P(t), Q(t)) + H_1(P(t), Q(t))\dot{W})$$

$$= \frac{\partial}{\partial q}(\frac{\partial \bar{S}}{\partial Q}^T(q, Q(t), t))$$

$$= \frac{\partial^2 \bar{S}}{\partial q \partial t}(q, Q(t), t) + \frac{\partial}{\partial P}(H(P(t), Q(t)) + H_1(P(t), Q(t))\dot{W})$$

$$= \frac{\partial^2 \bar{S}}{\partial q \partial t}(q, Q(t), t)$$

$$= \frac{\partial^2 \bar{S}}{\partial q \partial t}(q, Q(t), t) + \frac{\partial}{\partial q}(H(P(t), Q(t)) + H_1(P(t), Q(t))\dot{W})(q, Q(t), t).$$

$$= \frac{\partial^2 \bar{S}}{\partial q \partial t}(q, Q(t), t) + \frac{\partial}{\partial q}(H(P(t), Q(t)) + H_1(P(t), Q(t))\dot{W})(q, Q(t), t).$$

$$= \frac{\partial^2 \bar{S}}{\partial q \partial t}(q, Q(t), t) + \frac{\partial}{\partial q}(H(P(t), Q(t)) + H_1(P(t), Q(t))\dot{W})(q, Q(t), t).$$

$$= \frac{\partial^2 \bar{S}}{\partial q \partial t}(q, Q(t), t) + \frac{\partial}{\partial q}(H(P(t), Q(t)) + H_1(P(t), Q(t))\dot{W})(q, Q(t), t).$$

$$= \frac{\partial^2 \bar{S}}{\partial q \partial t}(q, Q(t), t) + \frac{\partial}{\partial q}(H(P(t), Q(t)) + H_1(P(t), Q(t))\dot{W})(q, Q(t), t).$$

$$= \frac{\partial^2 \bar{S}}{\partial q \partial t}(q, Q(t), t) + \frac{\partial}{\partial q}(H(P(t), Q(t)) + H_1(P(t), Q(t))\dot{W})(q, Q(t), t).$$

$$= \frac{\partial^2 \bar{S}}{\partial q \partial t}(q, Q(t), t) + \frac{\partial}{\partial q}(H(P(t), Q(t)) + H_1(P(t), Q(t))\dot{W})(q, Q(t), t).$$

$$= \frac{\partial^2 \bar{S}}{\partial q \partial t}(q, Q(t), t) + \frac{\partial}{\partial q}(H(P(t), Q(t)) + H_1(P(t), Q(t))\dot{W})(q, Q(t), t).$$

$$= \frac{\partial^2 \bar{S}}{\partial q \partial t}(q, Q(t), t) + \frac{\partial}{\partial q}(H(P(t), Q(t)) + H_1(P(t), Q(t))\dot{W})(q, Q(t), t).$$

$$= \frac{\partial^2 \bar{S}}{\partial q \partial t}(q, Q(t), t) + \frac{\partial}{\partial q}(H(P(t), Q(t)) + H_1(P(t), Q(t))\dot{W})(q, Q(t), t).$$

$$= \frac{\partial^2 \bar{S}}{\partial q \partial t}(q, Q(t), t) + \frac{\partial}{\partial q}(H(P(t), Q(t)) + H_1(P(t), Q(t))\dot{W})(q, Q(t), t).$$

$$= \frac{\partial^2 \bar{S}}{\partial q \partial t}(q, Q(t), t) + \frac{\partial}{\partial q}(H(P(t), Q(t)) + H_1(P(t), Q(t))\dot{W})(q, Q(t), t).$$

$$= \frac{\partial^2 \bar{S}}{\partial q \partial t}(q, Q(t), t) + \frac{\partial}{\partial q}(H(P(t), Q(t)) + H_1(P(t), Q(t))\dot{W}(q, Q(t), t).$$

Thus

$$\frac{\partial}{\partial q} \left(\frac{\partial \bar{S}}{\partial t} + H(P(t), Q(t)) + H_1(P(t), Q(t)) \dot{W} \right) = 0, \tag{5.2.6}$$

where $P(t) = \frac{\partial \bar{S}}{\partial Q}^T(q, Q(t), t)$. In (5.2.3) we have used the relation (4.1.14), and in (5.2.4) the first equation of (5.2.1). We have the following result.

Theorem 5.4. If $\bar{S}(q,Q(t),t)$ satisfies the following partial differential equation

$$\frac{\partial \bar{S}}{\partial t} + H(\frac{\partial \bar{S}}{\partial Q}^T, Q) + H_1(\frac{\partial \bar{S}}{\partial Q}^T, Q) \dot{W} = 0, \tag{5.2.7}$$

and the matrix $\frac{\partial^2 \bar{S}}{\partial q \partial Q}$ is invertible almost surely, then the mapping $(p,q) \mapsto (P(t),Q(t))$ defined by (5.2.1) is the phase trajectory of the stochastic Hamiltonian system (4.1.13)-(4.1.14).

Proof. The invertibility of the matrix $\frac{\partial^2 \bar{S}}{\partial q \partial Q}$ ensures that P(t) and Q(t) are well-defined by (5.2.1). If \bar{S} satisfies the equation (5.2.7), then the relation (5.2.6) holds. According to the calculations from (5.2.3) to (5.2.6), which are equivalent transformations based on the first equation of (5.2.1), (5.2.3) must equal zero. On the other hand, (5.2.1) yields (5.2.2). The invertibility of $\frac{\partial^2 \bar{S}}{\partial q \partial Q}$ gives

$$\dot{Q}(t) = \frac{\partial H^{T}}{\partial P}(P(t), Q(t)) + \frac{\partial H_{1}^{T}}{\partial P}(P(t), Q(t))\dot{W}, \tag{5.2.8}$$

which is the second equation of the stochastic Hamiltonian system (4.1.13)-(4.1.14). Differentiate the first equation of (5.2.1) with respect to t, we obtain

$$\dot{P}(t) = \frac{\partial^2 \bar{S}}{\partial Q \partial t}^T (q, Q(t), t) + \frac{\partial^2 \bar{S}}{\partial Q^2} (q, Q(t), t) \dot{Q}(t). \tag{5.2.9}$$

On the other hand, differentiating the equation (5.2.7) with respect to Q yields

$$\frac{\partial^{2}\bar{S}}{\partial Q\partial t}^{T}(q,Q(t),t) = -\frac{\partial^{2}\bar{S}}{\partial Q^{2}}(q,Q(t),t)\frac{\partial H}{\partial P}^{T}(P(t),Q(t)) - \frac{\partial H}{\partial Q}^{T}(P(t),Q(t)) (5.2.10)$$

$$- (\frac{\partial^{2}\bar{S}}{\partial Q^{2}}(q,Q(t),t)\frac{\partial H_{1}}{\partial P}^{T}(P(t),Q(t)) + \frac{\partial H_{1}}{\partial Q}^{T}(P(t),Q(t)))\dot{W}.$$
(5.2.11)

Substituting (5.2.8) and (5.2.10)-(5.2.11) into (5.2.9) gives

$$\dot{P}(t) = -\frac{\partial H}{\partial Q}^{T}(P(t), Q(t)) - \frac{\partial H_{1}}{\partial Q}^{T}(P(t), Q(t))\dot{W}, \qquad (5.2.12)$$

which is the first equation of the stochastic Hamiltonian system (4.1.13)-(4.1.14).

Remark. We call (5.2.7) the Hamilton-Jacobi partial differential equation with noise. The Stratonovich chain rule plays a vital role to ensure the validity of the derivation.

The relation between \bar{S} and \bar{S}^1 (5.1.4) implies that

$$\bar{S}^{1}(P,q,t) = P^{T}(Q-q) - \bar{S}(q,Q,t). \tag{5.2.13}$$

Differentiating both sides of the equation (5.2.13) with respect to t yields

$$\frac{\partial \bar{S}^1}{\partial t} = P^T \frac{\partial Q}{\partial t} - \frac{\partial \bar{S}}{\partial t} - \frac{\partial \bar{S}}{\partial Q} \frac{\partial Q}{\partial t} = -\frac{\partial \bar{S}}{\partial t}, \tag{5.2.14}$$

where the second equality is due to $P = \frac{\partial \bar{S}}{\partial Q}^T$. Substitute this relation and (5.2.14) into (5.2.7), the following theorem is motivated.

Theorem 5.5. If $\bar{S}^1(P,q,t)$ satisfies the following partial differential equation

$$\frac{\partial \bar{S}^1}{\partial t} = H(P, Q) + H_1(P, Q)\dot{W}, \qquad \bar{S}^1(P, q, 0) = 0, \tag{5.2.15}$$

where $Q = q + \frac{\partial \bar{S}^1}{\partial P}^T(P,q,t)$, then the mapping $(p,q) \mapsto (P(t),Q(t))$ defined by (5.1.9) is the phase trajectory of the stochastic Hamiltonian system (4.1.13)-(4.1.14).

Proof. Differentiating the first equation of (5.1.9) with respect to t gives

$$(I + \frac{\partial^2 \bar{S}^1}{\partial P \partial q}(P, q, t))\dot{P} = -\frac{\partial^2 \bar{S}^1}{\partial q \partial t}^T(P, q, t). \tag{5.2.16}$$

From (5.2.15),

$$\frac{\partial^2 \bar{S}^1}{\partial q \partial t} = \left(\frac{\partial H}{\partial Q} + \frac{\partial H_1}{\partial Q} \dot{W}\right) \frac{\partial Q}{\partial q}.$$
 (5.2.17)

Differentiating the second equation with respect to q gives

$$\frac{\partial Q}{\partial q} = I + \frac{\partial^2 \bar{S}^1}{\partial q \partial P}.$$
 (5.2.18)

Substituting (5.2.18) and (5.2.17) into (5.2.16) yields

$$(I + \frac{\partial^2 \bar{S}^1}{\partial P \partial q}(P, q, t))\dot{P} = -(I + \frac{\partial^2 \bar{S}^1}{\partial P \partial q}(P, q, t))(\frac{\partial H}{\partial Q}^T(P, Q) + \frac{\partial H_1}{\partial Q}^T(P, Q)\dot{W}), \quad (5.2.19)$$

which results in the first equation of the stochastic Hamiltonian system (4.1.13)-(4.1.14). Differentiating the second equation of (5.1.9) with respect to t gives

$$\dot{Q} = \frac{\partial^2 \bar{S}^1}{\partial P^2} (P, q, t) \dot{P} + \frac{\partial^2 \bar{S}^1}{\partial P \partial t}^T (P, q, t). \tag{5.2.20}$$

It follows from (5.2.15) that

$$\frac{\partial^2 \bar{S}^1}{\partial P \partial t} = \frac{\partial H}{\partial P} + \frac{\partial H_1}{\partial P} \dot{W} + (\frac{\partial H}{\partial Q} + \frac{\partial H_1}{\partial Q} \dot{W}) \frac{\partial Q}{\partial P}.$$
 (5.2.21)

The second equation of (5.1.9) yields

$$\frac{\partial Q}{\partial P} = \frac{\partial^2 \bar{S}^1}{\partial P^2}. (5.2.22)$$

Substituting (5.2.22), (5.2.21) and (5.2.19) into (5.2.20) gives

$$\dot{Q} = \frac{\partial H}{\partial P}^{T}(P, Q) + \frac{\partial H_{1}}{\partial P}^{T}(P, Q)\dot{W}, \qquad (5.2.23)$$

which is the second equation of the stochastic Hamiltonian system (4.1.13)-(4.1.14). The initial condition in (5.2.15) ensures that at t=0, the mapping $(p,q)\mapsto (P(t),Q(t))$ defined by (5.1.9) is the identity mapping.

Denote $u = \frac{P+p}{2}$, $v = \frac{Q+q}{2}$, the Hamilton-Jacobi partial differential equation with noise for $\bar{S}^3(u, v, t)$ can be derived in the same way.

Theorem 5.6. If $\bar{S}^3(u,v,t)$ satisfies the following partial differential equation

$$\frac{\partial \bar{S}^3}{\partial t} = H(P,Q) + H_1(P,Q)\dot{W}, \qquad \bar{S}^3(u,v,0) = 0, \tag{5.2.24}$$

where $P=u-\frac{1}{2}\frac{\partial \bar{S}^3}{\partial v}^T(u,v,t),\ Q=v+\frac{1}{2}\frac{\partial \bar{S}^3}{\partial u}^T(u,v,t),\ then\ the\ mapping\ (p,q)\mapsto (P(t),Q(t))$ defined by (5.1.15)-(5.1.16) is the phase trajectory of the stochastic Hamiltonian system (4.1.13)-(4.1.14).

Proof. The proof follows from differentiations of (5.1.15)-(5.1.16), as that of the proof of Theorem 5.5.

5.3 Symplectic Methods Based on \bar{S}^1

Since the generating functions with noise satisfy Hamilton-Jacobi partial differential equations with noise, we expect to approximate the solutions of the Hamilton-Jacobi equations with noise, in order to obtain approximations of generating functions. Enlightened by the methods in deterministic case, we assume certain forms of the solutions and substitute them into the Hamilton-Jacobi equations with noise, and compare coefficients to determine unknown terms in the assumed forms.

For $\bar{S}^1(P,q,t)$ which satisfies the equation (5.2.15), we assume

$$\bar{S}^{1}(P,q,t) = F_{1}(P,q)W(t) + F_{2}(P,q)\int_{0}^{t} W(s) \circ dW(s) + G_{1}(P,q)t \qquad (5.3.1)$$

+
$$F_3(P,q) \int_0^t s \circ dW(s) + G_2(P,q) \int_0^t W(s) ds$$
 (5.3.2)

+
$$F_4(P,q) \int_0^t sW(s) \circ dW(s) + G_3(P,q) \int_0^t sds$$
 (5.3.3)

+
$$F_5(P,q) \int_0^t s^2 \circ dW(s) + G_4(P,q) \int_0^t sW(s)ds$$
 (5.3.4)

+
$$F_6(P,q) \int_0^t s^2 W(s) \circ dW(s) + G_5(P,q) \int_0^t s^2 ds$$
 (5.3.5)

+
$$F_7(P,q) \int_0^t s^3 \circ dW(s) + G_6(P,q) \int_0^t s^2 W(s) ds$$
 (5.3.6)

$$+ \cdots,$$
 $(5.3.7)$

by which the initial condition $\bar{S}^1(P,q,0)=0$ is satisfied, since W(0)=0 with probability 1.

Lemma 5.7. ([25]) For a stochastic differential equation system with r noises, suppose

$$I_{i_1,\dots,i_j}(h) = \int_t^{t+h} dW_{i_j}(\theta) \int_t^{\theta} dW_{i_{j-1}}(\theta_1) \int_t^{\theta_1} \dots \int_t^{\theta_{j-2}} dW_{i_1}(\theta_{j-1}), \tag{5.3.8}$$

where i_1, \ldots, i_j takes values from the set $\{0, 1, \ldots, r\}$, and $dW_0(\theta_k) = d\theta_k$. Then it holds

$$\left(\mathbb{E}(I_{i_1,\dots,i_j})^2\right)^{\frac{1}{2}} = O\left(h^{\sum_{k=1}^j \frac{2-i_k}{2}}\right),\tag{5.3.9}$$

where

$$\mathbf{1}_k = \begin{cases} 0, & i_k = 0, \\ 1, & i_k \neq 0. \end{cases}$$
 (5.3.10)

In other words, the order of smallness of the integral (5.3.8) is determined by $d\theta$ and $dW_k(\theta)$, k = 1, ..., r, where $d\theta$ contributes 1 to the order of smallness, and $dW_k(\theta)$ contributes $\frac{1}{2}$.

For example, the first term in (5.3.1) is of order of smallness $\frac{1}{2}$, and the second and third terms are of order 1. The two integrals in (5.3.2) are both of order $\frac{3}{2}$. In fact, from (5.3.2) to (5.3.6), the order of the integrals involved increases $\frac{1}{2}$ from each equation to the next. This is the reason why we construct \bar{S}^1 in such a manner.

Now substitute the assumption on $\bar{S}^1(P,q,t)$ into the Hamilton-Jacobi equation with noise (5.2.15). We have

$$\frac{\partial \bar{S}^{1}}{\partial t} = \left(G_{1} + G_{2}W + G_{3}t + G_{4}tW + G_{5}t^{2} + G_{6}t^{2}W + \ldots \right) + \left(F_{1} + F_{2}W + F_{3}t + F_{4}tW + F_{5}t^{2} + F_{6}t^{2}W + \ldots \right) \dot{W}.$$
(5.3.11)

Thus

$$H(P,Q) = G_1 + G_2W + G_3t + G_4tW + G_5t^2 + G_6t^2W + \dots,$$
 (5.3.12)

$$H_1(P,Q) = F_1 + F_2W + F_3t + F_4tW + F_5t^2 + F_6t^2W + \dots,$$
 (5.3.13)

Denote

$$a = \frac{\partial H}{\partial p}^{T}, \qquad b = \frac{\partial H_1}{\partial p}^{T},$$
 (5.3.14)

equation (4.1.11) is rewritten as

$$dq = adt + b \circ dW. \tag{5.3.15}$$

Expand H(P,Q) at the point (P,q) progressively according to equation (5.3.15), as the Wagner-Platen expansion does, but here we deal with Stratonovich integrals instead of

Itô ones. We have

$$\begin{split} H(P,Q) &= H(P,q) + \int_0^t H_q(P,q(s))a(P,q(s))ds + \int_0^t H_q(P,q(s))b(P,q(s)) \circ dW(s) \\ &= H(P,q) + H_q(P,q)a(P,q)t + H_q(P,q)b(P,q)W(t) + \int_0^t \int_0^s [H_{qq}(P,q(u)) \\ &= a(P,q(u)) + H_q(P,q(u))a_q(P,q(u))]a(P,q(u))duds + \int_0^t \int_0^s [H_{qq}(P,q(u)) \\ &= a(P,q(u)) + H_q(P,q(u))a_q(P,q(u))]b(P,q(u)) \circ dW(u)ds + \int_0^t \int_0^s [H_{qq}(P,q(u)) b(P,q(u)) + H_q(P,q(u))]a(P,q(u))]a(P,q(u))du \\ &= \int_0^t \int_0^s [H_{qq}(P,q(u)) b(P,q(u)) + H_q(P,q(u))b_q(P,q(u))]a(P,q(u))du \\ &= \circ dW(s) + \int_0^t \int_0^s [H_{qq}(P,q(u)) b(P,q(u)) + H_q(P,q(u))b_q(P,q(u))] \\ &= b(P,q(u)) \circ dW(u) \circ dW(s) \\ &= H(P,q) + H_q(P,q)a(P,q)t + H_q(P,q)b(P,q)W(t) + [H_{qq}(P,q)a(P,q) \\ &+ H_q(P,q)a_q(P,q)]a(P,q) + H_q(P,q)b(P,q) + H_q(P,q)a_q(P,q)]b(P,q) \\ &= \int_0^t W(s)ds + [H_{qq}(P,q)b(P,q) + H_q(P,q)b_q(P,q)]a(P,q) \int_0^t s \circ dW(s) \\ &+ [H_{qq}(P,q)b(P,q) + H_q(P,q)b_q(P,q)]b(P,q) \int_0^t W(s) \circ dW(s) \\ &+ \int_0^t \int_0^s \int_0^u \{[H_{qqq}(P,q(v))a(P,q(v)) + 2H_{qq}(P,q(v))a_q(P,q(v)) + H_q(P,q(v))a_q(P,q(v)) + H_q(P,q(v))a_q(P$$

$$+ \int_{0}^{t} \int_{0}^{s} \int_{0}^{u} \left\{ [H_{qqq}(P, q(v))b(P, q(v)) + 2H_{qq}(P, q(v))b_{q}(P, q(v)) + H_{q}(P, q(v))b_{q}(P, q(v)) + [H_{qq}(P, q(v))b(P, q(v)) + H_{q}(P, q(v))b_{q}(P, q(v))] a_{q}(P, q(v)) + [H_{qq}(P, q(v))b(P, q(v)) + dW(v)du \circ dW(s) + \int_{0}^{t} \int_{0}^{s} \int_{0}^{u} \left\{ [H_{qqq}(P, q(v))b(P, q(v)) + 2H_{qq}(P, q(v))b_{q}(P, q(v)) + H_{q}(P, q(v))b_{q}(P, q(v))] b(P, q(v)) + [H_{qq}(P, q(v))b(P, q(v)) + H_{q}(P, q(v))b_{q}(P, q(v))] b_{q}(P, q(v)) \right\} a(P, q(v))dv \circ dW(u) \circ dW(s) + \int_{0}^{t} \int_{0}^{s} \int_{0}^{u} \left\{ [H_{qqq}(P, q(v))b(P, q(v)) + 2H_{qq}(P, q(v))b_{q}(P, q(v)) + H_{q}(P, q(v))b_{q}(P, q(v))] b(P, q(v)) + [H_{qq}(P, q(v))b(P, q(v)) + H_{q}(P, q(v))b_{q}(P, q(v))] b(P, q(v)) + [H_{qq}(P, q(v))b(P, q(v)) + H_{q}(P, q(v))b_{q}(P, q(v))] b_{q}(P, q(v)) \right\} b(P, q(v)) \circ dW(v) \circ dW(u) \circ dW(s) = \cdots$$

$$(5.3.16)$$

Compare the expansion of H(P,Q) with the righthand side of equation (5.3.12), let coefficients of terms with same order of smallness be equal, we obtain

$$G_1 = H,$$
 (5.3.17)

$$G_2 = H_q b,$$
 (5.3.18)

$$G_3 = H_q a + \frac{1}{2} [H_{qq} b + H_q b_q] b, (5.3.19)$$

$$G_4 = [H_{qq}a + H_q a_q]b + [H_{qq}b + H_q b_q]a + [(H_{qqq}b + 2H_{qq}b_q + H_q b_{qq})b + (H_{qq}b + H_q b_q)b_q]b, \vdots$$

where the functions G_i (i = 1, 2, ...), a, b, H and derivatives of H are evaluated at (P, q).

Expand $H_1(P,Q)$ at (P,q) in the same way as H(P,Q), and compare its expansion with the righthand side of (5.3.13), we find the functions F_i (i = 1, 2, ...).

$$F_1 = H_1,$$
 (5.3.20)

$$F_2 = H_{1_q}b, (5.3.21)$$

$$F_3 = H_{1_q}a + \frac{1}{2}[H_{1_{qq}}b + H_{1_q}b_q]b, (5.3.22)$$

$$F_{4} = [H_{1_{qq}}a + H_{1_{q}}a_{q}]b + [H_{1_{qq}}b + H_{1_{q}}b_{q}]a + [(H_{1_{qqq}}b + 2H_{1_{qq}}b_{q} + H_{1_{q}}b_{qq})b + (H_{1_{qq}}b + H_{1_{q}}b_{q})b_{q}]b,$$

:

Thus, an approximation of $\bar{S}^1(P,q,t)$ can be constructed according to (5.3.1)-(5.3.7) by truncation to certain term. The higher order of smallness the terms involved in the truncated \bar{S}^1 have, the higher order has the resulted numerical method. Explicitly, the mean-square order of a method is determined in the following way.

Theorem 5.8. ([25]) A method of mean-square order m ($m \in \mathbb{Z}$) includes all integrals $I_{i_1,...,i_j}$ of order m and below. A method of mean-square order $m + \frac{1}{2}$ includes all

integrals of order $m + \frac{1}{2}$ and below, and also a deterministic integral of order m + 1.

Based on this theorem, we can truncate the assumption of \bar{S}^1 to a term with proper order of smallness to obtain required mean-square order of the method.

Example 5.1. For the linear stochastic oscillator (3.1.7)-(3.1.8)

$$dy = -xdt + \sigma dW, \quad y(0) = y_0,$$

$$dx = ydt, \quad x(0) = x_0,$$

we have

$$H = \frac{1}{2}(x^2 + y^2), \qquad H_1 = -\sigma x,$$

and $a=y,\,b=0.$ We truncate the assumption for \bar{S}^1 to the order of smallness 1:

$$\bar{S}^1(P,q,t) \approx F_1 W + F_2 \int_0^t W \circ dW + G_1 t.$$
 (5.3.23)

According to (5.3.17), (5.3.20) and (5.3.21), for the linear stochastic oscillator we have

$$F_1 = -\sigma x$$
, $F_2 = 0$, $G_1 = \frac{1}{2}(x^2 + y^2)$. (5.3.24)

Thus, for step size h,

$$\bar{S}^{1}(y_{n+1}, x_n, h) = \frac{h}{2}(x_n^2 + y_{n+1}^2) - \sigma x_n \Delta W_n.$$
 (5.3.25)

The scheme (5.1.9) generated by \bar{S}^1 gives

$$y_n = y_{n+1} + \frac{\partial \bar{S}^1}{\partial x_n}(y_{n+1}, x_n), \quad x_{n+1} = x_n + \frac{\partial \bar{S}^1}{\partial y_{n+1}}(y_{n+1}, x_n),$$
 (5.3.26)

which for (5.3.25) results in

$$x_{n+1} = x_n + hy_{n+1}, (5.3.27)$$

$$y_{n+1} = y_n - hx_n + \sigma \Delta W_n. ag{5.3.28}$$

This is the symplectic Euler-Maruyama method, and is the adjoint method of the partitioned Euler-Maruyama method (3.3.5)-(3.3.6).

Theorem 5.9. The numerical method (5.3.27)-(5.3.28) for the linear stochastic oscillator (3.1.7)-(3.1.8) is symplectic and of mean-square order 1.

Proof. Its symplecticity can be directly verified by checking $dx_{n+1} \wedge dy_{n+1} = dx_n \wedge dy_n$ on the scheme, and its mean-square order 1 is due to Theorem 5.8 and our way of truncation.

To obtain a method of order $\frac{3}{2}$, we need to truncate the assumption of \bar{S}^1 to

$$\bar{S}^1(P,q,t) \approx F_1 W + F_2 \int_0^t W \circ dW + G_1 t + F_3 \int_0^t s \circ dW + G_2 \int_0^t W ds + G_3 \int_0^t s ds.$$
 (5.3.29)

For the linear stochastic oscillator, (5.3.18), (5.3.19), and (5.3.22) give

$$F_3 = -\sigma y, \quad G_2 = 0, \quad G_3 = xy.$$
 (5.3.30)

Thus,

$$\bar{S}^{1}(y_{n+1}, x_n, h) = \frac{h}{2}(x_n^2 + y_{n+1}^2) - \sigma x_n \Delta W_n - \sigma y_{n+1} \int_0^h s \circ dW + y_{n+1} x_n \int_0^h s ds. \quad (5.3.31)$$

Substitute (5.3.31) to (5.3.26), we obtain the scheme

$$y_n = y_{n+1} + hx_n - \sigma \Delta W_n + \frac{h^2}{2} y_{n+1}, \qquad (5.3.32)$$

$$x_{n+1} = x_n + hy_{n+1} - \sigma \int_0^h s \circ dW + \frac{h^2}{2} x_n,$$
 (5.3.33)

which can also be written in the form

$$\begin{pmatrix} x_{n+1} \\ y_{n+1} \end{pmatrix} = \begin{pmatrix} \frac{4+h^4}{4+2h^2} & \frac{2h}{2+h^2} \\ -\frac{2h}{2+h^2} & \frac{2}{2+h^2} \end{pmatrix} \begin{pmatrix} x_n \\ y_n \end{pmatrix} + \begin{pmatrix} -\sigma \int_0^h s \circ dW + \frac{2h\sigma}{2+h^2} \Delta W_n \\ \frac{2\sigma}{2+h^2} \Delta W_n \end{pmatrix}.$$
(5.3.34)

Theorem 5.10. The numerical method (5.3.34) generated by \bar{S}^1 in (5.3.31) for the linear stochastic oscillator (3.1.7)-(3.1.8) is symplectic and of mean-square order $\frac{3}{2}$.

Proof. The mean-square order of convergence is guaranteed by Theorem 5.8 and our truncation (5.3.29) of \bar{S}^1 . We check the symplecticity of the scheme. According to (5.3.34),

$$dx_{n+1} \wedge dy_{n+1} = \left(\frac{4+h^4}{(2+h^2)^2} + \frac{4h^2}{(2+h^2)^2}\right) dx_n \wedge dy_n = dx_n \wedge dy_n.$$
 (5.3.35)

By using the scheme (5.3.34), the term $\int_0^h s \circ dW$ must be properly modeled. It is given in [25] that, $\int_0^h W ds$ is a sum of two independent normally distributed random variables:

$$\int_0^h W(s)ds = \frac{1}{2}hW(h) + \left(\int_0^h W(s)ds - \frac{1}{2}hW(h)\right),\tag{5.3.36}$$

where the first term on the righthand side of the equation is $\mathcal{N}(0, \frac{h^3}{4})$ distributed, and the other is $\mathcal{N}(0, \frac{h^3}{12})$ distributed. Thus we have

$$\int_{0}^{h} s \circ dW = hW(h) - \int_{0}^{h} W(s)ds = \frac{1}{2}hW(h) - \left(\int_{0}^{h} W(s)ds - \frac{1}{2}hW(h)\right)
= \sqrt{\frac{h^{3}}{4}}\xi_{1} - \sqrt{\frac{h^{3}}{12}}\xi_{2},$$
(5.3.37)

where ξ_1 and ξ_2 are two independent $\mathcal{N}(0,1)$ distributed random variables, and the first equality results from the Stratonovich chain rule.

In [25], explicit modeling of integrals of order $\frac{3}{2}$ such as the discussion above is given, and modeling of integrals of order 2 is also analyzed. Modeling of higher order of integrals is required by construction of higher order methods, and is still at the beginning of development.

Example 5.2. In this example, we consider the Kubo oscillator (3.1.16)-(3.1.17). Note that there is a constant a in (3.1.16)-(3.1.17), which is different from our assumption of function a in (5.3.14). To distinguish them, we denote in this example the function a and b in (5.3.14) with \tilde{a} and \tilde{b} respectively. For the Kubo oscillator,

$$H = \frac{a}{2}(p^2 + q^2), \quad H_1 = \frac{\sigma}{2}(p^2 + q^2), \quad \tilde{a} = ap, \quad \tilde{b} = \sigma p.$$
 (5.3.38)

According to (5.3.17)-(5.3.19),

$$G_1 = \frac{a}{2}(p^2 + q^2), \quad G_2 = a\sigma pq, \quad G_3 = a^2pq + \frac{1}{2}a\sigma^2p^2.$$
 (5.3.39)

(5.3.20)-(5.3.22) gives

$$F_1 = \frac{\sigma}{2}(p^2 + q^2), \quad F_2 = \sigma^2 pq, \quad F_3 = a\sigma pq + \frac{1}{2}\sigma^3 p^2.$$
 (5.3.40)

We first construct a method of mean-square order 1 by the following truncation of \bar{S}^1

$$\bar{S}^{1}(p_{n+1}, q_{n}, h) = F_{1}\Delta W_{n} + F_{2} \int_{0}^{h} W \circ dW + G_{1}h$$

$$= \frac{\sigma}{2}(p_{n+1}^{2} + q_{n}^{2})\Delta W_{n} + \frac{h}{2}\sigma^{2}p_{n+1}q_{n} + \frac{ah}{2}(p_{n+1}^{2} + q_{n}^{2}). \quad (5.3.41)$$

Substituting (5.3.41) into (5.1.9) gives

$$p_{n+1} = p_n - ahq_n - \frac{h}{2}\sigma^2 p_{n+1} - \sigma q_n \Delta W_n,$$
 (5.3.42)

$$q_{n+1} = q_n + ahp_{n+1} + \frac{h}{2}\sigma^2 q_n + \sigma p_{n+1}\Delta W_n, \qquad (5.3.43)$$

which is a scheme given by Milstein et. al. in [27] and [29]. Here we have reproduced it via generating function. Note that we have used

$$\int_{0}^{h} W \circ dW = \frac{W^{2}(h)}{2}, \quad \text{and} \quad \mathbb{E}(W^{2}(h)) = h$$
 (5.3.44)

to approximate $\int_0^h W \circ dW$ by $\frac{h}{2}$ in (5.3.41).

For a method of mean-square order $\frac{3}{2}$, we need the following truncation of \bar{S}^1 :

$$\bar{S}^{1}(p_{n+1}, q_{n}, h) = F_{1}\Delta W_{n} + F_{2} \int_{0}^{h} W \circ dW + G_{1}h + F_{3} \int_{0}^{h} s \circ dW + G_{2} \int_{0}^{h} W ds
+ G_{3} \int_{0}^{h} s ds
= \frac{\sigma}{2} (p_{n+1}^{2} + q_{n}^{2}) \Delta W_{n} + \frac{h}{2} \sigma^{2} p_{n+1} q_{n} + \frac{ah}{2} (p_{n+1}^{2} + q_{n}^{2})
+ (a\sigma p_{n+1}q_{n} + \frac{1}{2}\sigma^{3} p_{n+1}^{2}) \int_{0}^{h} s \circ dW + a\sigma p_{n+1}q_{n} \int_{0}^{h} W ds
+ \frac{h^{2}}{2} (a^{2} p_{n+1}q_{n} + \frac{1}{2}a\sigma^{2} p_{n+1}^{2}).$$
(5.3.45)

Applying (5.1.9) with \bar{S}^1 given in (5.3.45) yields

$$-(ah + \frac{h^2}{2}a\sigma^2 + \sigma\Delta W_n + \sigma^3 \int_0^h s \circ dW)p_{n+1} + q_{n+1} = \left(1 + \frac{h\sigma^2}{2} + \frac{h^2a^2}{2} + a\sigma h\Delta W_n\right)q_n,$$

$$\left(1 + \frac{h\sigma^2}{2} + \frac{h^2a^2}{2} + a\sigma h\Delta W_n\right)p_{n+1} = p_n - (ah + \sigma\Delta W_n)q_n.$$
(5.3.46)

Theorem 5.11. The numerical method (5.3.46) for the Kubo oscillator (3.1.16)-(3.1.17) is symplectic and of mean-square order $\frac{3}{2}$.

Proof. Since the truncation of \bar{S}^1 in (5.3.45) contains all integrals of order of smallness less than or equal to $\frac{3}{2}$, and a deterministic integral of order 2 in the assumption of \bar{S}^1 (5.3.1)-(5.3.7), Theorem 5.8 guarantees the mean-square order $\frac{3}{2}$ of the method. Symplecticity of the method (5.3.46) can be verified the same way as that for (5.3.34) in Theorem 5.10.

By modeling ΔW_n and $\int_0^h s \circ dW$, we use truncation (3.2.13) of the $\mathcal{N}(0,1)$ distributed random variables to ensure the realizability of the method, as introduced in section 3.2.

5.4 Symplectic Methods Based on \bar{S}^3

Methods based on \bar{S}^3 can be similarly constructed as that on \bar{S}^1 . Let

$$\bar{S}^{3}(u,v,t) = F_{1}(u,v)W(t) + F_{2}(u,v) \int_{0}^{t} W(s) \circ dW(s) + G_{1}(u,v)t \qquad (5.4.1)$$

$$+ F_{3}(u,v) \int_{0}^{t} s \circ dW(s) + G_{2}(u,v) \int_{0}^{t} W(s)ds \qquad (5.4.2)$$

+
$$F_4(u,v) \int_0^t sW(s) \circ dW(s) + G_3(u,v) \int_0^t sds$$
 (5.4.3)

+
$$F_5(u,v) \int_0^t s^2 \circ dW(s) + G_4(u,v) \int_0^t sW(s)ds$$
 (5.4.4)

+
$$F_6(u,v) \int_0^t s^2 W(s) \circ dW(s) + G_5(u,v) \int_0^t s^2 ds$$
 (5.4.5)

+
$$F_7(u,v) \int_0^t s^3 \circ dW(s) + G_6(u,v) \int_0^t s^2 W(s) ds$$
 (5.4.6)

$$+ \cdots, \qquad (5.4.7)$$

which satisfies the initial condition $\bar{S}^3(u, v, 0) = 0$ of the Hamilton-Jacobi equation with noise (5.2.24). Then we have

$$\frac{\partial \bar{S}^3}{\partial t} = \left(G_1 + G_2 W + G_3 t + G_4 t W + G_5 t^2 + G_6 t^2 W + \ldots \right)
+ \left(F_1 + F_2 W + F_3 t + F_4 t W + F_5 t^2 + F_6 t^2 W + \ldots \right) \dot{W},$$
(5.4.8)

where the functions G_i and F_i (i = 1, 2, ...) are evaluated at (u, v). Substituting (5.4.8) into (5.2.24) gives

$$H(P,Q) = G_1 + G_2W + G_3t + G_4tW + G_5t^2 + G_6t^2W + \dots,$$
 (5.4.9)

$$H_1(P,Q) = F_1 + F_2W + F_3t + F_4tW + F_5t^2 + F_6t^2W + \dots$$
 (5.4.10)

Rewrite the stochastic Hamiltonian system (4.1.10)-(4.1.11) in the form

$$dp = a_1 dt + b_1 \circ dW, \qquad dq = a_2 dt + b_2 \circ dW,$$
 (5.4.11)

where

$$a_1 = -\frac{\partial H}{\partial q}^T, \quad b_1 = -\frac{\partial H_1}{\partial q}^T,$$
 (5.4.12)

$$a_2 = \frac{\partial H}{\partial p}^T, \quad b_2 = \frac{\partial H_1}{\partial p}^T.$$
 (5.4.13)

Expand H(P,Q) at (u,v) according to (5.4.11), and let $t_0 = \frac{t}{2}$, we have

$$\begin{split} H(P,Q) &= H(u,v) + \int_{t_0}^t H_v(u,v(s))a_2(u,v(s))ds + \int_{t_0}^t H_v(u,v(s))b_2(u,v(s)) \circ dW(s) \\ &+ \int_{t_0}^t \left\{ H_u(u(s),v)a_1(u(s),v) + \int_{t_0}^t [H_{uv}(u(s),v(s))a_1(u(s),v(s)) \\ &+ H_u(u(s),v(s))a_{1_v}(u(s),v(s))]a_2(u(s),v(s))ds \\ &+ \int_{t_0}^t [H_{uv}(u(s),v(s))a_1(u(s),v(s)) \\ &+ H_u(u(s),v(s))a_{1_v}(u(s),v(s))]b_2(u(s),v(s)) \circ dW(s) \right\} ds \\ &+ \int_{t_0}^t \left\{ H_u(u(s),v)b_1(u(s),v) + \int_{t_0}^t [H_{uv}(u(s),v(s))b_1(u(s),v(s)) \\ &+ H_u(u(s),v(s))b_{1_v}(u(s),v(s))]a_2(u(s),v(s))ds \\ &+ \int_{t_0}^t [H_{uv}(u(s),v(s))b_1(u(s),v(s)) \\ &+ H_u(u(s),v(s))b_{1_v}(u(s),v(s))]b_2(u(s),v(s)) \circ dW(s) \right\} \circ dW(s) \\ &= H(u,v) + H_v(u,v)a_2(u,v)\frac{h}{2} + H_v(u,v)b_2(u,v)\frac{1}{\sqrt{2}}W(h) \\ &+ [H_{vv}(u,v)b_2(u,v) + H_vb_{2_v}(u,v)]b_2(u,v)\frac{h}{4} \\ &+ \frac{h}{2}(H_u(u,v)a_1(u,v)) + H_u(u,v)b_1(u,v)\frac{1}{\sqrt{2}}W(h) \\ &+ [H_{uu}(u,v)b_1(u,v) + H_u(u,v)b_{1_u}(u,v)]b_2(u,v)\frac{h}{4} \\ &+ [H_{uv}(u,v)b_1(u,v) + H_u(u,v)b_{1_v}(u,v)]b_2(u,v)\frac{h}{2} + R, \end{split}$$
 (5.4.14)

where the remainder term R contains all terms of order of smallness larger than or equal to $\frac{3}{2}$.

Compare the expansion (5.4.14) with the righthand side of equation (5.4.9), let coefficients of terms with the same order of smallness be equal, we obtain

$$G_{1} = H(u,v),$$

$$G_{2} = \frac{1}{\sqrt{2}}(H_{v}b_{2} + H_{u}b_{1}),$$

$$G_{3} = \frac{1}{2}\left[\frac{1}{2}(H_{vv}b_{2} + H_{v}b_{2v})b_{2} + \frac{1}{2}(H_{uu}b_{1} + H_{u}b_{1u})b_{1} + (H_{uv}b_{1} + H_{u}b_{1v})b_{2}\right],$$

$$\vdots$$

$$(5.4.15)$$

$$(5.4.15)$$

Similarly, expanding $H_1(P,Q)$ at (u,v) and comparing the expansion with the righthand

side of equation (5.4.10) gives

$$F_1 = H_1(u, v), (5.4.18)$$

$$F_2 = \frac{1}{\sqrt{2}}(H_{1v}b_2 + H_{1u}b_1) = 0, (5.4.19)$$

$$F_{3} = \frac{1}{2}[H_{1_{v}}a_{2} + H_{1_{u}}a_{1} + \frac{1}{2}(H_{1_{vv}}b_{2} + H_{1_{v}}b_{2_{v}})b_{2} + \frac{1}{2}(H_{1_{uu}}b_{1} + H_{1_{u}}b_{1_{u}})b_{1} + (H_{1_{uv}}b_{1} + H_{1_{u}}b_{1_{v}})b_{2}],$$

$$(5.4.20)$$

:

Substitute the functions G_i and F_i (i = 1, 2, ...) into the assumption of \bar{S}^3 in (5.4.1)-(5.4.7), and then apply the scheme (5.1.15)-(5.1.16), symplectic schemes for the stochastic Hamiltonian system (4.1.10)-(4.1.11) will be created.

Example 5.3. We construct symplectic methods for the linear stochastic oscillator (3.1.7)-(3.1.8) via \bar{S}^3 .

For a method of mean-square order 1, we need the truncation

$$\bar{S}^{3}(u, v, h) = F_{1} \Delta W_{n} + F_{2} \int_{0}^{h} W \circ dW + G_{1} h$$

$$= \frac{h}{2} (u^{2} + v^{2}) - \sigma v \Delta W_{n}. \qquad (5.4.21)$$

Substituting (5.4.21) into (5.1.15)-(5.1.16) yields

$$x_{n+1} = x_n + h \frac{y_n + y_{n+1}}{2}, (5.4.22)$$

$$y_{n+1} = y_n - h \frac{x_n + x_{n+1}}{2} + \sigma \Delta W_n, \qquad (5.4.23)$$

which is the midpoint rule (3.3.8)-(3.3.9).

A method of mean-square order $\frac{3}{2}$ can be obtained by the following truncation of \bar{S}^3 :

$$\bar{S}^{3}(u,v,h) = F_{1}\Delta W_{n} + F_{2} \int_{0}^{h} W \circ dW + G_{1}h + F_{3} \int_{0}^{h} s \circ dW + G_{2} \int_{0}^{h} W ds
+ G_{3} \int_{0}^{h} s ds
= \frac{h}{2}(u^{2} + v^{2}) - \sigma v \Delta W_{n} + \frac{h^{2}\sigma^{2}}{8} - \frac{\sigma u}{2} \int_{0}^{h} s \circ dW
+ \frac{\sigma u}{\sqrt{2}} \int_{0}^{h} W ds.$$
(5.4.24)

According to (5.1.15)-(5.1.16), the symplectic scheme generated by \bar{S}^3 is

$$x_{n+1} = x_n + h \frac{y_n + y_{n+1}}{2} - \frac{\sigma}{2} \int_0^h s \circ dW + \frac{\sigma}{\sqrt{2}} \int_0^h W ds,$$
 (5.4.25)

$$y_{n+1} = y_n - h \frac{x_n + x_{n+1}}{2} + \sigma \Delta W_n. (5.4.26)$$

Denote

$$m = -\frac{\sigma}{2} \int_0^h s \circ dW + \frac{\sigma}{\sqrt{2}} \int_0^h W ds, \qquad (5.4.27)$$

the scheme (5.4.25)-(5.4.26) can also be written as

$$\begin{pmatrix} x_{n+1} \\ y_{n+1} \end{pmatrix} = \begin{pmatrix} \frac{4-h^2}{4+h^2} & \frac{4h}{4+h^2} \\ -\frac{4h}{4+h^2} & \frac{4-h^2}{4+h^2} \end{pmatrix} \begin{pmatrix} x_n \\ y_n \end{pmatrix} + \frac{4}{4+h^2} \begin{pmatrix} m + \frac{\sigma h}{2} \Delta W_n \\ -\frac{h}{2} m + \sigma \Delta W_n \end{pmatrix}.$$
 (5.4.28)

Theorem 5.12. The numerical method (5.4.25)-(5.4.26) for the linear stochastic oscillator (3.1.7)-(3.1.8) is symplectic and of mean-square order $\frac{3}{2}$.

Proof. Its proof follows the same way as Theorem 5.10.

The analysis for (5.3.36) and (5.3.37) implies that we can model $\int_0^h W ds$ by

$$\int_{0}^{h} W ds = \sqrt{\frac{h^{3}}{4}} \xi_{1} + \sqrt{\frac{h^{3}}{12}} \xi_{2}, \tag{5.4.29}$$

where the $\mathcal{N}(0,1)$ distributed random variables ξ_1 and ξ_2 are identical with that in (5.3.37).

Example 5.4. Applying \bar{S}^3 to the Kubo oscillator (3.1.16)-(3.1.17) can reproduce a midpoint rule given by Milstein et. al. in [29]. In order to achieve it, let

$$\bar{S}^{3}(u,v,h) = F_{1}\Delta W_{n} + F_{2} \int_{0}^{h} W \circ dW + G_{1}h$$

$$= \frac{a}{2}(u^{2} + v^{2})h + \frac{\sigma}{2}(u^{2} + v^{2})\Delta W_{n}.$$
(5.4.30)

Substituting (5.4.30) into (5.1.15)-(5.1.16) gives the midpoint rule

$$p_{n+1} = p_n - ah \frac{q_n + q_{n+1}}{2} - \sigma \frac{q_n + q_{n+1}}{2} \Delta W_n, \qquad (5.4.31)$$

$$q_{n+1} = q_n + ah\frac{p_n + p_{n+1}}{2} + \sigma \frac{p_n + p_{n+1}}{2} \Delta W_n.$$
 (5.4.32)

According to our way of truncation on \bar{S}^3 , this method has mean-square order 1. A method of mean-square order $\frac{3}{2}$ can be constructed by assuming

$$\bar{S}^{3}(u,v,h) = F_{1}\Delta W_{n} + F_{2} \int_{0}^{h} W \circ dW + G_{1}h + F_{3} \int_{0}^{h} s \circ dW + G_{2} \int_{0}^{h} W ds
+ G_{3} \int_{0}^{h} s ds
= \frac{a}{2}(u^{2} + v^{2})h + \frac{\sigma}{2}(u^{2} + v^{2})\Delta W_{n} + \frac{a\sigma^{2}h^{2}}{8}(v^{2} - u^{2})
+ \frac{1}{4}\sigma^{3}(v^{2} - u^{2}) \int_{0}^{h} s \circ dW,$$
(5.4.33)

which gives by applying (5.1.15)-(5.1.16) the scheme

$$p_{n+1} = p_n - (ah + \sigma \Delta W_n + \frac{ah^2\sigma^2}{4} + \frac{\sigma^3}{2} \int_0^h s \circ dW) \frac{q_n + q_{n+1}}{2}, \quad (5.4.34)$$

$$q_{n+1} = q_n + (ah + \sigma \Delta W_n - \frac{ah^2\sigma^2}{4} - \frac{\sigma^3}{2} \int_0^h s \circ dW) \frac{p_n + p_{n+1}}{2}.$$
 (5.4.35)

Denote

$$k = ah + \sigma \Delta W_n + \frac{ah^2\sigma^2}{4} + \frac{\sigma^3}{2} \int_0^h s \circ dW,$$
 (5.4.36)

$$l = ah + \sigma \Delta W_n - \frac{ah^2\sigma^2}{4} - \frac{\sigma^3}{2} \int_0^h s \circ dW,$$
 (5.4.37)

the scheme (5.4.34)-(5.4.35) can also be written in the form

$$\begin{pmatrix} p_{n+1} \\ q_{n+1} \end{pmatrix} = \begin{pmatrix} \frac{4-kl}{4+kl} & \frac{-4k}{4+kl} \\ \frac{4l}{4+kl} & \frac{4-kl}{4+kl} \end{pmatrix} \begin{pmatrix} p_n \\ q_n \end{pmatrix}.$$
 (5.4.38)

Theorem 5.13. The numerical method (5.4.34)-(5.4.35) for the Kubo oscillator (3.1.16)-(3.1.17) is symplectic and of mean-square order $\frac{3}{2}$.

Proof. The construction of \bar{S}^3 and Theorem 5.8 implies the mean-square order $\frac{3}{2}$. Symplecticity of the scheme can be shown by checking $dp_{n+1} \wedge dq_{n+1} = dp_n \wedge dq_n$ as in Theorem 5.10.

Chapter 6

Generating Functions with Two Noises

In this chapter, generating functions for stochastic Hamiltonian systems with two noises are discussed. Hamilton-Jacobi partial differential equations with two noises are given, based on which generating functions with two noises are constructed through performing Wagner-Platen expansion in the sense of Stratonovich with respect to two noises. Symplectic schemes are created using the obtained generating functions for a model of synchrotron oscillations and a system with two additive noises. The methods of dealing with two noises in this chapter can be naturally generalized to systems with more noises.

6.1 \bar{S}^1 with Two Noises

(4.1.18) gives the generalized action integral \bar{S} with r noises. Results in (4.2.1)-(4.2.3) and Theorem 4.3 are also valid for systems with r noises. Therefore, for the stochastic Hamiltonian system with two noises

$$dp = -\frac{\partial H}{\partial q}^{T} dt - \frac{\partial H_{1}}{\partial q}^{T} \circ dW_{1} - \frac{\partial H_{2}}{\partial q}^{T} \circ dW_{2}, \tag{6.1.1}$$

$$dq = \frac{\partial H}{\partial p}^{T} dt + \frac{\partial H_{1}}{\partial p}^{T} \circ dW_{1} + \frac{\partial H_{2}}{\partial p}^{T} \circ dW_{2}, \tag{6.1.2}$$

we can obtain the following result about its action integral with noises \bar{S} , which is a generalization of Theorem 5.4.

Theorem 6.1. If $\bar{S}(q,Q(t),t)$ satisfies the following partial differential equation

$$\frac{\partial \bar{S}}{\partial t} + H(\frac{\partial \bar{S}}{\partial Q}^T, Q) + H_1(\frac{\partial \bar{S}}{\partial Q}^T, Q)\dot{W}_1 + H_2(\frac{\partial \bar{S}}{\partial Q}^T, Q)\dot{W}_2 = 0, \tag{6.1.3}$$

and the matrix $\frac{\partial^2 \bar{S}}{\partial q \partial Q}$ is invertible, then the mapping $(p,q) \mapsto (P(t),Q(t))$ defined by (5.2.1) is the phase trajectory of the stochastic Hamiltonian system (6.1.1)-(6.1.2).

Proof. The proof follows the same way as that of Theorem 5.4, with consideration of relation (6.1.1)-(6.1.2).

From the proof of Theorem 5.1, it is clear that the definition of the first kind of generating function \bar{S}^1 in (5.1.4), and the scheme generated by \bar{S}^1 (5.1.9) can both be used in case of more noises. Thus we have the following generalization of Theorem 5.5.

Theorem 6.2. If $\bar{S}^1(P,q,t)$ satisfies the following partial differential equation

$$\frac{\partial \bar{S}^1}{\partial t} = H(P,Q) + H_1(P,Q)\dot{W}_1 + H_2(P,Q)\dot{W}_2, \qquad \bar{S}^1(P,q,0) = 0, \tag{6.1.4}$$

where $Q = q + \frac{\partial \bar{S}^1}{\partial P}^T(P,q,t)$, then the mapping $(p,q) \mapsto (P(t),Q(t))$ defined by (5.1.9) is the phase trajectory of the stochastic Hamiltonian system (6.1.1)-(6.1.2).

Proof. It can be proved in the same way as Theorem 5.5. \Box

For the solution $\bar{S}^1(P,q,t)$ of (6.1.4), we make the following assumption.

$$\bar{S}^{1}(P,q,t) = F_{1}(P,q)W_{1}(t) + K_{1}(P,q)W_{2}(t)
+ F_{2}(P,q) \int_{0}^{t} W_{1} \circ dW_{1} + K_{2}(P,q) \int_{0}^{t} W_{2} \circ dW_{2}
+ G_{1}(P,q)t + \bar{F}_{2}(P,q) \int_{0}^{t} W_{2} \circ dW_{1} + \bar{K}_{2}(P,q) \int_{0}^{t} W_{1} \circ dW_{2} \quad (6.1.6)
+ G_{2}(P,q) \int_{0}^{t} W_{1}ds + \bar{G}_{2}(P,q) \int_{0}^{t} W_{2}ds
+ \tilde{F}_{2}(P,q) \int_{0}^{t} W_{1}W_{2} \circ dW_{1} + \tilde{K}_{2}(P,q) \int_{0}^{t} W_{1}W_{2} \circ dW_{2}
+ F_{3}(P,q) \int_{0}^{t} s \circ dW_{1} + K_{3}(P,q) \int_{0}^{t} s \circ dW_{2} \quad (6.1.7)
+ \tilde{G}_{2}(P,q) \int_{0}^{t} W_{1}W_{2}ds + G_{3}(P,q) \int_{0}^{t} sds
+ F_{4}(P,q) \int_{0}^{t} sW_{1} \circ dW_{1} + K_{4}(P,q) \int_{0}^{t} sW_{2} \circ dW_{2}
+ \tilde{F}_{4}(P,q) \int_{0}^{t} sW_{2} \circ dW_{1} + \tilde{K}_{4}(P,q) \int_{0}^{t} sW_{1} \circ dW_{2} \quad (6.1.8)
+ \cdots , \qquad (6.1.9)$$

where the terms in (6.1.5) are of order of smallness $\frac{1}{2}$, the following terms till (6.1.6) are of order 1, and the next terms till (6.1.7) are of order $\frac{3}{2}$, and so on.

Consequently, we have

$$\frac{\partial \bar{S}^{1}}{\partial t} = G_{1} + G_{2}W_{1} + \bar{G}_{2}W_{2} + \tilde{G}_{2}W_{1}W_{2} + G_{3}t + G_{4}tW_{1} + \bar{G}_{4}tW_{2}
+ \tilde{G}_{4}tW_{1}W_{2} + G_{5}t^{2} + G_{6}t^{2}W_{1} + \bar{G}_{6}t^{2}W_{2} + \dots
+ \dot{W}_{1}(F_{1} + F_{2}W_{1} + \bar{F}_{2}W_{2} + \tilde{F}_{2}W_{1}W_{2} + F_{3}t + F_{4}tW_{1} + \bar{F}_{4}tW_{2}
+ \tilde{F}_{4}tW_{1}W_{2} + F_{5}t^{2} + F_{6}t^{2}W_{1} + \dots)
+ \dot{W}_{2}(K_{1} + K_{2}W_{2} + \bar{K}_{2}W_{1} + \tilde{K}_{2}W_{1}W_{2} + K_{3}t + K_{4}tW_{2} + \bar{K}_{4}tW_{1}
+ \tilde{K}_{4}tW_{1}W_{2} + K_{5}t^{2} + K_{6}t^{2}W_{2} + \dots),$$
(6.1.10)

where the functions G_i , \bar{G}_i , \bar{G}_i , \bar{F}_i , \bar{F}_i , \bar{F}_i , \bar{K}_i , and \bar{K}_i (i = 1, 2, ...) are evaluated at (P, q). Compare (6.1.10) with the righthand side of (6.1.4), we have

$$H(P,Q) = G_1 + G_2W_1 + \bar{G}_2W_2 + \tilde{G}_2W_1W_2 + G_3t + G_4tW_1 + \bar{G}_4tW_2 + \tilde{G}_4tW_1W_2 + G_5t^2 + G_6t^2W_1 + \bar{G}_6t^2W_2 + \dots$$
(6.1.11)

$$H_1(P,Q) = F_1 + F_2W_1 + \bar{F}_2W_2 + \tilde{F}_2W_1W_2 + F_3t + F_4tW_1 + \bar{F}_4tW_2 + \tilde{F}_4tW_1W_2 + F_5t^2 + F_6t^2W_1 + \dots$$
(6.1.12)

$$H_2(P,Q) = K_1 + K_2W_2 + \bar{K}_2W_1 + \tilde{K}_2W_1W_2 + K_3t + K_4tW_2 + \bar{K}_4tW_1 + \tilde{K}_4tW_1W_2 + K_5t^2 + K_6t^2W_2 + \dots$$
(6.1.13)

For convenience, rewrite equation (6.1.1)-(6.1.2) in the form

$$dp = a_1 dt + b_1 \circ dW_1 + \tilde{b}_1 \circ dW_2, (6.1.14)$$

$$dq = a_2 dt + b_2 \circ dW_1 + \tilde{b}_2 \circ dW_2, (6.1.15)$$

where

$$a_1 = -\frac{\partial H}{\partial q}^T, \quad b_1 = -\frac{\partial H_1}{\partial q}^T, \quad \tilde{b}_1 = -\frac{\partial H_2}{\partial q}^T,$$
 (6.1.16)

$$a_2 = \frac{\partial H^T}{\partial p}, \qquad b_2 = \frac{\partial H_1^T}{\partial p}, \qquad \tilde{b}_2 = \frac{\partial H_2^T}{\partial p}.$$
 (6.1.17)

Expand H(P,Q) at (P,q) progressively based on (6.1.14)-(6.1.15), we have

$$\begin{split} H(P,Q) &= H(P,q) + \int_{0}^{t} H_{q}(P,q(s))a_{2}(P,q(s))ds + \int_{0}^{t} H_{q}(P,q(s))b_{2}(P,q(s)) \\ &\circ dW_{1}(s) + \int_{0}^{t} H_{q}(P,q(s))\tilde{b}_{2}(P,q(s)) \circ dW_{2}(s) \\ &= H(P,q) + \int_{0}^{t} \left\{ H_{q}(P,q)a_{2}(P,q) + \int_{0}^{s} [H_{qq}(P,q(u))a_{2}(P,q(u)) \\ &+ H_{q}(P,q(u))a_{2q}(P,q(u))]a_{2}(P,q(u))du + \int_{0}^{s} [H_{qq}(P,q(u))a_{2}(P,q(u)) \\ &+ H_{q}(P,q(u))a_{2q}(P,q(u))]b_{2}(P,q(u)) \circ dW_{1}(u) + \int_{0}^{s} [H_{qq}(P,q(u)) \\ &+ H_{q}(P,q(u))a_{2q}(P,q(u))]b_{2}(P,q(u)) \circ dW_{1}(u) + \int_{0}^{s} [H_{qq}(P,q(u)) \\ &+ u_{2}(P,q(u)) + H_{q}(P,q(u))a_{2q}(P,q(u))]\tilde{b}_{2}(P,q(u)) \circ dW_{2}(u) \right\} ds \\ &+ \int_{0}^{t} \left\{ H_{q}(P,q)b_{2}(P,q) + \int_{0}^{s} [H_{qq}(P,q(u))b_{2}(P,q(u)) \\ &+ H_{q}(P,q(u))b_{2q}(P,q(u))]a_{2}(P,q(u)) \circ dW_{1}(u) + \int_{0}^{s} [H_{qq}(P,q(u))b_{2}(P,q(u)) \\ &+ H_{q}(P,q(u))b_{2q}(P,q(u))]b_{2}(P,q(u)) \circ dW_{1}(u) + \int_{0}^{s} [H_{qq}(P,q(u)) \circ dW_{1}(s) \\ &+ \int_{0}^{t} \left\{ H_{q}(P,q)\tilde{b}_{2}(P,q) + \int_{0}^{s} [H_{qq}(P,q(u))\tilde{b}_{2}(P,q(u)) \circ dW_{2}(u) \right\} \circ dW_{1}(s) \\ &+ H_{q}(P,q(u))\tilde{b}_{2q}(P,q(u))]a_{2}(P,q(u)) du + \int_{0}^{s} [H_{qq}(P,q(u))\tilde{b}_{2}(P,q(u)) \\ &+ H_{q}(P,q(u))\tilde{b}_{2q}(P,q(u))]a_{2}(P,q(u)) \circ dW_{1}(u) + \int_{0}^{s} [H_{qq}(P,q(u))\tilde{b}_{2}(P,q(u)) \\ &+ H_{q}(P,q(u))\tilde{b}_{2q}(P,q(u))]b_{2}(P,q(u)) \circ dW_{1}(u) + \int_{0}^{s} [H_{qq}(P,q(u))\tilde{b}_{2}(P,q(u)) \\ &+ H_{q}(P,q(u))\tilde{b}_{2q}(P,q(u))]b_{2}(P,q(u)) \circ dW_{1}(u) + \int_{0}^{s} [H_{qq}(P,q(u))\tilde{b}_{2}(P,q(u)) \\ &+ H_{q}(P,q(u))\tilde{b}_{2q}(P,q(u))]b_{2}(P,q(u)) \circ dW_{1}(u) + \int_{0}^{s} [H_{qq}(P,q(u))\tilde{b}_{2}(P,q(u)) \\ &+ H_{q}(P,q)\tilde{b}_{2}(P,q) + H_{q}(P,q)b_{2q}(P,q)]\tilde{b}_{2}(P,q) H_{1}(t) + H_{q}(P,q)\tilde{b}_{2}(P,q) \\ &+ [H_{qq}(P,q)\tilde{b}_{2}(P,q) + H_{q}(P,q)\tilde{b}_{2q}(P,q)]\tilde{b}_{2}(P,q) \int_{0}^{t} W_{1}(s) \circ dW_{1}(s) \\ &+ [H_{qq}(P,q)\tilde{b}_{2}(P,q) + H_{q}(P,q)\tilde{b}_{2q}(P,q)]\tilde{b}_{2}(P,q) \int_{0}^{t} W_{2}(s) \circ dW_{2}(s) \\ &+ [H_{qq}(P,q)\tilde{b}_{2}(P,q) + H_{q}(P,q)\tilde{b}_{2q}(P,q)]\tilde{b}_{2}(P,q) \int_{0}^{t} W_{2}(s) \circ dW_{2}(s) \\ &+ R. \end{split}$$

where the remainder R is of order $\frac{3}{2}$ of smallness.

Compare the expansion (6.1.18) with the righthand side of equation (6.1.11), let coefficients of terms with the same order of smallness be equal, we get

$$G_{1} = H(P,q), \qquad (6.1.19)$$

$$G_{2} = H_{q}(P,q)b_{2}(P,q), \qquad (6.1.20)$$

$$\bar{G}_{2} = H_{q}(P,q)\tilde{b}_{2}(P,q), \qquad (6.1.21)$$

$$\tilde{G}_{2} = [H_{qq}(P,q)b_{2}(P,q) + H_{q}(P,q)b_{2q}(P,q)]\tilde{b}_{2}(P,q)$$

$$+ [H_{qq}(P,q)\tilde{b}_{2}(P,q) + H_{q}(P,q)\tilde{b}_{2q}(P,q)]b_{2}(P,q), \qquad (6.1.22)$$

$$G_{3} = H_{q}(P,q)a_{2}(P,q) + \frac{1}{2}[H_{qq}(P,q)b_{2}(P,q) + H_{q}(P,q)b_{2q}(P,q)]b_{2}(P,q)$$

$$+ \frac{1}{2}[H_{qq}(P,q)\tilde{b}_{2}(P,q) + H_{q}(P,q)\tilde{b}_{2q}(P,q)]\tilde{b}_{2}(P,q), \qquad (6.1.23)$$

:

The same approach applied to $H_1(P,Q)$ gives

$$F_{1} = H_{1}(P,q), \qquad (6.1.24)$$

$$F_{2} = H_{1_{q}}(P,q)b_{2}(P,q), \qquad (6.1.25)$$

$$\bar{F}_{2} = H_{1_{q}}(P,q)\tilde{b}_{2}(P,q), \qquad (6.1.26)$$

$$\tilde{F}_{2} = [H_{1_{qq}}(P,q)b_{2}(P,q) + H_{1_{q}}(P,q)b_{2_{q}}(P,q)]\tilde{b}_{2}(P,q)$$

$$+ [H_{1_{qq}}(P,q)\tilde{b}_{2}(P,q) + H_{1_{q}}(P,q)\tilde{b}_{2_{q}}(P,q)]b_{2}(P,q), \qquad (6.1.27)$$

$$F_{3} = H_{1_{q}}(P,q)a_{2}(P,q) + \frac{1}{2}[H_{1_{qq}}(P,q)b_{2}(P,q) + H_{1_{q}}(P,q)b_{2_{q}}(P,q)]b_{2}(P,q)$$

$$+ \frac{1}{2}[H_{1_{qq}}(P,q)\tilde{b}_{2}(P,q) + H_{1_{q}}(P,q)\tilde{b}_{2_{q}}(P,q)]\tilde{b}_{2}(P,q), \qquad (6.1.28)$$

$$F_{4} = (H_{1_{qq}}a_{2} + H_{1_{q}}a_{2_{q}})b_{2} + (H_{1_{qq}}b_{2} + H_{1_{q}}b_{2_{q}})a_{2}$$

$$+ [(H_{1_{qq}}a_{2} + H_{1_{q}}a_{2_{q}})\tilde{b}_{2} + (H_{1_{qq}}\tilde{b}_{2} + H_{1_{q}}\tilde{b}_{2_{q}})a_{2}$$

$$+ [(H_{1_{qq}}a_{2} + H_{1_{q}}a_{2_{q}})\tilde{b}_{2} + (H_{1_{qq}}\tilde{b}_{2} + H_{1_{q}}\tilde{b}_{2_{q}})a_{2}$$

$$+ [(H_{1_{qq}}a_{2} + H_{1_{q}}a_{2_{q}})\tilde{b}_{2} + (H_{1_{qq}}\tilde{b}_{2} + H_{1_{q}}\tilde{b}_{2_{q}})a_{2}$$

$$+ [(H_{1_{qq}}a_{2} + H_{1_{q}}a_{2_{q}})\tilde{b}_{2} + (H_{1_{qq}}\tilde{b}_{2} + H_{1_{q}}\tilde{b}_{2_{q}})\tilde{b}_{2_{q}}]\tilde{b}_{2}, \qquad (6.1.30)$$

:

Expansion of $H_2(P,Q)$ at (P,q) and the equation (6.1.13) yields

$$K_1 = H_2(P,q),$$
 (6.1.31)

$$K_2 = H_{2q}(P,q)b_2(P,q),$$
 (6.1.32)

$$\bar{K}_2 = H_{2q}(P,q)\tilde{b}_2(P,q),$$
(6.1.33)

$$\tilde{K}_{2} = [H_{2qq}(P,q)b_{2}(P,q) + H_{2q}(P,q)b_{2q}(P,q)]\tilde{b}_{2}(P,q)
+ [H_{2qq}(P,q)\tilde{b}_{2}(P,q) + H_{2q}(P,q)\tilde{b}_{2q}(P,q)]b_{2}(P,q),$$
(6.1.34)

$$K_{3} = H_{2q}(P,q)a_{2}(P,q) + \frac{1}{2}[H_{2qq}(P,q)b_{2}(P,q) + H_{2q}(P,q)b_{2q}(P,q)]b_{2}(P,q) + \frac{1}{2}[H_{2qq}(P,q)\tilde{b}_{2}(P,q) + H_{2q}(P,q)\tilde{b}_{2q}(P,q)]\tilde{b}_{2}(P,q),$$

$$(6.1.35)$$

$$K_{4} = (H_{2qq}a_{2} + H_{2q}a_{2q})\tilde{b}_{2} + (H_{2qq}\tilde{b}_{2} + H_{2q}\tilde{b}_{2q})a_{2} + [(H_{2qqq}\tilde{b}_{2} + 2H_{2qq}\tilde{b}_{2q} + H_{2q}\tilde{b}_{2qq})\tilde{b}_{2} + (H_{2qq}\tilde{b}_{2} + H_{2q}\tilde{b}_{2q})\tilde{b}_{2q}]\tilde{b}_{2},$$
(6.1.36)

$$\bar{K}_{4} = (H_{2qq}a_{2} + H_{2q}a_{2q})b_{2} + (H_{2qq}b_{2} + H_{2q}b_{2q})a_{2}
+ [(H_{2qqq}b_{2} + 2H_{2qq}b_{2q} + H_{2q}b_{2qq})b_{2} + (H_{2qq}b_{2} + H_{2q}b_{2q})b_{2q}]b_{2},$$
(6.1.37)

Example 6.1. As given in Example 3.3, for the model of synchrotron oscillations

$$dp = -\omega^2 \sin(q) dt - \sigma_1 \cos(q) \circ dW_1 - \sigma_2 \sin(q) \circ dW_2, \quad p(0) = p_0,$$

$$dq = pdt, \quad q(0) = q_0,$$

we have

$$H = -\omega^2 \cos(q) + \frac{p^2}{2}, \quad H_1 = \sigma_1 \sin(q), \quad H_2 = -\sigma_2 \cos(q).$$

Use the notations in (6.1.14)-(6.1.15), we have for this system

$$a_1 = -\omega^2 \sin(q), \quad b_1 = -\sigma_1 \cos(q), \quad \tilde{b}_1 = -\sigma_2 \sin(q),$$
 (6.1.38)

$$a_2 = p, \quad b_2 = \tilde{b}_2 = 0.$$
 (6.1.39)

According to (6.1.19)-(6.1.37), we obtain

$$G_1 = -\omega^2 \cos(q) + \frac{p^2}{2}, \quad F_1 = \sigma_1 \sin(q), \quad F_2 = \bar{F}_2 = 0,$$
 (6.1.40)

$$K_1 = -\sigma_2 \cos(q), \qquad K_2 = \bar{K}_2 = 0.$$
 (6.1.41)

Based on these functions, \bar{S}^1 for a method of mean-square order 1 can be constructed according to the assumption (6.1.5)-(6.1.9), as given below.

$$\bar{S}^{1}(p_{n+1}, q_n, h) = \left(-\omega^2 \cos(q_n) + \frac{p_{n+1}^2}{2}\right)h + \sigma_1 \sin(q_n)\Delta_n W_1 - \sigma_2 \cos(q_n)\Delta_n W_2. \quad (6.1.42)$$

Substitute (6.1.42) into (5.1.9), we obtain the following scheme,

$$p_{n+1} = p_n - h\omega^2 \sin(q_n) - \sigma_1 \cos(q_n) \Delta_n W_1 - \sigma_2 \sin(q_n) \Delta_n W_2,$$
 (6.1.43)

$$q_{n+1} = q_n + hp_{n+1}, (6.1.44)$$

77

which is the adjoint method of a method given by Milstein et. al. in [29].

Theorem 6.3. The method (6.1.43)-(6.1.44) for the stochastic Hamiltonian system (3.1.22)-(3.1.23) is symplectic and of mean-square order 1.

Proof. From the scheme (6.1.43)-(6.1.44), it follows

$$dp_{n+1} \wedge dq_{n+1} = (1 - \omega^2 \cos(q_n)h^2 + \sigma_1 \sin(q_n)h\Delta_n W_1 - \sigma_2 \cos(q_n)h\Delta_n W_2 + \omega^2 \cos(q_n)h^2 - \sigma_1 \sin(q_n)h\Delta_n W_1 + \sigma_2 \cos(q_n)h\Delta_n W_2)dp_n \wedge dq_n = dp_n \wedge dq_n.$$

$$(6.1.45)$$

Since our truncation of \bar{S}^1 contains all integrals with order of smallness less than or equal to 1 in the assumption (6.1.5)-(6.1.9), Theorem 5.8 ensures mean-square order 1 of the method (6.1.43)-(6.1.44).

For a method of mean-square order $\frac{3}{2}$, we need the following functions:

$$G_2 = \bar{G}_2 = \tilde{F}_2 = \tilde{K}_2 = 0, \quad F_3 = \sigma_1 p \cos(q),$$
 (6.1.46)

$$K_3 = \sigma_2 p \sin(q), \quad G_3 = \omega^2 p \sin(q).$$
 (6.1.47)

The corresponding \bar{S}^1 is

$$\bar{S}^{1}(p_{n+1}, q_{n}, h) = (-\omega^{2} \cos(q_{n}) + \frac{p_{n+1}^{2}}{2})h + \sigma_{1} \sin(q_{n})\Delta_{n}W_{1} - \sigma_{2} \cos(q_{n})\Delta_{n}W_{2}
+ \sigma_{1}p_{n+1}\cos(q_{n}) \int_{0}^{h} s \circ dW_{1}(s) + \sigma_{2}p_{n+1}\sin(q_{n}) \int_{0}^{h} s \circ dW_{2}(s)
+ \omega^{2}p_{n+1}\sin(q_{n})\frac{h^{2}}{2}.$$
(6.1.48)

The scheme generated by it according to (5.1.9) is

$$p_{n+1} = p_n - h\omega^2 \sin(q_n) - \frac{h^2}{2}\omega^2 p_{n+1}\cos(q_n) - \sigma_1 \cos(q_n)\Delta_n W_1$$

$$+ \sigma_1 p_{n+1}\sin(q_n) \int_0^h s \circ dW_1(s) - \sigma_2 \sin(q_n)\Delta_n W_2$$

$$- \sigma_2 p_{n+1}\cos(q_n) \int_0^h s \circ dW_2(s), \qquad (6.1.49)$$

$$q_{n+1} = q_n + hp_{n+1} + \frac{h^2}{2}\omega^2 \sin(q_n) + \sigma_1 \cos(q_n) \int_0^h s \circ dW_1(s)$$

$$+ \sigma_2 \sin(q_n) \int_0^h s \circ dW_2(s). \qquad (6.1.50)$$

Theorem 6.4. The method (6.1.49)-(6.1.50) for the stochastic Hamiltonian system (3.1.22)-(3.1.23) is symplectic and of mean-square order $\frac{3}{2}$.

Proof. $dp_{n+1} \wedge dq_{n+1} = dp_n \wedge dq_n$ can be directly checked on scheme (6.1.49)-(6.1.50).

The mean-square order $\frac{3}{2}$ results from the truncation of \bar{S}^1 and Theorem 5.8.

Example 6.2. It is studied in [28] that, for the system with two additive noises (3.1.27)-(3.1.28)

$$dp = -qdt + \gamma \circ dW_2(t), \quad p(0) = p_0,$$

$$dq = pdt + \sigma \circ dW_1(t), \quad q(0) = q_0,$$

the symplectic Euler-Maruyama method

$$p_{n+1} = p_n - hq_n + \gamma \Delta_n W_2, (6.1.51)$$

$$q_{n+1} = q_n + hp_{n+1} + \sigma \Delta_n W_1 \tag{6.1.52}$$

simulates the original system (3.1.27)-(3.1.28) accurately over long time intervals. We can reproduce this method via generating function \bar{S}^1 . As indicated by (3.1.32), for the system (3.1.27)-(3.1.28), we have

$$H = \frac{1}{2}(p^2 + q^2), \quad H_1 = \sigma p, \quad H_2 = -\gamma q,$$

and

$$F_1 = \sigma P, \quad K_1 = -\gamma q, \quad F_2 = 0, \quad K_2 = -\sigma \gamma,$$

 $G_1 = \frac{1}{2}(P^2 + q^2), \quad \bar{F}_2 = 0, \quad \bar{K}_2 = 0.$ (6.1.53)

Thus, for a method of mean-square order 1,

$$\bar{S}^{1}(p_{n+1}, q_n, h) = \sigma p_{n+1} \Delta_n W_1 - \gamma q_n \Delta_n W_2 - \frac{h}{2} \sigma \gamma + \frac{h}{2} (p_{n+1}^2 + q_n^2), \tag{6.1.54}$$

which generates the symplectic Euler-Maruyama scheme (6.1.51)-(6.1.52) via relation (5.1.9).

Give more terms to the truncated \bar{S}^1 , i.e., add terms in (6.1.5)-(6.1.9) with coefficients

$$G_2 = \sigma q, \quad \bar{G}_2 = 0, \quad \tilde{F}_2 = 0, \quad \tilde{K}_2 = 0,$$

 $F_3 = 0, \quad K_3 = -\gamma P, \quad G_3 = Pq + \frac{\sigma^2}{2}$ (6.1.55)

to \bar{S}^1 in (6.1.54), we get

$$\bar{S}^{1}(p_{n+1}, q_{n}, h) = \sigma p_{n+1} \Delta_{n} W_{1} - \gamma q_{n} \Delta_{n} W_{2} - \frac{h}{2} \sigma \gamma + \frac{h}{2} (p_{n+1}^{2} + q_{n}^{2})
+ \sigma q_{n} \int_{0}^{h} W_{1}(s) ds - \gamma p_{n+1} \int_{0}^{h} s \circ dW_{2}(s) + \frac{h^{2}}{2} p_{n+1} q_{n} + \frac{h^{2}}{4} \sigma^{2},$$
(6.1.56)

which gives via (5.1.9) the following scheme

$$p_{n+1} = p_n + \gamma \Delta_n W_2 - \sigma \int_0^h W_1(s) ds - q_n h - \frac{h^2}{2} p_{n+1}, \qquad (6.1.57)$$

$$q_{n+1} = q_n + \sigma \Delta_n W_1 - \gamma \int_0^h s \circ dW_2(s) + p_{n+1}h + \frac{h^2}{2}q_n. \tag{6.1.58}$$

Theorem 6.5. The numerical method (6.1.57)-(6.1.58) for the stochastic Hamiltonian system (3.1.27)-(3.1.28) is symplectic and of mean-square order $\frac{3}{2}$.

The proof follows the same way as that of Theorem 6.4.

6.2 \bar{S}^3 with Two Noises

The relation between \bar{S}^3 and \bar{S} (5.1.14), as well as the Hamilton-Jacobi partial differential equation with two noises (6.1.3) motivates the following theorem.

Theorem 6.6. If $\bar{S}^3(u,v,t)$ satisfies the following partial differential equation

$$\frac{\partial \bar{S}^3}{\partial t} = H(P,Q) + H_1(P,Q)\dot{W}_1 + H_2(P,Q)\dot{W}_2, \qquad \bar{S}^3(u,v,0) = 0, \tag{6.2.1}$$

where $P = u - \frac{1}{2} \frac{\partial \bar{S}^3}{\partial v}^T(u, v, t)$, $Q = v + \frac{1}{2} \frac{\partial \bar{S}^3}{\partial u}^T(u, v, t)$, then the mapping $(p, q) \mapsto (P(t), Q(t))$ defined by (5.1.15)-(5.1.16) is the phase trajectory of the stochastic Hamiltonian system (6.1.1)-(6.1.2).

Proof. The proof follows the same way as that of Theorem 5.6, with consideration of the equations with two noises (6.1.1)-(6.1.2).

Similar to the approach for \bar{S}^1 , we suppose

$$\bar{S}^{3}(u,v,t) = F_{1}(u,v)W_{1}(t) + K_{1}(u,v)W_{2}(t)
+ F_{2}(u,v) \int_{0}^{t} W_{1} \circ dW_{1} + K_{2}(u,v) \int_{0}^{t} W_{2} \circ dW_{2}
+ G_{1}(u,v)t + \bar{F}_{2}(u,v) \int_{0}^{t} W_{2} \circ dW_{1} + \bar{K}_{2}(u,v) \int_{0}^{t} W_{1} \circ dW_{2} \quad (6.2.3)
+ G_{2}(u,v) \int_{0}^{t} W_{1}ds + \bar{G}_{2}(u,v) \int_{0}^{t} W_{2}ds
+ \tilde{F}_{2}(u,v) \int_{0}^{t} W_{1}W_{2} \circ dW_{1} + \tilde{K}_{2}(u,v) \int_{0}^{t} W_{1}W_{2} \circ dW_{2}
+ F_{3}(u,v) \int_{0}^{t} s \circ dW_{1} + K_{3}(u,v) \int_{0}^{t} s \circ dW_{2} \quad (6.2.4)
+ \tilde{G}_{2}(u,v) \int_{0}^{t} W_{1}W_{2}ds + G_{3}(u,v) \int_{0}^{t} sds
+ F_{4}(u,v) \int_{0}^{t} sW_{1} \circ dW_{1} + K_{4}(u,v) \int_{0}^{t} sW_{2} \circ dW_{2}
+ \bar{F}_{4}(u,v) \int_{0}^{t} sW_{2} \circ dW_{1} + \bar{K}_{4}(u,v) \int_{0}^{t} sW_{1} \circ dW_{2} \quad (6.2.5)
+ \cdots \qquad (6.2.6)$$

Thus,

$$\frac{\partial \bar{S}^{3}}{\partial t} = G_{1} + G_{2}W_{1} + \bar{G}_{2}W_{2} + \tilde{G}_{2}W_{1}W_{2} + G_{3}t + G_{4}tW_{1} + \bar{G}_{4}tW_{2}
+ \tilde{G}_{4}tW_{1}W_{2} + G_{5}t^{2} + G_{6}t^{2}W_{1} + \bar{G}_{6}t^{2}W_{2} + \dots
+ \dot{W}_{1}(F_{1} + F_{2}W_{1} + \bar{F}_{2}W_{2} + \tilde{F}_{2}W_{1}W_{2} + F_{3}t + F_{4}tW_{1} + \bar{F}_{4}tW_{2}
+ \tilde{F}_{4}tW_{1}W_{2} + F_{5}t^{2} + F_{6}t^{2}W_{1} + \dots)
+ \dot{W}_{2}(K_{1} + K_{2}W_{2} + \bar{K}_{2}W_{1} + \tilde{K}_{2}W_{1}W_{2} + K_{3}t + K_{4}tW_{2} + \bar{K}_{4}tW_{1}
+ \tilde{K}_{4}tW_{1}W_{2} + K_{5}t^{2} + K_{6}t^{2}W_{2} + \dots),$$
(6.2.7)

where the functions G_i , \bar{G}_i , \bar{G}_i , \bar{F}_i , \bar{F}_i , \bar{F}_i , \bar{K}_i , and \bar{K}_i (i = 1, 2, ...) are evaluated at (u, v).

Compare (6.2.7) with the righthand side of (6.2.1), it is obtained that

$$H(P,Q) = G_1 + G_2W_1 + \bar{G}_2W_2 + \tilde{G}_2W_1W_2 + G_3t + G_4tW_1 + \bar{G}_4tW_2 + \tilde{G}_4tW_1W_2 + G_5t^2 + G_6t^2W_1 + \bar{G}_6t^2W_2 + \dots$$
(6.2.8)

$$H_1(P,Q) = F_1 + F_2W_1 + \bar{F}_2W_2 + \tilde{F}_2W_1W_2 + F_3t + F_4tW_1 + \bar{F}_4tW_2 + \tilde{F}_4tW_1W_2 + F_5t^2 + F_6t^2W_1 + \dots$$
(6.2.9)

$$H_2(P,Q) = K_1 + K_2W_2 + \bar{K}_2W_1 + \tilde{K}_2W_1W_2 + K_3t + K_4tW_2 + \bar{K}_4tW_1 + \tilde{K}_4tW_1W_2 + K_5t^2 + K_6t^2W_2 + \dots$$
(6.2.10)

Denote $t_0 = \frac{t}{2}$, and expand H(P,Q) at (u,v) based on (6.1.14)-(6.1.15), we have

$$\begin{split} H(P,Q) &= H(u,v) + \int_{t_0}^t H_q(u,q(s))a_2(u,q(s))ds + \int_{t_0}^t H_q(u,q(s))b_2(u,q(s)) \circ dW_1(s) \\ &+ \int_{t_0}^t H_q(u,q(s))\tilde{b}_2(u,q(s)) \circ dW_2(s) + \int_{t_0}^t \left\{ H_u(p(s),v)a_1(p(s),v) \right. \\ &+ \int_{t_0}^t \left[H_{uv}(p(s),q(s))a_1(p(s),q(s)) + H_u(p(s),q(s))a_{1_v}(p(s),q(s)) \right] a_2(p(s),q(s)) ds \\ &+ \int_{t_0}^t \left[H_{uv}(p(s),q(s))a_1(p(s),q(s)) \right. \\ &+ H_u(p(s),q(s))a_{1_v}(p(s),q(s)) \right] b_2(p(s),q(s)) \circ dW_1(s) \\ &+ \left. \int_{t_0}^t \left[H_{uv}(p(s),q(s))a_1(p(s),q(s)) \right] b_2(p(s),q(s)) \circ dW_2(s) \right\} ds \end{split}$$

$$\begin{split} &+\int_{t_0}^t \left\{ H_u(p(s),v)b_1(p(s),v) + \int_{t_0}^t [H_{uv}(p(s),q(s))b_1(p(s),q(s)) \\ &+ H_u(p(s),q(s))b_{1v}(p(s),q(s))]a_2(p(s),q(s))ds + \int_{t_0}^t [H_{uv}(p(s),q(s))b_1(p(s),q(s)) \\ &+ H_u(p(s),q(s))b_{1v}(p(s),q(s))]b_2(p(s),q(s)) \circ dW_1(s) \\ &+ \int_{t_0}^t [H_{uv}(p(s),q(s))b_1(p(s),q(s))] \bar{b}_2(p(s),q(s)) \circ dW_2(s) \right\} \circ dW_1(s) \\ &+ H_u(p(s),q(s))b_{1v}(p(s),q(s))] \bar{b}_2(p(s),q(s)) \circ dW_2(s) \right\} \circ dW_1(s) \\ &+ \int_{t_0}^t \left\{ H_u(p(s),v) \bar{b}_1(p(s),v) + \int_{t_0}^t [H_{uv}(p(s),q(s)) \bar{b}_1(p(s),q(s)) \\ &+ H_u(p(s),q(s)) \bar{b}_{1v}(p(s),q(s))] a_2(p(s),q(s)) ds + \int_{t_0}^t [H_{uv}(p(s),q(s)) \bar{b}_1(p(s),q(s)) \\ &+ H_u(p(s),q(s)) \bar{b}_{1v}(p(s),q(s))] b_2(p(s),q(s)) \circ dW_1(s) \\ &+ \int_{t_0}^t [H_{uv}(p(s),q(s)) \bar{b}_1(p(s),q(s))] \bar{b}_2(p(s),q(s)) \circ dW_2(s) \right\} \circ dW_2(s) \\ &= H(u,v) + \int_{t_0}^t \left\{ H_v(u,v)a_2(u,v) + \int_{t_0}^s [H_{vv}(u,q(l))a_2(u,q(l)) \\ &+ H_v(u,q(l))a_2(u,q(l))] b_2(u,q(l)) \circ dW_1(l) \\ &+ \int_{t_0}^s [H_{vv}(u,q(l))a_2(u,q(l))] b_2(u,q(l)) \circ dW_1(l) \\ &+ \int_{t_0}^s \left\{ H_v(u,v)b_2(u,v) + \int_{t_0}^s [H_{vv}(u,q(l))a_2(u,q(l)) \circ dW_2(l) \right\} ds \\ &+ \int_{t_0}^t \left\{ H_v(u,v)b_2(u,v) + \int_{t_0}^s [H_{vv}(u,q(l))b_2(u,q(l)) \circ dW_2(l) \right\} \circ dW_1(s) \\ &+ H_v(u,q(l))b_2(u,q(l))] b_2(u,q(l)) \circ dW_1(l) \\ &+ H_v(u,q(l))b_2(u,q(l))] b_2(u,q(l)) \circ dW_1(l) \\ &+ \int_{t_0}^s [H_{vv}(u,q(l))b_2(u,q(l)) + H_v(u,q(l))b_2(u,q(l)) \circ dW_2(l) \right\} \circ dW_1(s) \\ &+ \int_{t_0}^t \left\{ H_v(u,v) \bar{b}_2(u,v) + \int_{t_0}^s [H_{vv}(u,q(l))b_2(u,q(l)) \circ dW_2(l) \right\} \circ dW_1(s) \\ &+ \int_{t_0}^t \left\{ H_v(u,v) \bar{b}_2(u,v) + \int_{t_0}^s [H_{vv}(u,q(l))b_2(u,q(l)) + H_v(u,q(l))b_2(u,q(l)) + H_v(u,q(l))b_2(u,q(l)) + H_v(u,q(l))b_2(u,q(l)) + H_v(u,q(l))b_2(u,q(l)) + H_v(u,q(l))b_2(u,q(l)) + H_v(u,q(l))\bar{b}_2(u,q(l)) + H_v(u,q(l))\bar{b}_2$$

$$\begin{split} &+\int_{t_0}^t \left\{ H_u(v,v) a_1(u,v) + \int_{t_0}^s [H_{uu}(p(l),v) a_1(p(l),v) \\ &+ H_u(p(l),v) a_{1u}(p(l),v)] a_1(p(l),v) d \\ &+\int_{t_0}^s [H_{uu}(p(l),v) a_1(p(l),v) + H_u(p(l),v) a_{1u}(p(l),v)] b_1(p(l),v) \circ dW_1(l) \\ &+\int_{t_0}^s [H_{uu}(p(l),v) a_1(p(l),v) + H_u(p(l),v) a_{1u}(p(l),v)] \bar{b}_1(p(l),v) \circ dW_2(l) \right\} ds \\ &+\int_{t_0}^s \left\{ [H_{uv}(p(s),v) a_1(p(s),v) + H_u(p(s),v) a_{1v}(p(s),v)] a_2(p(s),v) \right. \\ &+ \left. \frac{t}{2} \int_{t_0}^t \left\{ [H_{uv}(p(s),v) a_1(p(s),v) + H_u(p(s),v) a_{1v}(p(s),q(l)) a_1(p(s),q(l)) \right. \\ &+ \left. \frac{t}{2} \int_{t_0}^t \left\{ [H_{uvv}(p(s),q(l)) a_1(p(s),q(l)) + 2H_{uv}(p(s),q(l)) a_1(p(s),q(l)) \right. \\ &+ \left. \frac{t}{2} \int_{t_0}^t \left\{ [H_{uvv}(p(s),q(l)) a_1(p(s),q(l)) + 2H_{uv}(p(s),q(l)) a_1(p(s),q(l)) \right. \\ &+ \left. \frac{t}{2} \int_{t_0}^t \left\{ [H_{uvv}(p(s),q(l)) a_1(p(s),q(l)) + 2H_{uv}(p(s),q(l)) a_1(p(s),q(l)) \right. \\ &+ \left. \frac{t}{2} \int_{t_0}^t \left\{ [H_{uvv}(p(s),q(l)) a_1(p(s),q(l)) + 2H_{uv}(p(s),q(l)) a_1(p(s),q(l)) \right. \\ &+ \left. \frac{t}{2} \int_{t_0}^t \left\{ [H_{uvv}(p(s),q(l)) a_1(p(s),q(l)) + 2H_{uv}(p(s),q(l)) a_1(p(s),q(l)) + H_u(p(s),q(l)) a_1(p(s),q(l)) \right. \\ &+ \left. \frac{t}{2} \int_{t_0}^t \left\{ [H_{uvv}(p(s),q(l)) a_1(p(s),q(l)) + 2H_{uv}(p(s),q(l)) a_1(p(s),q(l)) + H_u(p(s),q(l)) a_1(p(s),q(l)) \right. \\ &+ \left. \frac{t}{2} \int_{t_0}^t \left\{ [H_{uvv}(p(s),q(l)) a_1(p(s),q(l)) + 2H_{uv}(p(s),q(l)) a_1(p(s),q(l)) \right. \\ &+ \left. \frac{t}{2} \int_{t_0}^t \left\{ [H_{uvv}(p(s),q(l)) a_1(p(s),q(l)) + 2H_{uv}(p(s),q(l)) a_1(p(s),q(l)) \right. \\ &+ \left. \frac{t}{2} \int_{t_0}^t \left\{ [H_{uvv}(p(s),q(l)) a_1(p(s),q(l)) + 2H_{uv}(p(s),q(l)) a_1(p(s),q(l)) \right. \\ &+ \left. \frac{t}{2} \int_{t_0}^t \left\{ [H_{uvv}(p(s),q(l)) a_1(p(s),q(l)) + 2H_{uv}(p(s),q(l)) a_1(p(s),q(l)) \right. \\ &+ \left. \frac{t}{2} \int_{t_0}^t \left\{ [H_{uvv}(p(s),q(l)) a_1(p(s),q(l)) + 2H_{uv}(p(s),q(l)) a_1(p(s),q(l)) \right. \\ &+ \left. \frac{t}{2} \int_{t_0}^t \left\{ [H_{uvv}(p(s),q(l)) a_1(p(s),q(l)) + 2H_{uv}(p(s),q(l)) a_1(p(s),q(l)) \right. \\ &+ \left. \frac{t}{2} \int_{t_0}^t \left\{ [H_{uvv}(p(s),q(l)) a_1(p(s),q(l)) + 2H_{uv}(p(s),q(l)) a_1(p(s),q(l)) \right. \\ &+ \left. \frac{t}{2} \int_{t_0}^t \left\{ [H_{uvv}(p(s),q(l)) a_1(p(s),q(l)) + 2H_{uv}(p(s),q(l)) a_1(p(s),q(l)) \right. \\ &+ \left. \frac{t}{2} \int_{t_$$

$$\begin{array}{ll} &+ \ H_u(p(s),q(l))a_{1w}(p(s),q(l))]\tilde{b}_2(p(s),q(l)) + \ [H_{uv}(p(s),q(l))a_1(p(s),q(l))\\ &+ \ H_u(p(s),q(l))a_{1v}(p(s),q(l))]\tilde{b}_{2v}(p(s),q(l)) \right\} a_2(p(s),q(l))dl\\ &+ \ H_u(p(s),q(l))a_{1w}(p(s),q(l))a_1(p(s),q(l)) + 2H_{uv}(p(s),q(l))a_{1v}(p(s),q(l))\\ &+ \ H_u(p(s),q(l))a_{1w}(p(s),q(l))]\tilde{b}_2(p(s),q(l)) + [H_{uv}(p(s),q(l))a_1(p(s),q(l))\\ &+ \ H_u(p(s),q(l))a_{1v}(p(s),q(l))]\tilde{b}_2(p(s),q(l)) + [D_{uv}(p(s),q(l))a_1(p(s),q(l))\\ &+ \ H_u(p(l),v)b_{1u}(p(l),v) + \int_{t_0}^{s} [H_{uu}(p(l),v)b_1(p(l),v)]\tilde{b}_2(p(s),q(l)) + [U_{uv}(p(s),q(l))a_1(p(s),q(l))\\ &+ \ H_u(p(l),v)b_{1u}(p(l),v)]a_1(p(l),v)dl\\ &+ \ \int_{t_0}^{s} [H_{uu}(p(l),v)b_1(p(l),v) + H_u(p(l),v)b_{1u}(p(l),v)]\tilde{b}_1(p(l),v)\circ dW_1(l)\\ &+ \ \int_{t_0}^{s} [H_{uu}(p(l),v)b_1(p(l),v) + H_u(p(l),v)b_{1u}(p(l),v)]\tilde{b}_1(p(l),v)\circ dW_2(l)\\ &+ \ U_1(t) \int_{t_0}^{s} [H_{uu}(p(l),v)b_1(p(s),v) + H_u(p(l),v)b_{1u}(p(l),v)]\tilde{b}_1(p(l),v)\circ dW_2(l)\\ &+ \ W_1(t) \int_{t_0}^{s} [H_{uv}(p(s),q(l))b_1(p(s),q(l)) + 2H_{uv}(p(s),q(l))b_1(p(s),q(l))\\ &+ \ H_u(p(s),q(l))b_1(p(s),q(l)) + 2H_{uv}(p(s),q(l))b_1(p(s),q(l))\\ &+ \ H_u(p(s),q(l))b_1(p(s),q(l))]b_2(p(s),q(l)) + [H_{uv}(p(s),q(l))b_1(p(s),q(l))\\ &+$$

$$\begin{split} & + \ H_{u}(p(s),q(l))b_{1_{vv}}(p(s),q(l))[\tilde{b}_{2}(p(s),q(l)) + [H_{uv}(p(s),q(l))b_{1}(p(s),q(l))]\\ & + \ H_{u}(p(s),q(l))b_{1_{v}}(p(s),q(l))[\tilde{b}_{2},p(s),q(l))]\\ & + \ \int_{t_{0}}^{s} \left\{ [H_{uvv}(p(s),q(l))b_{1}(p(s),q(l)) + 2H_{uv}(p(s),q(l))b_{1_{v}}(p(s),q(l))\\ & + \ H_{u}(p(s),q(l))b_{1_{vv}}(p(s),q(l))[\tilde{b}_{2}(p(s),q(l)) + [H_{uv}(p(s),q(l))b_{1_{v}}(p(s),q(l))\\ & + \ H_{u}(p(s),q(l))b_{1_{v}}(p(s),q(l))[\tilde{b}_{2}(p(s),q(l))]\\ & + \ H_{u}(p(s),q(l))b_{1_{v}}(p(s),q(l))[\tilde{b}_{2}(p(s),q(l))]\\ & + \ H_{u}(p(s),q(l))b_{1_{v}}(p(s),q(l))[\tilde{b}_{2}(p(s),q(l))]\\ & + \ \int_{t_{0}}^{t} \left\{ H_{u}(u,v)\tilde{b}_{1}(u,v) + \int_{t_{0}}^{s} [H_{uu}(p(l),v)\tilde{b}_{1}(p(l),v)\\ & + \ H_{u}(p(l),v)\tilde{b}_{1_{u}}(p(l),v)]a_{1}(p(l),v)dl\\ & + \ \int_{t_{0}}^{s} [H_{uu}(p(l),v)\tilde{b}_{1}(p(l),v) + H_{u}(p(l),v)\tilde{b}_{1_{u}}(p(l),v)]b_{1}(p(l),v) \circ dW_{1}(l)\\ & + \ \int_{t_{0}}^{s} [H_{uu}(p(l),v)\tilde{b}_{1}(p(l),v) + H_{u}(p(l),v)\tilde{b}_{1_{u}}(p(l),v)]\tilde{b}_{1}(p(l),v) \circ dW_{2}(l)\\ & + \ \frac{W_{2}(t)}{\sqrt{2}} \int_{t_{0}}^{t} \left\{ [H_{uv}(p(s),v)\tilde{b}_{1}(p(s),v) + H_{u}(p(s),v)\tilde{b}_{1_{v}}(p(s),v)]b_{2}(p(s),v)\\ & + \ \frac{W_{2}(t)}{\sqrt{2}} \int_{t_{0}}^{t} \left\{ [H_{uv}(p(s),q(l))\tilde{b}_{1}(p(s),q(l)) + 2H_{uv}(p(s),q(l))\tilde{b}_{1_{v}}(p(s),q(l))\\ & + \ H_{u}(p(s),q(l))\tilde{b}_{1_{v}}(p(s),q(l))]b_{2}(p(s),q(l)) + [H_{uv}(p(s),q(l))\tilde{b}_{1_{v}}(p(s),q(l))\\ & + \ H_{u}(p(s),q(l))\tilde{b}_{1_{v}}(p(s),q(l))]b_{2}(p(s),q(l))\\ & + \ H_{u}(p(s),q(l))\tilde{b}_{1_{v}}(p(s),q(l))]b_{2}(p(s),q(l)) + [H_{uv}(p(s),q(l))\tilde{b}_{1_{v}}(p(s),q(l))\\ & + \ H_{u}(p(s),q(l))\tilde{b}_{1_{v}}(p(s),q(l))]b_{2}(p(s),q(l))\\ & + \ H_{u}(p(s),q(l))\tilde{b}_{1_{v}}(p(s),q(l))]\tilde{b}_{2}(p(s),q(l))\\ & + \ H_{u}(p(s),q(l))\tilde{b}_{1_{v}}(p(s),q($$

$$+ \ \, H_{u}(p(s),q(l))\tilde{b}_{1v}(p(s),q(l))]\tilde{b}_{2}(p(s),q(l)) + [H_{uv}(p(s),q(l))\tilde{b}_{1}(p(s),q(l)) \\ + \ \, H_{u}(p(s),q(l))\tilde{b}_{1v}(p(s),q(l))]\tilde{b}_{2v}(p(s),q(l)) \Big\} b_{2}(p(s),q(l)) \circ dW_{1}(l) \\ + \ \, \int_{t_{0}}^{s} \Big\{ [H_{uvv}(p(s),q(l))\tilde{b}_{1}(p(s),q(l))]\tilde{b}_{2}(p(s),q(l)) + 2H_{uv}(p(s),q(l))\tilde{b}_{1v}(p(s),q(l)) \\ + \ \, H_{u}(p(s),q(l))\tilde{b}_{1vv}(p(s),q(l))]\tilde{b}_{2}(p(s),q(l)) + [H_{uv}(p(s),q(l))\tilde{b}_{1}(p(s),q(l)) \\ + \ \, H_{u}(p(s),q(l))\tilde{b}_{1v}(p(s),q(l))]\tilde{b}_{2v}(p(s),q(l)) + [H_{uv}(p(s),q(l))\tilde{b}_{1v}(p(s),q(l)) \\ + \ \, H_{u}(p(s),q(l))\tilde{b}_{1v}(p(s),q(l)) \\ + \ \, H_$$

where R includes terms with order of smallness larger than or equal to $\frac{3}{2}$.

Compare the expansion (6.2.11) with the righthand side of equation (6.2.8), we have

$$G_{1} = H,$$

$$G_{2} = \frac{1}{\sqrt{2}}(H_{v}b_{2} + H_{u}b_{1}),$$

$$(6.2.12)$$

$$\bar{G}_{2} = \frac{1}{\sqrt{2}}(H_{v}\tilde{b}_{2} + H_{u}\tilde{b}_{1}),$$

$$(6.2.14)$$

$$\tilde{G}_{2} = \frac{1}{2}[b_{1}(H_{uu}\tilde{b}_{1} + H_{u}\tilde{b}_{1u}) + b_{2}(H_{vv}\tilde{b}_{2} + H_{v}\tilde{b}_{2v} + H_{uv}\tilde{b}_{1} + H_{u}\tilde{b}_{1v})$$

$$+ \tilde{b}_{1}(H_{uu}b_{1} + H_{u}b_{1u}) + \tilde{b}_{2}(H_{vv}b_{2} + H_{v}b_{2v} + H_{uv}b_{1} + H_{u}b_{1v})],$$

$$G_{3} = \frac{1}{2}[H_{v}a_{2} + H_{u}a_{1} + b_{1}(H_{uu}b_{1} + H_{u}b_{1u}) + b_{2}(H_{vv}b_{2} + H_{v}b_{2v} + H_{uv}\tilde{b}_{1} + H_{u}\tilde{b}_{1v})],$$

$$(6.2.14)$$

$$+ H_{uv}b_{1} + H_{u}b_{1u}) + \tilde{b}_{1}(H_{uu}b_{1} + H_{u}b_{1u}) + b_{2}(H_{vv}b_{2} + H_{v}b_{1v})],$$

:

Similarly, we get

$$F_1 = H_1,$$
 (6.2.16)

$$F_2 = \frac{1}{\sqrt{2}}(H_{1_v}b_2 + H_{1_u}b_1), \tag{6.2.17}$$

$$\bar{F}_2 = \frac{1}{\sqrt{2}} (H_{1_v} \tilde{b}_2 + H_{1_u} \tilde{b}_1),$$
(6.2.18)

$$\tilde{F}_{2} = \frac{1}{2} [b_{1}(H_{1_{uu}}\tilde{b}_{1} + H_{1_{u}}\tilde{b}_{1_{u}}) + b_{2}(H_{1_{vv}}\tilde{b}_{2} + H_{1_{v}}\tilde{b}_{2_{v}} + H_{1_{uv}}\tilde{b}_{1} + H_{1_{u}}\tilde{b}_{1_{v}})
+ \tilde{b}_{1}(H_{1_{uu}}b_{1} + H_{1_{u}}b_{1_{u}}) + \tilde{b}_{2}(H_{1_{vv}}b_{2} + H_{1_{v}}b_{2_{v}} + H_{1_{uv}}b_{1} + H_{1_{u}}b_{1_{v}})],$$
(6.2.19)

$$F_{3} = \frac{1}{2} [H_{1_{v}} a_{2} + H_{1_{u}} a_{1} + b_{1} (H_{1_{uu}} b_{1} + H_{1_{u}} b_{1_{u}}) + b_{2} (H_{1_{vv}} b_{2} + H_{1_{v}} b_{2_{v}}$$

$$+ H_{1_{uv}} b_{1} + H_{1_{u}} b_{1_{v}}) + \tilde{b}_{1} (H_{1_{uu}} \tilde{b}_{1} + H_{1_{u}} \tilde{b}_{1_{u}}) + \tilde{b}_{2} (H_{1_{vv}} \tilde{b}_{2} + H_{1_{v}} \tilde{b}_{2_{v}} + H_{1_{uv}} \tilde{b}_{1} + H_{1_{u}} \tilde{b}_{1_{v}})],$$

:

and

$$K_1 = H_2,$$
 (6.2.20)

$$K_2 = \frac{1}{\sqrt{2}}(H_{2v}b_2 + H_{2u}b_1), (6.2.21)$$

$$\bar{K}_2 = \frac{1}{\sqrt{2}} (H_{2v} \tilde{b}_2 + H_{2u} \tilde{b}_1), \tag{6.2.22}$$

$$\tilde{K}_{2} = \frac{1}{2} [b_{1}(H_{2uu}\tilde{b}_{1} + H_{2u}\tilde{b}_{1u}) + b_{2}(H_{2vv}\tilde{b}_{2} + H_{2v}\tilde{b}_{2v} + H_{2uv}\tilde{b}_{1} + H_{2u}\tilde{b}_{1v})
+ \tilde{b}_{1}(H_{2uu}b_{1} + H_{2u}b_{1u}) + \tilde{b}_{2}(H_{2vv}b_{2} + H_{2v}b_{2v} + H_{2uv}b_{1} + H_{2u}b_{1v})],$$
(6.2.23)

$$K_{3} = \frac{1}{2} [H_{2v}a_{2} + H_{2u}a_{1} + b_{1}(H_{2uu}b_{1} + H_{2u}b_{1u}) + b_{2}(H_{2vv}b_{2} + H_{2v}b_{2v} + H_{2u}b_{1v}) + \tilde{b}_{1}(H_{2uu}\tilde{b}_{1} + H_{2u}\tilde{b}_{1u}) + \tilde{b}_{2}(H_{2vv}\tilde{b}_{2} + H_{2v}\tilde{b}_{2v} + H_{2uv}\tilde{b}_{1} + H_{2u}\tilde{b}_{1v})],$$
:

Example 6.3. For the model of synchrotron oscillations (3.1.22)-(3.1.23),

$$G_1(u,v) = -\omega^2 \cos(v) + \frac{u^2}{2}, \quad F_1(u,v) = \sigma_1 \sin(v), \quad F_2(u,v) = \bar{F}_2(u,v) = 0,$$

$$(6.2.24)$$

$$K_1(u,v) = -\sigma_2 \cos(v), \qquad K_2(u,v) = \bar{K}_2(u,v) = 0.$$
 (6.2.25)

Let the truncation of \bar{S}^3 contain terms till order 1 of smallness in the assumption (6.2.2)-(6.2.6), i.e.,

$$\bar{S}^{3}(u,v,h) = F_{1}\Delta_{n}W_{1} + K_{1}\Delta_{n}W_{2} + F_{2}\int_{0}^{h}W_{1} \circ dW_{1} + K_{2}\int_{0}^{h}W_{2} \circ dW_{2}
+ \bar{F}_{2}\int_{0}^{h}W_{2} \circ dW_{1} + \bar{K}_{2}\int_{0}^{h}W_{1} \circ dW_{2}
= (-\omega^{2}\cos(v) + \frac{u^{2}}{2})h + \sigma_{1}\sin(v)\Delta_{n}W_{1} - \sigma_{2}\cos(v)\Delta_{n}W_{2}.$$
(6.2.26)

Substituting (6.2.26) into (5.1.15)-(5.1.16) results in the scheme

$$p_{n+1} = p_n - \sin(\frac{q_n + q_{n+1}}{2})(\omega^2 h + \sigma_2 \Delta_n W_2) - \cos(\frac{q_n + q_{n+1}}{2})\sigma_1 \Delta_n W_1, (6.2.27)$$

$$q_{n+1} = q_n + h \frac{p_n + p_{n+1}}{2}. \tag{6.2.28}$$

Theorem 6.7. The numerical method (6.2.27)-(6.2.28) for the stochastic Hamiltonian system (3.1.22)-(3.1.23) is symplectic and of mean-square order 1.

Proof. Apply the implicit function theorem, we can calculate in a straightforward way that

$$\begin{pmatrix}
\frac{\partial p_{n+1}}{\partial p_n} & \frac{\partial p_{n+1}}{\partial q_n} \\
\frac{\partial q_{n+1}}{\partial p_n} & \frac{\partial q_{n+1}}{\partial q_n}
\end{pmatrix}^T J \begin{pmatrix}
\frac{\partial p_{n+1}}{\partial p_n} & \frac{\partial p_{n+1}}{\partial q_n} \\
\frac{\partial q_{n+1}}{\partial p_n} & \frac{\partial q_{n+1}}{\partial q_n}
\end{pmatrix} = J,$$
(6.2.29)

where $J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$. This proves symplecticity of the method according to Definition 2.3.

The mean-square order 1 follows from our truncation of \bar{S}^3 .

Example 6.4. In this example, we construct numerical methods for the system with two additive noises (3.1.27)-(3.1.28) via $\bar{S}^3(u, v, h)$.

For (3.1.27)-(3.1.28),

$$H = \frac{1}{2}(u^{2} + v^{2}), \quad H_{1} = \sigma u, \quad H_{2} = -\gamma v,$$

$$F_{1} = \sigma u, \quad K_{1} = -\gamma v, \quad F_{2} = 0, \quad K_{2} = -\frac{\sigma \gamma}{\sqrt{2}},$$

$$G_{1} = \frac{1}{2}(u^{2} + v^{2}), \quad \bar{F}_{2} = \frac{\sigma \gamma}{\sqrt{2}}, \quad \bar{K}_{2} = 0.$$

$$(6.2.30)$$

Thus, \bar{S}^3 for a method of mean-square order 1 has the form

$$\bar{S}^{3}(u,v,h) = \sigma u \Delta_{n} W_{1} - \gamma v \Delta_{n} W_{2} - \frac{\sigma \gamma}{\sqrt{2}} \int_{0}^{h} W_{2}(s) \circ dW_{2}(s)$$

$$+ \frac{1}{2} (u^{2} + v^{2})h + \frac{\sigma \gamma}{\sqrt{2}} \int_{0}^{h} W_{2}(s) \circ dW_{1}(s), \qquad (6.2.31)$$

which gives via relation (5.1.15)-(5.1.16) the scheme

$$p_{n+1} + \frac{h}{2}q_{n+1} = p_n - \frac{h}{2}q_n + \gamma \Delta_n W_2,$$
 (6.2.32)

$$-\frac{h}{2}p_{n+1} + q_{n+1} = \frac{h}{2}p_n + q_n + \sigma\Delta_n W_1. \tag{6.2.33}$$

Theorem 6.8. The numerical method (6.2.32)-(6.2.33) for the stochastic Hamiltonian system (3.1.27)-(3.1.28) is symplectic and of mean-square order 1.

According to (6.2.2)-(6.2.6) and Theorem 5.8, for a method of mean-square order $\frac{3}{2}$, we need the following functions:

$$G_2 = \frac{\sigma v}{\sqrt{2}}, \quad \bar{G}_2 = \frac{\gamma u}{\sqrt{2}}, \quad \tilde{F}_2 = 0, \quad \tilde{K}_2 = 0,$$

$$F_3 = -\frac{\sigma v}{2}, \quad K_3 = -\frac{\gamma u}{2}, \quad G_3 = \frac{\sigma^2 + \gamma^2}{2}. \tag{6.2.34}$$

Thus, a method of mean-square order $\frac{3}{2}$ can be generated by

$$\bar{S}^{3}(u,v,h) = \sigma u \Delta_{n} W_{1} - \gamma v \Delta_{n} W_{2} - \frac{\sigma \gamma}{\sqrt{2}} \int_{0}^{h} W_{2}(s) \circ dW_{2}(s) + \frac{1}{2} (u^{2} + v^{2}) h
+ \frac{\sigma \gamma}{\sqrt{2}} \int_{0}^{h} W_{2}(s) \circ dW_{1}(s) + \frac{\sigma v}{\sqrt{2}} \int_{0}^{h} W_{1}(s) ds + \frac{\gamma u}{\sqrt{2}} \int_{0}^{h} \int_{0}^{h} W_{2}(s) ds
- \frac{\sigma v}{2} \int_{0}^{h} s \circ dW_{1} - \frac{\gamma u}{2} \int_{0}^{h} s \circ dW_{2} + \frac{h^{2}}{4} (\sigma^{2} + \gamma^{2})$$
(6.2.35)

via relation (5.1.15)-(5.1.16). The resulted scheme is

$$p_{n+1} + \frac{h}{2}q_{n+1} = p_n - \frac{h}{2}q_n + \gamma \Delta_n W_2 - \frac{\sigma}{\sqrt{2}} \int_0^h W_1(s) ds + \frac{\sigma}{2} \int_0^h s \circ dW_1(s),$$

$$-\frac{h}{2}p_{n+1} + q_{n+1} = \frac{h}{2}p_n + q_n + \sigma \Delta_n W_1 + \frac{\gamma}{\sqrt{2}} \int_0^h W_2(s) ds - \frac{\gamma}{2} \int_0^h s \circ dW_2(s).$$

$$(6.2.37)$$

Theorem 6.9. The numerical method (6.2.36)-(6.2.37) for the stochastic Hamiltonian system (3.1.27)-(3.1.28) is symplectic and of mean-square order $\frac{3}{2}$.

Remark. In the case of two noises, such terms

$$\int_0^h W_i \circ dW_j \tag{6.2.38}$$

may appear in the numerical schemes, as shown in the righthand side of the first equality of (6.2.26) when \bar{F}_2 or \bar{K}_2 does not vanish. Numerical simulation of multiple stochastic integrals is usually difficult, especially as the multiplicity increases. In [25], integrals of the form (6.2.38) in Itô sense are simulated. We modify the method and make it appropriate for Stratonovich integrals.

Divide the interval [0,h] into l subintervals with length $\frac{h}{l}$. Thus we write

$$\int_0^h W_i(s) \circ dW_j(s) \doteq \sum_{k=1}^l W_i(\frac{s_{k-1} + s_k}{2})(W_j(s_k) - W_j(s_{k-1}))$$
 (6.2.39)

according to the definition of Stratonovich integrals (1.1.15). Since each $\Delta_k W_i$ (k = 1, ..., l) is $\mathcal{N}(0, \frac{h}{l})$ distributed, and independent to each other, we can write

$$W_i(\frac{s_{k-1} + s_k}{2}) = \sqrt{\frac{h}{l}} \sum_{r=1}^{k-1} \xi_{ir} + \sqrt{\frac{h}{2l}} \xi_{ik},$$
 (6.2.40)

where ξ_{ir} (r = 1, ..., k-1) and ξ_{ik} are independent $\mathcal{N}(0, 1)$ distributed random variables. The second term on the righthand side of the equality is due to the length $\frac{h}{2l}$ of the half interval $[s_{k-1}, \frac{s_{k-1}+s_k}{2}]$. Similarly,

$$W_j(s_k) - W_j(s_{k-1}) = \sqrt{\frac{h}{l}} \xi_{jk},$$
 (6.2.41)

where ξ_{jk} is $\mathcal{N}(0,1)$ distributed and independent to ξ_{ir} $(k, r = 1, \ldots, l)$. Thus we have

$$\int_0^h W_i(s) \circ dW_j(s) \doteq \frac{h}{l} \sum_{k=1}^l \sum_{r=1}^{k-1} \xi_{ir} \xi_{jk} + \frac{h}{\sqrt{2}l} \sum_{k=1}^l \xi_{ik} \xi_{jk}. \tag{6.2.42}$$

Chapter 7

Generating Functions for Some Symplectic Methods

In this chapter, generating functions are derived for some stochastic symplectic methods proposed in literature (Milstein et al. [27], [28], [29]), and symplectic Runge-Kutta methods (3.7) in [28] for systems with additive noises are generalized to that for systems with general noises, for which three kinds of generating functions are also derived.

7.1 A Partitioned Runge-Kutta Method

Consider the partitioned Runge-Kutta method (4.9)-(4.10) in [29]

$$\mathcal{P}_{i} = p + h \sum_{j=1}^{s} \alpha_{ij} f(t + c_{j}h, \mathcal{Q}_{j}) + \sum_{j=1}^{s} \sum_{r=1}^{m} \sigma_{r}(t + d_{j}h, \mathcal{Q}_{j}) (\lambda_{ij}\varphi_{r} + \mu_{ij}\psi_{r}), (7.1.1)$$

$$Q_i = q + h \sum_{j=1}^s \hat{\alpha}_{ij} g(\mathcal{P}_j), \qquad i = 1, \dots, s$$

$$(7.1.2)$$

$$P = p + h \sum_{i=1}^{s} \beta_{i} f(t + c_{i}h, Q_{i}) + \sum_{i=1}^{s} \sum_{r=1}^{m} \sigma_{r}(t + d_{i}h, Q_{i})(\nu_{i}\varphi_{r} + \chi_{i}\psi_{r}), \quad (7.1.3)$$

$$Q = q + h \sum_{i=1}^{s} \hat{\beta}_{i} g(\mathcal{P}_{i}), \qquad (7.1.4)$$

where φ_r , ψ_r do not depend on p and q, the parameters α_{ij} , $\hat{\alpha}_{ij}$, β_i , $\hat{\beta}_i$, λ_{ij} , μ_{ij} , ν_i , χ_i satisfy the conditions

$$\beta_i \hat{\alpha}_{ij} + \hat{\beta}_j \alpha_{ji} - \beta_i \hat{\beta}_j = 0, \tag{7.1.5}$$

$$\nu_i \hat{\alpha}_{ij} + \hat{\beta}_j \lambda_{ji} - \nu_i \hat{\beta}_j = 0, \tag{7.1.6}$$

$$\chi_i \hat{\alpha}_{ij} + \hat{\beta}_j \mu_{ji} - \chi_i \hat{\beta}_j = 0, \tag{7.1.7}$$

 c_i , d_i are arbitrary parameters, and

$$f = -H_q, \quad g = H_p, \quad \sigma_r = -H_{r_q}, \quad H_{r_p} = 0.$$
 (7.1.8)

92CHAPTER 7. GENERATING FUNCTIONS FOR SOME SYMPLECTIC METHODS

Here is the separable case

$$H(t, p, q) = T(t, p) + U(t, q), \quad f = -U_q, \quad g = T_p,$$
 (7.1.9)
 $H_r(t, p, q) = U_r(t, q), \quad \sigma_r = -U_{r_q}.$ (7.1.10)

Theorem 7.1. Under the conditions (7.1.5)-(7.1.7), the partitioned Runge-Kutta method (7.1.1)-(7.1.4) for a separable Hamiltonian system with (7.1.8)-(7.1.10) can be written as (5.1.9) with

$$\bar{S}^{1}(P,q,h) = h \sum_{i=1}^{s} (\beta_{i}U(t+c_{i}h,\mathcal{Q}_{i}) + \hat{\beta}_{i}T(t+c_{i}h,\mathcal{P}_{i}))
+ \sum_{i=1}^{s} \sum_{r=1}^{m} U_{r}(t+c_{i}h,\mathcal{Q}_{i})(\nu_{i}\varphi_{i} + \chi_{i}\psi_{i}) + F,$$
(7.1.11)

where

$$F = -h^2 \sum_{ij} \beta_i \hat{\alpha}_{ij} U_q^T (t + c_i h, \mathcal{Q}_i) T_p (t + c_j h, \mathcal{P}_j)$$

$$- h \sum_{ij} \sum_{r=1}^m U_{r_q}^T (t + c_i h, \mathcal{Q}_i) T_p (t + c_j h, \mathcal{P}_j) (\nu_i \hat{\alpha}_{ij} \varphi_r + \chi_i \hat{\alpha}_{ij} \psi_r).$$
 (7.1.12)

Proof. Denote $U(t+c_ih, \mathcal{Q}_i) = U[i]$, $U_q(t+c_ih, \mathcal{Q}_i) = U_q[i]$, \cdots . It follows from (7.1.11)-(7.1.12) that

$$\frac{\partial \bar{S}^{1}}{\partial P} = h \sum_{i=1}^{s} \beta_{i} U_{q}[i]^{T} \left(h \sum_{j=1}^{s} \hat{\alpha}_{ij} \frac{\partial}{\partial P} T_{p}[j] \right)
+ h \sum_{i=1}^{s} \hat{\beta}_{i} T_{p}[i] \left(\frac{\partial p}{\partial P} + h \sum_{j=1}^{s} \alpha_{ij} \frac{\partial}{\partial P} (-U_{q}[j]) - \sum_{j=1}^{s} \sum_{r=1}^{m} \frac{\partial}{\partial P} U_{r_{q}}[j] (\lambda_{ij} \varphi_{r} + \mu_{ij} \psi_{r}) \right)
+ \sum_{i=1}^{s} \sum_{r=1}^{m} U_{r_{q}} \left(h \sum_{j=1}^{s} \alpha_{ij} \frac{\partial}{\partial P} T_{p}[j] \right) (\nu_{i} \varphi_{r} + \chi_{i} \psi_{r}) + \frac{\partial}{\partial P} F.$$
(7.1.13)

By

$$\frac{\partial p}{\partial P} = I + h \sum_{j=1}^{s} \beta_j \frac{\partial}{\partial P} U_q[j] + \sum_{j=1}^{s} \sum_{r=1}^{m} \frac{\partial}{\partial P} U_{r_q}[j] (\nu_j \varphi_r + \chi_j \psi_r), \tag{7.1.14}$$

$$\frac{\partial \bar{S}^{1}}{\partial P} = h \sum_{i=1}^{s} \hat{\beta}_{i} T_{p}[i] + h^{2} \sum_{ij} \beta_{i} \hat{\alpha}_{ij} U_{q}[i]^{T} \frac{\partial}{\partial P} T_{p}[j]
+ h^{2} \sum_{ij} \hat{\beta}_{i} \beta_{j} T_{p}[i]^{T} \frac{\partial}{\partial P} U_{q}[j] - h^{2} \sum_{ij} \hat{\beta}_{i} \alpha_{ij} T_{p}[i]^{T} \frac{\partial}{\partial P} U_{q}[j]
+ h \sum_{ij} \sum_{r=1}^{m} T_{p}[i]^{T} \frac{\partial}{\partial P} U_{r_{q}}[j][(\hat{\beta}_{i} \nu_{j} \varphi_{r} + \hat{\beta}_{i} \chi_{j} \psi_{r}) - (\hat{\beta}_{i} \lambda_{ij} \varphi_{r} + \hat{\beta}_{i} \mu_{ij} \psi_{r})]
+ h \sum_{ij} \sum_{r=1}^{m} U_{r_{q}}[i]^{T} \frac{\partial}{\partial P} T_{p}[j](\nu_{i} \hat{\alpha}_{ij} \varphi_{r} + \chi_{i} \hat{\alpha}_{ij} \psi_{r}) + \frac{\partial}{\partial P} F
= h \sum_{i=1}^{s} \hat{\beta}_{i} T_{p}[i] + h^{2} \sum_{ij} \beta_{i} \hat{\alpha}_{ij} \frac{\partial}{\partial P} (U_{q}[i]^{T} T_{p}[j])
+ h \sum_{ij} \sum_{r=1}^{m} \frac{\partial}{\partial P} [U_{r_{q}}[i]^{T} T_{p}[j](\nu_{i} \hat{\alpha}_{ij} \varphi_{r} + \chi_{i} \hat{\alpha}_{ij} \psi_{r})] + \frac{\partial}{\partial P} F,$$
(7.1.15)

therefore,

$$\frac{\partial \bar{S}^1}{\partial P} = h \sum_{i=1}^s \hat{\beta}_i T_p[i]. \tag{7.1.16}$$

In the same way we get

$$\frac{\partial \bar{S}^{1}}{\partial q} = h \sum_{i=1}^{s} \beta_{i} U_{q}[i] + \sum_{i=1}^{s} \sum_{r=1}^{m} U_{r_{q}}[i] (\nu_{i} \varphi_{r} + \chi_{i} \psi_{r}). \tag{7.1.17}$$

7.2 A Method for Systems with Additive Noises

For the stochastic Hamiltonian system with additive noises

$$dp = f(t, p, q)dt + \sum_{r=1}^{s} \sigma_r(t)dW_r(t), \quad p(t_0) = p,$$
 (7.2.1)

$$dq = g(t, p, q)dt + \sum_{r=1}^{s} \gamma_r(t)dW_r(t), \quad q(t_0) = q,$$
 (7.2.2)

consider the following relation ([28])

$$P = p + hf(t_0 + \beta h, \alpha P + (1 - \alpha)p, (1 - \alpha)Q + \alpha q) + \sum_{r=1}^{m} \sigma_r(t)\Delta W_r, \quad (7.2.3)$$

$$Q = q + hg(t_0 + \beta h, \alpha P + (1 - \alpha)p, (1 - \alpha)Q + \alpha q) + \sum_{r=1}^{m} \gamma_r(t)\Delta W_r, \quad (7.2.4)$$

where $\alpha, \beta \in [0, 1], f = -H_q, g = H_p$.

Theorem 7.2. The method (7.2.3)-(7.2.4) can be written as (5.1.9) with

$$\bar{S}^{1}(P,q,h) = hH(t_{0} + \beta h, \alpha P + (1-\alpha)p, (1-\alpha)Q + \alpha q) + \sum_{r=1}^{m} (\gamma_{r}(t)P - \sigma_{r}(t)q)\Delta W_{r} + F,$$
(7.2.5)

where

$$F = h^{2}(\alpha - 1)H_{q}^{T}H_{p}. (7.2.6)$$

Proof. From (7.2.5)-(7.2.6) we have

$$\frac{\partial \bar{S}^{1}}{\partial q} = hH_{q}^{T}(\alpha I + (1 - \alpha)(I + h\frac{\partial}{\partial q}H_{p})) + hH_{p}^{T}(1 - \alpha)\frac{\partial p}{\partial q} - \sum_{r=1}^{m} \sigma_{r}(t)\Delta W_{r} + \frac{\partial F}{\partial q}$$

$$= hH_{q}^{T} + h^{2}(1 - \alpha)H_{q}^{T}\frac{\partial}{\partial q}H_{p} + h^{2}(1 - \alpha)H_{p}^{T}\frac{\partial}{\partial p}H_{q} - \sum_{r=1}^{m} \sigma_{r}(t)\Delta W_{r} + \frac{\partial F}{\partial q}$$

$$= hH_{q}^{T} - \sum_{r=1}^{m} \sigma_{r}(t)\Delta W_{r} + h^{2}(1 - \alpha)\frac{\partial}{\partial q}(H_{q}^{T}H_{p}) + \frac{\partial F}{\partial q}$$

$$= hH_{q}^{T} - \sum_{r=1}^{m} \sigma_{r}(t)\Delta W_{r}. \tag{7.2.7}$$

Similarly, it can be verified that

$$\frac{\partial \bar{S}^1}{\partial P} = hH_p^T + \sum_{r=1}^m \gamma_r(t)\Delta W_r. \tag{7.2.8}$$

7.3 Generating Function for Phase Trajectory of a SDE

Consider the stochastic Hamiltonian system with two additive noise (3.1.27)-(3.1.28)

$$dq = pdt + \sigma dW_1(t), \quad q(0) = q_0,$$

$$dp = -qdt + \gamma dW_2(t), \quad p(0) = p_0.$$

Let $X = (q, p)^T$, we know from (3.1.29) that the exact solution of the system (3.1.27)-(3.1.28) can also be written as

$$X(t+h) = FX(t) + u(t,h), (7.3.1)$$

where

$$F = \begin{pmatrix} \cos h & \sin h \\ -\sin h & \cos h \end{pmatrix}, \qquad u(t,h) = \begin{pmatrix} u_1 \\ u_2 \end{pmatrix}$$
 (7.3.2)

with

$$u_1 = \sigma \int_t^{t+h} \cos(t+h-s)dW_1(s) + \gamma \int_t^{t+h} \sin(t+h-s)dW_2(s),$$
 (7.3.3)

$$u_2 = -\sigma \int_t^{t+h} \sin(t+h-s)dW_1(s) + \gamma \int_t^{t+h} \cos(t+h-s)dW_2(s). \quad (7.3.4)$$

Now we write $X(t+h) = (Q, P)^T$, $X(t) = (q, p)^T$, then

$$Q = q\cos h + p\sin h + u_1, \tag{7.3.5}$$

$$P = -q\sin h + p\cos h + u_2. (7.3.6)$$

Theorem 7.3. The solution of (7.3.5)-(7.3.6) can be written as (5.1.1) with

$$\bar{S}(q,Q,h) = -pq\sin^2 h + \frac{1}{2}(p^2 - q^2)\sin h\cos h + pu_2\sin h + qu_2\cos h, \quad (7.3.7)$$

where
$$p = \frac{Q}{\sin h} - q \cot h - \frac{u_1}{\sin h}. \tag{7.3.8}$$

Proof. From (7.3.7)-(7.3.8),

$$\frac{\partial \bar{S}}{\partial Q} = \frac{\partial \bar{S}}{\partial p} \frac{\partial p}{\partial Q} = (-q \sin^2 h + p \sin h \cos h + u_2 \sin h)(\frac{1}{\sin h})$$

$$= -q \sin h + p \cos h + u_2, \qquad (7.3.9)$$

and the first relation (7.3.5) is a direct consequence of (7.3.8).

7.4 Generalization of a Symplectic Runge-Kutta Method

For Hamiltonian system with additive noises (7.2.1)-(7.2.2), the following symplectic Runge-Kutta method is proposed ([28]), which is also given in section 3.2 with equation number (3.2.5)-(3.2.6):

$$\mathcal{P}_{i} = p + h \sum_{j=1}^{s} \alpha_{ij} f(t_{0} + c_{j}h, \mathcal{P}_{j}, \mathcal{Q}_{j}) + \varphi_{i},$$

$$\mathcal{Q}_{i} = q + h \sum_{j=1}^{s} \alpha_{ij} g(t_{0} + c_{j}h, \mathcal{P}_{j}, \mathcal{Q}_{j}) + \psi_{i},$$

$$P = p + h \sum_{i=1}^{s} \beta_{i} f(t_{0} + c_{i}h, \mathcal{P}_{i}, \mathcal{Q}_{i}) + \eta,$$

$$Q = q + h \sum_{i=1}^{s} \beta_{i} g(t_{0} + c_{i}h, \mathcal{P}_{i}, \mathcal{Q}_{i}) + \zeta,$$

$$(7.4.1)$$

where φ_i , ψ_i , η , ζ do not depend on p and q, the parameters α_{ij} and β_i satisfy the conditions

$$\beta_i \alpha_{ij} + \beta_j \alpha_{ji} - \beta_i \beta_j = 0, \quad i, j = 1, \dots, s, \tag{7.4.2}$$

96CHAPTER 7. GENERATING FUNCTIONS FOR SOME SYMPLECTIC METHODS

and c_i are arbitrary parameters. In fact, stochastic symplectic Runge-Kutta methods can be generalized to cases of any type of noises. For convenience, we discuss the following system with one noise, cases of more noises can be treated in the same way:

$$dp = -H_q(t, p, q)dt - \hat{H}_q(t, p, q) \circ dW(t), \quad p(t_0) = p, \tag{7.4.3}$$

$$dq = H_p(t, p, q)dt + \hat{H}_p(t, p, q) \circ dW(t), \qquad q(t_0) = q. \tag{7.4.4}$$

Consider the following method

$$\mathcal{P}_{i} = p - h \sum_{j=1}^{s} \alpha_{ij} H_{q}(t_{0} + c_{j}h, \mathcal{P}_{j}, \mathcal{Q}_{j}) - \sum_{j=1}^{s} \alpha_{ij} \hat{H}_{q}(t_{0} + c_{j}h, \mathcal{P}_{j}, \mathcal{Q}_{j}) \Delta W_{j}, (7.4.5)$$

$$Q_{i} = q + h \sum_{j=1}^{s} \alpha_{ij} H_{p}(t_{0} + c_{j}h, \mathcal{P}_{j}, \mathcal{Q}_{j}) + \sum_{j=1}^{s} \alpha_{ij} \hat{H}_{p}(t_{0} + c_{j}h, \mathcal{P}_{j}, \mathcal{Q}_{j}) \Delta W_{j}, (7.4.6)$$

$$P = p - h \sum_{i=1}^{s} \beta_{i} H_{q}(t_{0} + c_{i}h, \mathcal{P}_{i}, \mathcal{Q}_{i}) - \sum_{i=1}^{s} \beta_{i} \hat{H}_{q}(t_{0} + c_{i}h, \mathcal{P}_{i}, \mathcal{Q}_{i}) \Delta W_{i}, \quad (7.4.7)$$

$$Q = q + h \sum_{i=1}^{s} \beta_{i} H_{p}(t_{0} + c_{i}h, \mathcal{P}_{i}, \mathcal{Q}_{i}) + \sum_{i=1}^{s} \beta_{i} \hat{H}_{q}(t_{0} + c_{i}h, \mathcal{P}_{i}, \mathcal{Q}_{i}) \Delta W_{i}, \quad (7.4.8)$$

with relation (7.4.2).

Theorem 7.4. The method (7.4.5)-(7.4.8) with relation (7.4.2) is symplectic and can be written as (5.1.9) with

$$\bar{S}^{1}(P,q,h) = h \sum_{i=1}^{s} \beta_{i} H(t_{0} + c_{i}h, \mathcal{P}_{i}, \mathcal{Q}_{i}) + \sum_{i=1}^{s} \beta_{i} \hat{H}(t_{0} + c_{i}h, \mathcal{P}_{i}, \mathcal{Q}_{i}) \Delta W_{i} + F,$$
(7.4.9)

where

$$F = -\left(h^2 \sum_{ij} \beta_i \alpha_{ij} H_q^T(t_0 + c_i h, \mathcal{P}_i, \mathcal{Q}_i) H_p(t_0 + c_j h, \mathcal{P}_j, \mathcal{Q}_j) \right.$$

$$+ h \sum_{ij} \beta_i \alpha_{ij} (\hat{H}_q(t_0 + c_i h, \mathcal{P}_i, \mathcal{Q}_i) H_p(t_0 + c_j h, \mathcal{P}_j, \mathcal{Q}_j) \Delta W_i$$

$$+ \hat{H}_p^T(t_0 + c_i h, \mathcal{P}_i, \mathcal{Q}_i) H_q(t_0 + c_j h, \mathcal{P}_j, \mathcal{Q}_j) \Delta W_i$$

$$+ \sum_{ij} \beta_i \alpha_{ij} \hat{H}_q^T(t_0 + c_i h, \mathcal{P}_i, \mathcal{Q}_i) \hat{H}_p(t_0 + c_j h, \mathcal{P}_j, \mathcal{Q}_j) \Delta W_i \Delta W_j \right). \quad (7.4.10)$$

Proof. Denote $H(t_0 + c_i h, \mathcal{P}_i, \mathcal{Q}_i) = H[i]$, $H_q(t_0 + c_i h, \mathcal{P}_i, \mathcal{Q}_i) = H_{q_i}$, \cdots . By straightforward calculation as in Theorem 7.1 and the relation (7.4.2), one can verify that

$$\frac{\partial \bar{S}^1}{\partial q} = h \sum_{i=1}^s \beta_i H_q[i] + \sum_{i=1}^s \beta_i \hat{H}_q[i] \Delta W_i, \qquad (7.4.11)$$

$$\frac{\partial \bar{S}^1}{\partial P} = h \sum_{i=1}^s \beta_i H_p[i] + \sum_{i=1}^s \beta_i \hat{H}_p[i] \Delta W_i. \tag{7.4.12}$$

Consequently, the method (7.4.5)-(7.4.8) is symplectic by Theorem 5.1.

Similarly, we can verify the following two results.

Theorem 7.5. The method (7.4.5)-(7.4.8) with relation (7.4.2) is equivalent to (5.1.12) with

$$\bar{S}^{2}(p,Q,h) = h \sum_{i=1}^{s} \beta_{i} H[i] + \sum_{i=1}^{s} \beta_{i} \hat{H}[i] \Delta W_{i}
+ \sum_{ij} \beta_{i} \alpha_{ij} (h^{2} H_{p}[i]^{T} H_{q}[j] + h H_{p}[j]^{T} \hat{H}_{q}[j] \Delta W_{i}
+ h H_{q}[i]^{T} \hat{H}_{p}[j] \Delta W_{i} + \hat{H}_{p}[i] \hat{H}_{q}[j] \Delta W_{i} \Delta W_{j}).$$
(7.4.13)

Theorem 7.6. The method (7.4.5)-(7.4.8) with relation (7.4.2) is equivalent to (5.1.15)-(5.1.16) with

$$\bar{S}^{3}(\frac{1}{2}(P+p), \frac{1}{2}(Q+q), h) = h \sum_{i=1}^{s} \beta_{i} H[i] + \sum_{i=1}^{s} \beta_{i} \hat{H}[i] \Delta W_{i}
+ \sum_{ij} \beta_{i} \alpha_{ij} \left(\frac{h^{2}}{2} (H_{p}[i]^{T} H_{q}[j] - H_{q}[i]^{T} H_{p}[j]) \right)
+ \frac{h}{2} ((H_{p}[j]^{T} \hat{H}_{q}[j] - \hat{H}_{q}[i]^{T} H_{p}[j])
+ (H_{q}[i]^{T} \hat{H}_{p}[j] - \hat{H}_{p}[i]^{T} H_{q}[j])) \Delta W_{i}
+ \frac{1}{2} (\hat{H}_{p}[i]^{T} \hat{H}_{q}[j] - \hat{H}_{q}[i]^{T} \hat{H}_{p}[j]) \Delta W_{i} \Delta W_{j} \right) . (7.4.14)$$

98CHAPTER 7	GENERATING	FUNCTIONS FOR	R.SOMESYMPLECTICMETHODS
JOULLAL LIJULE.		TO CONCOUNT OF COME	1. ()() V 17 () 1 V 1 1/17(/ 1 1(/ V 17 1 1 (/ /

Chapter 8

Backward Error Analysis

Backward error analysis studies qualitative behavior of numerical methods by constructing modified equations of them. The discrete points of numerical solutions settle on exact integration curves of the modified equations. In deterministic case, one can use generating functions of a symplectic method to build its modified equation, which is a Hamiltonian system ([12]). We construct in this chapter modified equations with noises for stochastic symplectic methods, by using their generating functions with noises. This gives insight into the stochastic symplectic methods, and support to the stochastic generating function theory proposed in previous chapters.

8.1 Deterministic Modified Equations and Generating Functions

For an ordinary differential equation

$$\dot{y} = f(y) \tag{8.1.1}$$

and a numerical method $\Phi_h(y)$ which gives the discrete solution

$$y_0, y_1, y_2, \cdots,$$

a modified equation of the method is of the form

$$\dot{\tilde{y}} = f(\tilde{y}) + h f_2(\tilde{y}) + h^2 f_3(\tilde{y}) + \dots$$
 (8.1.2)

such that $y_n = \tilde{y}(nh)$. The idea of backward analysis is to study the difference between the two vector fields f(y) and $f_h(y)$, instead of the local error $y_1 - \varphi_h(y_0)$ and the global error $y_n - \varphi_{nh}(y_0)$ in the solution space, where φ_t denotes the exact flow of the differential equation (8.1.1).

The series in (8.1.2) is usually divergent and has to be truncated suitably. Using Taylor expansion of $\Phi_h(y)$ at y in powers of h, and that of $\tilde{y}(t+h)$ at y based on the assumption $\tilde{y}(t) = y$, and comparing like powers of h, the coefficient functions $f_i(y)$ in (8.1.2) can be

determined as

$$f_{2}(y) = d_{2}(y) - \frac{1}{2!}f'f(y),$$

$$f_{3}(y) = d_{3}(y) - \frac{1}{3!}(f''(f,f)(y) + f'f'f(y)) - \frac{1}{2!}(f'f_{2}(y) + f'_{2}f(y)),$$

$$\vdots$$
(8.1.3)

where $d_i(y)$ are coefficient functions in the Taylor expansion of $\Phi_h(y)$

$$\Phi_h(y) = y + hf(y) + h^2 d_2(y) + h^3 d_3(y) + \dots$$
(8.1.4)

Any one-step symplectic method $\Phi_h:(p,q)\mapsto(P,Q)$ can be generated by a generating function S(P,q,h) through the relation

$$p = P + \frac{\partial S}{\partial q}^{T}(P, q, h), \qquad Q = q + \frac{\partial S}{\partial P}^{T}(P, q, h).$$
 (8.1.5)

It is verified that the modified equation of a symplectic method is a Hamiltonian system, and the Hamiltonian of the modified equation can be found explicitly, as stated in the following results.

Theorem 8.1. ([12]) Assume that the symplectic method Φ_h has a generating function

$$S(P,q,h) = hS_1(P,q) + h^2S_2(P,q) + h^3S_3(P,q) + \dots$$
(8.1.6)

with smooth $S_j(P,q)$ defined on an open set D. Then, the modified equation is a Hamiltonian system with

$$\tilde{H}(p,q) = H(p,q) + hH_2(p,q) + h^2H_3(p,q) + \dots,$$
(8.1.7)

where the functions $H_i(p,q)$ are defined and smooth on the whole of D.

The proof is based on the fact that the phase flow of a Hamiltonian system can be generated by a generating function $\tilde{S}(P,q,t)$ which satisfies a Hamilton-Jacobi partial differential equation, and that the generating function $\tilde{S}(P,q,t)$ should equal S(P,q,h) at t=h owing to the definition of a modified equation. It is first assumed that the modified equation is a Hamiltonian system with (8.1.7), and then to find the functions H_j according to the two facts stated above. The proof also gives a method of constructing the modified equation of a symplectic method by applying its generating function.

Since we have developed generating functions for stochastic symplectic methods, it is natural to raise the question whether we could construct modified equations for sympletic methods using their generating functions with noises? In the following sections we deal with this problem.

8.2 Stochastic Modified Equations Based on \bar{S}^1

In this section we propose the definition of stochastic modified equations, and give a theorem asserting property of modified equations of stochastic symplectic methods, as well as their construction via generating function \bar{S}^1 .

Definition 8.2. Given a stochastic differential equation in Stratonovich sense

$$dy = f(y)dt + g(y) \circ dW \tag{8.2.1}$$

and a numerical method $\Phi_h(y)$, which produces approximations

$$y_0, y_1, y_2, \ldots,$$

the stochastic modified equation of the method is a stochastic differential equation of the form

$$d\tilde{y} = f_h(\tilde{y})dt + g_h(\tilde{y}) \circ dW \tag{8.2.2}$$

such that $y_n = \tilde{y}(nh)$.

For a stochastic symplectic method $\Phi_h:(p,q)\mapsto(P,Q)$ generated by $\bar{S}^1(P,q,h)$ through the relation (5.1.9)

$$p = P + \frac{\partial \bar{S}^1}{\partial q}^T (P, q, h), \qquad Q = q + \frac{\partial \bar{S}^1}{\partial P}^T (P, q, h),$$

we can prove that its modified equation is a stochastic Hamiltonian system, which can be determined explicitly, as given in the following theorem and its proof. We first discuss the case of one noise.

Theorem 8.3. Given a stochastic Hamiltonian system

$$dy = J^{-1}\nabla H(y)dt + J^{-1}\nabla H_1(y) \circ dW(t), \tag{8.2.3}$$

where $y = \begin{pmatrix} p \\ q \end{pmatrix}$. Assume that the symplectic method Φ_h has a generating function

$$\bar{S}^{1}(P,q,h) = F_{1}(P,q)W(h) + F_{2}(P,q) \int_{0}^{h} W(s) \circ dW(s) + G_{1}(P,q) \int_{0}^{h} ds
+ F_{3}(P,q) \int_{0}^{h} s \circ dW(s) + G_{2}(P,q) \int_{0}^{h} W(s) ds
+ F_{4}(P,q) \int_{0}^{h} sW(s) \circ dW(s) + G_{3}(P,q) \int_{0}^{h} sds + \dots$$
(8.2.4)

Then, the modified equation of Φ_h is a stochastic Hamiltonian system

$$dy = J^{-1}\nabla \tilde{H}(y)dt + J^{-1}\nabla \tilde{H}_1(y) \circ dW(t), \tag{8.2.5}$$

where

$$\tilde{H}(p,q) = H(p,q) + H_2(p,q)W + H_3(p,q)h + H_4(p,q)hW + H_5(p,q)h^2 + \dots,$$

$$\tilde{H}_1(p,q) = H_1(p,q) + \bar{H}_2(p,q)W + \bar{H}_3(p,q)h + \bar{H}_4(p,q)hW + \bar{H}_5(p,q)h^2 + \dots.$$
(8.2.6)

Proof. We first assume that the modified equation is really a stochastic Hamiltonian system with Hamiltonians in (8.2.6)-(8.2.7). In the following we use the Hamilton-Jacobi partial differential equation with noise and the definition of stochastic modified equation to determine the functions $H_j(p,q)$ and $\bar{H}_j(p,q)$. If the process can be performed successfully, then the assertion is proved. At the same time, we find the expression of the stochastic modified equation (8.2.5).

According to the Hamilton-Jacobi theory, let $\tilde{S}^1(P,q,t)$ be the generating function that generates the phase trajectory $\{\tilde{P}(t), \tilde{Q}(t)\}$ of the stochastic Hamiltonian system (8.2.5) through the relation

$$p = \tilde{P}(t) + \frac{\partial \tilde{S}^1}{\partial q}^T, \qquad \tilde{Q}(t) = q + \frac{\partial \tilde{S}^1}{\partial P}^T,$$
 (8.2.8)

then by Theorem 5.5, it is sufficient that $\tilde{S}^1(P,q,t)$ satisfies the Hamilton-Jacobi partial differential equation with noise

$$\frac{\partial \tilde{S}^{1}}{\partial t} = \tilde{H}(P, q + \frac{\partial \tilde{S}^{1}}{\partial P}) + \tilde{H}_{1}(P, q + \frac{\partial \tilde{S}^{1}}{\partial P})\dot{W}. \tag{8.2.9}$$

Suppose

$$\tilde{S}^{1}(P,q,t) = \tilde{S}_{1}(P,q,h)W(t) + \tilde{S}_{2}(P,q,h) \int_{0}^{t} W(s) \circ dW(s) + \tilde{T}_{1}(P,q,h)t
+ \tilde{S}_{3}(P,q,h) \int_{0}^{t} s \circ dW(s) + \tilde{T}_{2}(P,q,h) \int_{0}^{t} W(s)ds
+ \tilde{S}_{4}(P,q,h) \int_{0}^{t} sW(s) \circ dW(s) + \tilde{T}_{3}(P,q,h) \int_{0}^{t} sds + \dots$$
(8.2.10)

Then we have

$$\frac{\partial \tilde{S}^{1}}{\partial t} = (\tilde{T}_{1} + \tilde{T}_{2}W + \tilde{T}_{3}t + \tilde{T}_{4}tW + \tilde{T}_{5}t^{2} + \dots)
+ (\tilde{S}_{1} + \tilde{S}_{2}W + \tilde{S}_{3}t + \tilde{S}_{4}tW + \tilde{S}_{5}t^{2} + \dots)\dot{W},$$
(8.2.11)

where the functions \tilde{T}_i and \tilde{S}_i are evaluated at (P, q, h).

Substitute (8.2.11) into (8.2.9), we obtain

$$\tilde{H}(P, q + \frac{\partial \tilde{S}^1}{\partial P}) = \tilde{T}_1 + \tilde{T}_2 W + \tilde{T}_3 t + \tilde{T}_4 t W + \tilde{T}_5 t^2 + \dots,$$
 (8.2.12)

$$\tilde{H}_1(P, q + \frac{\partial \tilde{S}^1}{\partial P}) = \tilde{S}_1 + \tilde{S}_2 W + \tilde{S}_3 t + \tilde{S}_4 t W + \tilde{S}_5 t^2 + \dots$$
 (8.2.13)

Expand $\tilde{H}(P,q+\frac{\partial \tilde{S}^1}{\partial P})$ at (P,q) according to Wagner-Platen expansion in Stratonovich sense and the relation (8.2.5) with $y=\begin{pmatrix} p\\q \end{pmatrix}$, as in (5.3.16), and let coefficients of terms

of the same order of smallness on both sides of (8.2.12) be equal, we have

$$\tilde{T}_{1} = \tilde{H},
\tilde{T}_{2} = \tilde{H}_{q}\tilde{H}_{1_{p}},
\tilde{T}_{3} = \tilde{H}_{q}\tilde{H}_{p} + \frac{1}{2}(\tilde{H}_{qq}\tilde{H}_{1_{p}} + \tilde{H}_{q}\tilde{H}_{1_{pq}})\tilde{H}_{1_{p}},
\vdots$$
(8.2.14)

where \tilde{T}_i are evaluated at (P, q, h).

The same approach applied to $\tilde{H}_1(P, q + \frac{\partial \tilde{S}^1}{\partial P})$ gives

$$\tilde{S}_{1} = \tilde{H}_{1},
\tilde{S}_{2} = \tilde{H}_{1q}\tilde{H}_{1p},
\tilde{S}_{3} = \tilde{H}_{1q}\tilde{H}_{p} + \frac{1}{2}(\tilde{H}_{1qq}\tilde{H}_{1p} + \tilde{H}_{1q}\tilde{H}_{1pq})\tilde{H}_{1p},
\vdots$$
(8.2.15)

with \tilde{S}_i at (P, q, h).

According to the Definition 8.2 of stochastic modified equation, it should hold that $\begin{pmatrix} \tilde{P}(h) \\ \tilde{Q}(h) \end{pmatrix} = \begin{pmatrix} P \\ Q \end{pmatrix}$, which requires

$$\tilde{S}^1(P,q,h) = \bar{S}^1(P,q,h).$$
 (8.2.16)

Substitute (8.2.10) into (8.2.16), we get

$$\tilde{S}_{1}(P,q,h)W(h) + \tilde{S}_{2}(P,q,h) \int_{0}^{h} W(s) \circ dW(s) + \tilde{T}_{1}(P,q,h)h
+ \tilde{S}_{3}(P,q,h) \int_{0}^{h} s \circ dW(s) + \tilde{T}_{2}(P,q,h) \int_{0}^{h} W(s)ds
+ \tilde{S}_{4}(P,q,h) \int_{0}^{h} sW(s) \circ dW(s) + \tilde{T}_{3}(P,q,h) \int_{0}^{h} sds + \dots
= F_{1}(P,q)W(h) + F_{2}(P,q) \int_{0}^{h} W(s) \circ dW(s) + G_{1}(P,q) \int_{0}^{h} ds
+ F_{3}(P,q) \int_{0}^{h} s \circ dW(s) + G_{2}(P,q) \int_{0}^{h} W(s)ds
+ F_{4}(P,q) \int_{0}^{h} sW(s) \circ dW(s) + G_{3}(P,q) \int_{0}^{h} sds + \dots$$
(8.2.17)

Substitute (8.2.14)-(8.2.15) and (8.2.6)-(8.2.7) into the left hand-side of (8.2.17) and let coefficients of terms of the same order of smallness on both sides of (8.2.17) be equal, we

obtain

$$H_{1} = F_{1},$$

$$\bar{H}_{2} = F_{2} - H_{1q}H_{1p}$$

$$H = G_{1}$$

$$\bar{H}_{3} = F_{3} - \bar{H}_{2q}H_{1p} - H_{1q}\bar{H}_{2p} - H_{1q}H_{p}$$

$$- \frac{1}{2}(H_{1qq}H_{1p} + H_{1q}H_{1pq})H_{1p}$$

$$H_{2} = G_{2} - H_{q}H_{1p}$$

$$H_{3} = G_{3} - H_{q}\bar{H}_{2p} - H_{2}H_{1p} - H_{q}H_{p} - \frac{1}{2}(H_{qq}H_{1p} + H_{q}H_{1pq})H_{1p}$$

$$\vdots$$

$$(8.2.18)$$

It is obvious that the functions H_i and \bar{H}_i can be determined explicitly, owing to which the stochastic modified equation (8.2.5) is established.

Example 8.1. Consider the linear stochastic oscillator (3.1.7)-(3.1.8)

$$dy = -xdt + \sigma \circ dW, \qquad y(0) = y_0,$$

$$dx = ydt, \qquad x(0) = x_0,$$

where

$$H = \frac{1}{2}(x^2 + y^2), \qquad H_1 = -\sigma x,$$
 (8.2.19)

and the symplectic Euler-Maruyama method (5.3.27)-(5.3.28)

$$x_{n+1} = x_n + hy_{n+1}$$

$$y_{n+1} = y_n - hx_n + \sigma \Delta W_n,$$

which is generated by the generating function

$$\bar{S}^1 = F_1 W(h) + F_2 \int_0^h W \circ dW + G_1 h \tag{8.2.20}$$

with

$$F_1 = -\sigma x$$
, $F_2 = 0$, $G_1 = \frac{1}{2}(x^2 + y^2)$. (8.2.21)

According to (8.2.18), we have

$$H_2 = 0, \bar{H}_2 = 0, (8.2.22)$$

 $H_3 = -xy, \bar{H}_3 = \sigma y, (8.2.23)$

$$H_3 = -xy, \qquad \bar{H}_3 = \sigma y, \tag{8.2.23}$$

Thus we have

$$\tilde{H} = \frac{1}{2}(x^2 + y^2) - hxy + \dots, \quad \tilde{H}_1 = -\sigma x + h\sigma y + \dots$$
 (8.2.24)

After truncation to the second term of \tilde{H} and \tilde{H}_1 , we get the truncated modified equation

$$\begin{split} d\tilde{Y} &= J^{-1}\nabla \tilde{H}dt + J^{-1}\nabla \tilde{H}_{1} \circ dW \\ &\approx \begin{pmatrix} hy - x \\ y - hx \end{pmatrix} dt + \begin{pmatrix} \sigma \\ \sigma h \end{pmatrix} \circ dW, \end{split} \tag{8.2.25}$$

where $\tilde{Y} = \begin{pmatrix} y \\ x \end{pmatrix}$, i.e.

$$dy = (hy - x)dt + \sigma \circ dW, \quad y(0) = y_0,$$
 (8.2.26)

$$dx = (y - hx)dt + \sigma h \circ dW, \quad x(0) = x_0.$$
 (8.2.27)

In the next chapter, we can see through numerical test that phase trajectory of the numerical solution produced by symplectic Euler-Maruyama method (5.3.27)-(5.3.28) coincides with that of the truncated modified equation (8.2.26)-(8.2.27) very well. In order to simulate the solution of (8.2.26)-(8.2.27), we use its symplectic Euler-Maruyama discretization

$$y_{n+1} = y_n + h(hy_{n+1} - x_n) + \sigma \Delta W_n, \tag{8.2.28}$$

$$x_{n+1} = x_n + h(y_{n+1} - hx_n) + \sigma h \Delta W_n, \tag{8.2.29}$$

which is equivalent to

$$\begin{pmatrix} x_{n+1} \\ y_{n+1} \end{pmatrix} = \begin{pmatrix} \frac{-h^4 + 3h^2 - 1}{h^2 - 1} & \frac{-h}{h^2 - 1} \\ \frac{h}{h^2 - 1} & \frac{-1}{h^2 - 1} \end{pmatrix} \begin{pmatrix} x_n \\ y_n \end{pmatrix} + \begin{pmatrix} \frac{\sigma h^3 - 2\sigma h}{h^2 - 1} \\ \frac{-\sigma}{h^2 - 1} \end{pmatrix} \Delta W_n.$$
(8.2.30)

Example 8.2. For the Kubo oscilltor (3.1.16)-(3.1.17)

$$dp = -aqdt - \sigma q \circ dW(t), \qquad p(0) = p_0,$$

$$dq = apdt + \sigma p \circ dW(t), \qquad q(0) = q_0,$$

we have

$$H = \frac{a}{2}(p^2 + q^2), \qquad H_1 = \frac{\sigma}{2}(p^2 + q^2),$$

and the symplectic method (5.3.46)

$$-(ah + \frac{h^2}{2}a\sigma^2 + \sigma\Delta W_n + \sigma^3 \int_0^h s \circ dW)p_{n+1} + q_{n+1} = (1 + \frac{h\sigma^2}{2} + \frac{h^2a^2}{2} + a\sigma h\Delta W_n)q_n,$$

$$(1 + \frac{h\sigma^2}{2} + \frac{h^2a^2}{2} + a\sigma h\Delta W_n)p_{n+1} = p_n - (ah + \sigma\Delta W_n)q_n,$$

which is generated by (5.3.45)

$$\bar{S}^{1} = F_{1} \Delta W_{n} + F_{2} \int_{0}^{h} W \circ dW + G_{1}h + F_{3} \int_{0}^{h} s \circ dW + G_{2} \int_{0}^{h} W ds + G_{3} \int_{0}^{h} s ds$$

through the relation (5.1.9), where

$$F_1 = \frac{\sigma}{2}(p^2 + q^2), \quad F_2 = \sigma^2 pq, \quad F_3 = a\sigma pq + \frac{1}{2}\sigma^3 p^2,$$
 (8.2.31)

$$G_1 = \frac{a}{2}(p^2 + q^2), \quad G_2 = a\sigma pq, \quad G_3 = a^2pq + \frac{1}{2}a\sigma^2p^2.$$
 (8.2.32)

According to (8.2.6)-(8.2.7),

$$\tilde{H} = \frac{a}{2}(p^2 + q^2) + \dots,$$
 (8.2.33)

$$\tilde{H}_1 = \frac{\sigma}{2}(p^2 + q^2) - \frac{h}{2}\sigma^3 p^2 q + \dots,$$
 (8.2.34)

which after truncation to the given term results in the truncated modified equation

$$d\tilde{Y} = J^{-1}\nabla \tilde{H}(\tilde{Y})dt + J^{-1}\nabla \tilde{H}_{1}(\tilde{Y}) \circ dW$$

$$\approx \begin{pmatrix} -aq \\ ap \end{pmatrix} dt + \begin{pmatrix} \frac{h}{2}\sigma^{3}p^{2} - \sigma q \\ \sigma p - h\sigma^{3}pq \end{pmatrix} \circ dW, \tag{8.2.35}$$

where $\tilde{Y} = \begin{pmatrix} p \\ q \end{pmatrix}$. It can also be written in the form

$$dp = -aqdt + (\frac{h}{2}\sigma^3 p^2 - \sigma q) \circ dW, \quad p(0) = p_0,$$
 (8.2.36)

$$dq = apdt + (\sigma p - h\sigma^3 pq) \circ dW, \qquad q(0) = q_0.$$
 (8.2.37)

In numerical test, we simulate the solution of the modified equation (8.2.36)-(8.2.37) by its symplectic Euler-Maruyama discretization

$$p_{n+1} = p_n - ahq_n + (\frac{h}{2}\sigma^3 p_{n+1}^2 - \sigma q_n)\Delta W_n, \qquad (8.2.38)$$

$$q_{n+1} = q_n + ahp_{n+1} + (\sigma p_{n+1} - h\sigma^3 p_{n+1}q_n)\Delta W_n, \tag{8.2.39}$$

which can be realized by fixed point iteration.

8.3 Stochastic Modified Equations Based on \bar{S}^3

Construction of stochastic modified equation via generating function \bar{S}^3 is given in the following. The methods and results are similar to that of using generating function \bar{S}^1 .

Suppose a symplectic method $\Phi_h: (p,q) \mapsto (P,Q)$ is generated by $\bar{S}^3(u,v,h)$, where $u = \frac{P+p}{2}, v = \frac{Q+q}{2}$, via the relation (5.1.15)-(5.1.16)

$$P = p - \partial_2^T \bar{S}^3(u, v), \quad Q = q + \partial_1^T \bar{S}^3(u, v).$$

We can prove that the modified equation of the method Φ_h is a stochastic Hamiltonian system, phase trajectory of which is generated by a function $\tilde{S}^3(u, v, t)$ through the relation (5.1.15)-(5.1.16).

Theorem 8.4. Given a stochastic Hamiltonian system

$$dy = J^{-1}\nabla H(y)dt + J^{-1}\nabla H_1(y) \circ dW(t), \tag{8.3.1}$$

where $y = \begin{pmatrix} p \\ q \end{pmatrix}$. Assume that the symplectic method Φ_h has a generating function

$$\bar{S}^{3}(u,v,h) = F_{1}(u,v)W(h) + F_{2}(u,v) \int_{0}^{h} W(s) \circ dW(s) + G_{1}(u,v) \int_{0}^{h} ds
+ F_{3}(u,v) \int_{0}^{h} s \circ dW(s) + G_{2}(u,v) \int_{0}^{h} W(s) ds
+ F_{4}(u,v) \int_{0}^{h} sW(s) \circ dW(s) + G_{3}(u,v) \int_{0}^{h} sds + \dots,$$
(8.3.2)

where $u = \frac{P+p}{2}$, $v = \frac{Q+q}{2}$. Then, the modified equation of Φ_h is a stochastic Hamiltonian system

$$dy = J^{-1}\nabla \tilde{H}(y)dt + J^{-1}\nabla \tilde{H}_1(y) \circ dW(t), \tag{8.3.3}$$

where

$$\tilde{H}(p,q) = H(p,q) + H_2(p,q)W + H_3(p,q)h + H_4(p,q)hW + H_5(p,q)h^2 + \dots,$$

$$\tilde{H}_1(p,q) = H_1(p,q) + \bar{H}_2(p,q)W + \bar{H}_3(p,q)h + \bar{H}_4(p,q)hW + \bar{H}_5(p,q)h^2 + \dots$$

$$(8.3.4)$$

Proof. As in the proof of Theorem 8.3, we first assume that the function $\tilde{S}^3(u,v,t)$ generates via relation (5.1.15)-(5.1.16) the phase trajectory $\{P(t),Q(t)\}$ of the modified equation, which is a stochastic Hamiltonian system with Hamiltonians \tilde{H} and \tilde{H}_1 in (8.3.4)-(8.3.5), and then to find the functions H_i and \bar{H}_i . According to Theorem 5.6, it is sufficient that \tilde{S}^3 satisfies the following Hamilton-Jacobi equation with noise

$$\frac{\partial \tilde{S}^3}{\partial t} = \tilde{H}(P,Q) + \tilde{H}_1(P,Q)\dot{W}, \tag{8.3.6}$$

where

$$P = u - \frac{1}{2} \frac{\partial \tilde{S}^3}{\partial v}^T, \qquad Q = v + \frac{1}{2} \frac{\partial \tilde{S}^3}{\partial u}^T. \tag{8.3.7}$$

Suppose that

$$\tilde{S}^{3}(u,v,t) = \tilde{S}_{1}(u,v,h)W(t) + \tilde{S}_{2}(u,v,h) \int_{0}^{t} W \circ dW + \tilde{T}_{1}(u,v,h)t
+ \tilde{S}^{3}(u,v,h) \int_{0}^{t} s \circ dW(s) + \tilde{T}_{2}(u,v,h) \int_{0}^{t} W(s)ds
+ \tilde{S}_{4}(u,v,h) \int_{0}^{t} sW(s) \circ dW(s) + \tilde{T}_{3}(u,v,h) \int_{0}^{t} sds + \dots$$
(8.3.8)

Thus

$$\frac{\partial \tilde{S}^{3}}{\partial t} = (\tilde{T}_{1} + \tilde{T}_{2}W + \tilde{T}_{3}t + \tilde{T}_{4}tW + \tilde{T}_{5}t^{2} + \dots)
+ (\tilde{S}_{1} + \tilde{S}_{2}W + \tilde{S}_{3}t + \tilde{S}_{4}tW + \tilde{S}_{5}t^{2} + \dots)\dot{W},$$
(8.3.9)

where \tilde{T}_i and \tilde{S}_i are evaluated at (u, v, h). Substituting (8.3.9) into (8.3.6) yields

$$\tilde{H}(P,Q) = \tilde{T}_1 + \tilde{T}_2 W + \tilde{T}_3 t + \tilde{T}_4 t W + \tilde{T}_5 t^2 + \dots,$$
 (8.3.10)

$$\tilde{H}_1(P,Q) = \tilde{S}_1 + \tilde{S}_2 W + \tilde{S}_3 t + \tilde{S}_4 t W + \tilde{S}_5 t^2 + \dots$$
 (8.3.11)

Expand $\tilde{H}(P,Q)$ at (u,v) according to the formula of Wagner-Platen expansion in Stratonovich sense and the relation (8.3.3), and let coefficients of terms of the same order of smallness on both sides of (8.3.10) be equal, we obtain

$$\tilde{T}_{1} = \tilde{H},
\tilde{T}_{2} = \frac{1}{\sqrt{2}} (\tilde{H}_{v} \tilde{H}_{1_{u}} - \tilde{H}_{u} \tilde{H}_{1_{v}}),
\tilde{T}_{3} = \frac{1}{2} [\frac{1}{2} (\tilde{H}_{vv} \tilde{H}_{1_{u}} + \tilde{H}_{v} \tilde{H}_{1_{uv}}) \tilde{H}_{1_{u}} + \frac{1}{2} (\tilde{H}_{uu} \tilde{H}_{1_{v}} + \tilde{H}_{u} \tilde{H}_{1_{uv}}) \tilde{H}_{1_{v}}
- (\tilde{H}_{uv} \tilde{H}_{1_{v}} + \tilde{H}_{u} \tilde{H}_{1_{vv}}) \tilde{H}_{1_{u}}],
\vdots$$
(8.3.12)

The same approach applied to $\tilde{H}_1(P,Q)$ and the relation (8.3.11) gives

$$\tilde{S}_{1} = \tilde{H}_{1},
\tilde{S}_{2} = \frac{1}{\sqrt{2}} (\tilde{H}_{1_{v}} \tilde{H}_{1_{u}} - \tilde{H}_{1_{u}} \tilde{H}_{1_{v}}) = 0,
\tilde{S}_{3} = \frac{1}{2} [\tilde{H}_{1_{v}} \tilde{H}_{u} - \tilde{H}_{1_{u}} \tilde{H}_{v} + \frac{1}{2} (\tilde{H}_{1_{vv}} \tilde{H}_{1_{u}} + \tilde{H}_{1_{v}} \tilde{H}_{1_{uv}}) \tilde{H}_{1_{u}} + \frac{1}{2} (\tilde{H}_{1_{uu}} \tilde{H}_{1_{v}} + \tilde{H}_{1_{u}} \tilde{H}_{1_{uv}}) \tilde{H}_{1_{v}}
- (\tilde{H}_{1_{uv}} \tilde{H}_{1_{v}} + \tilde{H}_{1_{u}} \tilde{H}_{1_{vv}}) \tilde{H}_{1_{u}}],
\vdots$$
(8.3.13)

As (8.2.16) in the proof of Theorem 8.3, the definition of modified equation requires

$$\tilde{S}^{3}(u,v,h) = \bar{S}^{3}(u,v,h). \tag{8.3.14}$$

(8.3.2), (8.3.8) and (8.3.14) gives

$$\tilde{S}_{1}(u,v,h)W(h) + \tilde{S}_{2}(u,v,h) \int_{0}^{h} W \circ dW + \tilde{T}_{1}(u,v,h)h$$

$$+ \tilde{S}_{3}(u,v,h) \int_{0}^{h} s \circ dW + \tilde{T}_{2}(u,v,h) \int_{0}^{h} W ds$$

$$+ \tilde{S}_{4}(u,v,h) \int_{0}^{h} sW \circ dW + \tilde{T}_{3}(u,v,h) \int_{0}^{h} sds + \dots$$

$$= F_{1}(u,v)W(h) + F_{2}(u,v) \int_{0}^{h} W \circ dW + G_{1}(u,v)h$$

$$+ F_{3}(u,v) \int_{0}^{h} s \circ dW + G_{2}(u,v) \int_{0}^{h} W ds$$

$$+ F_{4}(u,v) \int_{0}^{h} sW \circ dW + G_{3}(u,v) \int_{0}^{h} sds + \dots$$
(8.3.15)

Substitute (8.3.12), (8.3.13) and (8.3.4)-(8.3.5) into (8.3.15), and let coefficients of terms of the same order of smallness on both sides of (8.3.15) be equal, we get

$$\begin{split} H_1 &= F_1, \\ \bar{H}_2 &= F_2, \\ H &= G_1, \\ \bar{H}_3 &= F_3 - \frac{1}{2} [H_{1_v} H_u - H_{1_u} H_v + \frac{1}{2} (H_{1_{vv}} H_{1_u} + H_{1_v} H_{1_{uv}}) H_{1_u} \\ &+ \frac{1}{2} (H_{1_{uu}} H_{1_v} + H_{1_u} H_{1_{uv}}) H_{1_v} - (H_{1_{uv}} H_{1_v} + H_{1_u} H_{1_{vv}}) H_{1_u}], \\ H_2 &= G_2 - \frac{1}{\sqrt{2}} (H_v H_{1_u} - H_u H_{1_v}), \\ H_3 &= G_3 - \frac{1}{\sqrt{2}} (H_v \bar{H}_{2_u} + H_{2_v} H_{1_u} - H_u \bar{H}_{2_v} - H_{2_u} H_{1_v}) - \frac{1}{2} [\frac{1}{2} (H_{vv} H_{1_u} + H_v H_{1_{uv}}) H_{1_u} \\ &+ \frac{1}{2} (H_{uu} H_{1_v} + H_u H_{1_{uv}}) H_{1_v} - (H_{uv} H_{1_v} + H_u H_{1_{vv}}) H_{1_u}], \\ \vdots &\vdots & (8.3.16) \end{split}$$

which ensures existence of (8.3.4)-(8.3.5).

Example 8.3. We study in this example the modified equation of the midpoint rule (5.4.22)-(5.4.23)

$$x_{n+1} = x_n + h \frac{y_n + y_{n+1}}{2},$$

 $y_{n+1} = y_n - h \frac{x_n + x_{n+1}}{2} + \sigma \Delta W_n$

for the linear stochastic oscillator (3.1.7)-(3.1.8)

$$dy = -xdt + \sigma \circ dW, \quad y(0) = y_0,$$

$$dx = ydt, \quad x(0) = x_0,$$

which has Hamiltonians

$$H = \frac{1}{2}(x^2 + y^2), \qquad H_1 = -\sigma x.$$
 (8.3.17)

According to Example 5.3, the midpoint rule (5.4.22)-(5.4.23) is generated by

$$\bar{S}^{3}(u,v,h) = F_{1}\Delta W_{n} + F_{2} \int_{0}^{h} W \circ dW + G_{1}h, \tag{8.3.18}$$

where

$$F_1 = -\sigma v, \quad F_2 = 0, \quad G_1 = \frac{1}{2}(u^2 + v^2).$$
 (8.3.19)

Substitute (8.3.17) and (8.3.19) into (8.3.16), we obtain

$$H_1 = -\sigma v, \quad \bar{H}_2 = 0, \quad H = \frac{1}{2}(u^2 + v^2),$$
 $H_2 = \frac{1}{\sqrt{2}}\sigma u, \quad \bar{H}_3 = \frac{1}{2}\sigma u, \quad H_3 = -\frac{3}{4}\sigma^2$
....
$$(8.3.20)$$

Thus, according to (8.3.4)-(8.3.5), the truncated Hamiltonians are

$$\tilde{H}(y,x) = \frac{1}{2}(y^2 + x^2) + \frac{1}{\sqrt{2}}\sigma y W(h) - \frac{3}{4}\sigma^2 h,$$
 (8.3.21)

$$\tilde{H}_1(y,x) = -\sigma x + \frac{1}{2}\sigma y h. \tag{8.3.22}$$

Consequently the truncated modified equation is

$$dY = J^{-1}\nabla \tilde{H}(Y)dt + J^{-1}\nabla \tilde{H}_{1}(Y) \circ dW$$

$$\approx \left(\frac{-x}{y + \frac{1}{\sqrt{2}}\sigma W(h)}\right)dt + \left(\frac{\sigma}{\frac{1}{2}\sigma h}\right) \circ dW, \tag{8.3.23}$$

which, with $Y = \begin{pmatrix} y \\ x \end{pmatrix}$, is equivalent to

$$dy = -xdt + \sigma \circ dW, \qquad y(0) = y_0, \qquad (8.3.24)$$

$$dy = -xdt + \sigma \circ dW, y(0) = y_0, (8.3.24)$$

$$dx = (y + \frac{\sigma}{\sqrt{2}}W(h))dt + \frac{\sigma}{2}h \circ dW, x(0) = x_0. (8.3.25)$$

In numerical tests in the next chapter, we simulate the solution of the truncated modified equation (8.3.24)-(8.3.25) by its midpoint discretization

$$y_{n+1} = y_n - h \frac{x_n + x_{n+1}}{2} + \sigma \Delta W_n, \tag{8.3.26}$$

$$x_{n+1} = x_n + h \frac{y_n + y_{n+1}}{2} + \frac{h}{\sqrt{2}} \sigma \Delta W_n + \frac{1}{2} \sigma h \Delta W_n,$$
 (8.3.27)

which can also be written as

$$\begin{pmatrix} x_{n+1} \\ y_{n+1} \end{pmatrix} = \begin{pmatrix} \frac{4-h^2}{4+h^2} & \frac{4h}{4+h^2} \\ \frac{-4h}{4+h^2} & \frac{4-h^2}{4+h^2} \end{pmatrix} \begin{pmatrix} x_n \\ y_n \end{pmatrix} + \frac{4}{4+h^2} \begin{pmatrix} (\frac{1}{\sqrt{2}}+1)\sigma h \\ \sigma - \frac{\sqrt{2}+1}{4}\sigma h^2 \end{pmatrix} \Delta W_n.$$
 (8.3.28)

Example 8.4. Consider the Kubo oscillator (3.1.16)-(3.1.17)

$$dp = -aqdt - \sigma q \circ dW(t), \qquad p(0) = p_0,$$

$$dq = apdt + \sigma p \circ dW(t), \qquad q(0) = q_0,$$

which has Hamiltonians

$$H = \frac{a}{2}(p^2 + q^2), \qquad H_1 = \frac{\sigma}{2}(p^2 + q^2),$$
 (8.3.29)

and its midpoint discretization (5.4.31)-(5.4.32)

$$p_{n+1} = p_n - ah \frac{q_n + q_{n+1}}{2} - \sigma \frac{q_n + q_{n+1}}{2} \Delta W_n,$$

$$q_{n+1} = q_n + ah \frac{p_n + p_{n+1}}{2} + \sigma \frac{p_n + p_{n+1}}{2} \Delta W_n,$$

which is generated by

$$\bar{S}^{3}(u,v,h) = F_{1}\Delta W_{n} + F_{2} \int_{0}^{h} W \circ dW + G_{1}h$$
(8.3.30)

with

$$F_1 = \frac{\sigma}{2}(P^2 + q^2), \quad F_2 = 0, \quad G_1 = \frac{a}{2}(P^2 + q^2).$$
 (8.3.31)

(8.3.16), (8.3.29) and (8.3.31) gives

$$H_1 = \frac{\sigma}{2}(p^2 + q^2), \quad H = \frac{a}{2}(p^2) + q^2, \quad \bar{H}_2 = 0,$$

$$H_2 = 0, \quad \bar{H}_3 = \frac{\sigma^3}{4}(p^2 - q^2), \quad H_3 = \frac{a\sigma^2}{4}(p^2 - q^2),$$

$$\dots \tag{8.3.32}$$

(8.3.4)-(8.3.5) and (8.3.32) thus yield

$$\tilde{H} = \frac{a}{2}(p^2 + q^2) + \frac{h}{4}a\sigma^2(p^2 - q^2) + \dots,$$
 (8.3.33)

$$\tilde{H}_1 = \frac{\sigma}{2}(p^2 + q^2) + \frac{h\sigma^3}{4}(p^2 - q^2) + \dots$$
 (8.3.34)

Consequently, the modified equation truncated to the given terms is

$$dy = J^{-1}\nabla \tilde{H}dt + J^{-1}\nabla \tilde{H}_{1} \circ dW(t)$$

$$\approx \left(\frac{ha\sigma^{2}q}{2} - aq \atop ap + \frac{ha\sigma^{2}p}{2}\right)dt + \left(\frac{h\sigma^{3}q}{2} - \sigma q \atop \sigma p + \frac{h\sigma^{3}p}{2}\right) \circ dW, \tag{8.3.35}$$

which can also be written as

$$dp = \left(\frac{ha\sigma^2q}{2} - aq\right)dt + \left(\frac{h\sigma^3q}{2} - \sigma q\right) \circ dW, \quad p(0) = p_0, \tag{8.3.36}$$

$$dq = (ap + \frac{ha\sigma^2 p}{2})dt + (\sigma p + \frac{h\sigma^3 p}{2}) \circ dW, \quad q(0) = q_0.$$
 (8.3.37)

In the numerical tests in Chapter 9, we simulate the solution of the truncated modified equation (8.3.36)-(8.3.37) with its midpoint discretization

$$\begin{pmatrix} p_{n+1} \\ q_{n+1} \end{pmatrix} = \frac{1}{1 - AB} \begin{pmatrix} 1 + AB & 2A \\ 2B & 1 + AB \end{pmatrix} \begin{pmatrix} p_n \\ q_n \end{pmatrix}, \tag{8.3.38}$$

where

$$A = \frac{1}{2}(C - D), \qquad B = \frac{1}{2}(C + D)$$
 (8.3.39)

with

$$C = \frac{h^2 a \sigma^2}{2} + \frac{h \sigma^3}{2} \Delta W_n, \quad D = ah + \sigma \Delta W_n.$$
 (8.3.40)

8.4 Modified Equations for Methods with Two Noises

In this section we discuss modified equation of symplectic methods for stochastic Hamiltonian system with two noises. We mainly use results in Chapter 6. Systems and methods with more noises can be treated similarly.

Suppose that a symplectic method with two noises $\Phi_h:(p,q)\mapsto(P,Q)$ is generated by $\bar{S}^1(P,q,h)$ via the relation (5.1.9)

$$p = P + \frac{\partial \bar{S}^1}{\partial a}^T, \quad Q = q + \frac{\partial \bar{S}^1}{\partial P}^T.$$

We prove in the following that its modified equation is a stochastic Hamiltonian system with two noises.

Theorem 8.5. Given a stochastic Hamiltonian system with two noises

$$dy = J^{-1}\nabla H(y)dt + J^{-1}\nabla H_1(y) \circ dW_1(t) + J^{-1}\nabla H_2(y) \circ dW_2(t), \tag{8.4.1}$$

where $y = \begin{pmatrix} p \\ q \end{pmatrix}$. Suppose that a symplectic method Φ_h has generating function

$$\bar{S}^{1}(P,q,h) = F_{1}(P,q)W_{1}(h) + K_{1}(P,q)W_{2}(h)
+ F_{2}(P,q) \int_{0}^{h} W_{1} \circ dW_{1} + K_{2}(P,q) \int_{0}^{h} W_{2} \circ dW_{2}
+ G_{1}(P,q)h + \bar{F}_{2}(P,q) \int_{0}^{h} W_{2} \circ dW_{1} + \bar{K}_{2}(P,q) \int_{0}^{h} W_{1} \circ dW_{2}
+ G_{2}(P,q) \int_{0}^{h} W_{1}ds + \bar{G}_{2}(P,q) \int_{0}^{h} W_{2}ds
+ \tilde{F}_{2}(P,q) \int_{0}^{h} W_{1}W_{2} \circ dW_{1} + \tilde{K}_{2}(P,q) \int_{0}^{h} W_{1}W_{2} \circ dW_{2}
+ F_{3}(P,q) \int_{0}^{h} s \circ dW_{1} + K_{3}(P,q) \int_{0}^{h} s \circ dW_{2}
+ \tilde{G}_{2}(P,q) \int_{0}^{h} W_{1}W_{2}ds + G_{3}(P,q) \int_{0}^{h} sds
+ \dots \qquad (8.4.2)$$

Then the modified equation of Φ_h is a stochastic Hamiltonian system with two noises

$$dy = J^{-1}\nabla \tilde{H}(y)dt + J^{-1}\nabla \tilde{H}_1(y) \circ dW_1(t) + J^{-1}\nabla \tilde{H}_2(y) \circ dW_2(t), \tag{8.4.3}$$

where

$$\tilde{H}(p,q) = H(p,q) + H_3(p,q)W_1 + H_4(p,q)W_2 + H_5(p,q)W_1W_2 + H_6(p,q)h
+ H_7(p,q)hW_1 + H_8(p,q)hW_2 + H_9(p,q)hW_1W_2 + H_{10}(p,q)h^2 + \dots (8.4.4)
\tilde{H}_1(p,q) = H_1(p,q) + \bar{H}_2(p,q)W_1 + \bar{H}_3(p,q)W_2 + \bar{H}_4(p,q)W_1W_2 + \bar{H}_5(p,q)h
+ \bar{H}_6(p,q)hW_1 + \bar{H}_7(p,q)hW_2 + \bar{H}_8(p,q)hW_1W_2 + \bar{H}_9(p,q)h^2 + \dots (8.4.5)
\tilde{H}_2(p,q) = H_2(p,q) + \hat{H}_2(p,q)W_2 + \hat{H}_3(p,q)W_1 + \hat{H}_4(p,q)W_1W_2 + \hat{H}_5(p,q)h
+ \hat{H}_6(p,q)hW_2 + \hat{H}_7(p,q)hW_1 + \hat{H}_8(p,q)hW_1W_2 + \hat{H}_9(p,q)h^2 + \dots (8.4.6)$$

Proof. Suppose the phase trajectory of the stochastic Hamiltonian system with two noises (8.4.3) is generated by the function $\tilde{S}^1(P,q,t)$ through the relation (5.1.9). According to Theorem 6.2, it is sufficient that $\tilde{S}^1(P,q,t)$ satisfies the following Hamilton-Jacobi equation with two noises

$$\frac{\partial \tilde{S}^1}{\partial t} = \tilde{H}(P,Q) + \tilde{H}_1(P,Q)\dot{W}_1 + \tilde{H}_2(P,Q)\dot{W}_2, \tag{8.4.7}$$

where $Q = q + \frac{\partial \tilde{S}^1}{\partial P}^T$. Suppose

$$\tilde{S}^{1}(P,q,t) = \tilde{S}_{1}(P,q,h)W_{1}(t) + \tilde{U}_{1}(P,q,h)W_{2}(t)
+ \tilde{S}_{2}(P,q,h) \int_{0}^{t} W_{1} \circ dW_{1} + \tilde{U}_{2}(P,q,h) \int_{0}^{t} W_{2} \circ dW_{2}
+ \tilde{T}_{1}(P,q,h)t + \hat{S}_{2}(P,q,h) \int_{0}^{t} W_{2} \circ dW_{1} + \hat{U}_{2}(P,q,h) \int_{0}^{t} W_{1} \circ dW_{2}
+ \tilde{T}_{2}(P,q,h) \int_{0}^{t} W_{1}ds + \hat{T}_{2}(P,q,h) \int_{0}^{t} W_{2}ds
+ \tilde{S}_{2}(P,q,h) \int_{0}^{t} W_{1}W_{2} \circ dW_{1} + \tilde{U}_{2}(P,q,h) \int_{0}^{t} W_{1}W_{2} \circ dW_{2}
+ \tilde{S}_{3}(P,q,h) \int_{0}^{t} s \circ dW_{1} + U_{3}(P,q,h) \int_{0}^{t} s \circ dW_{2}
+ \tilde{T}_{2}(P,q,h) \int_{0}^{t} W_{1}W_{2}ds + \tilde{T}_{3}(P,q,h) \int_{0}^{t} s ds
+ \dots \qquad (8.4.8)$$

Thus

$$\frac{\partial \tilde{S}^{1}}{\partial t} = \tilde{T}_{1} + \tilde{T}_{2}W_{1} + \hat{T}_{2}W_{2} + \tilde{T}_{2}W_{1}W_{2} + \tilde{T}_{3}t + \tilde{T}_{4}tW_{1} + \hat{T}_{4}tW_{2}
+ \tilde{T}_{4}tW_{1}W_{2} + \tilde{T}_{5}t^{2} + \dots
+ \dot{W}_{1}(\tilde{S}_{1} + \tilde{S}_{2}W_{1} + \hat{S}_{2}W_{2} + \tilde{S}_{2}W_{1}W_{2} + \tilde{S}_{3}t + \tilde{S}_{4}tW_{1} + \hat{S}_{4}tW_{2}
+ \dot{S}_{4}tW_{1}W_{2} + \tilde{S}_{5}t^{2} + \dots)
+ \dot{W}_{2}(\tilde{U}_{1} + \tilde{U}_{2}W_{2} + \hat{U}_{2}W_{1} + \check{U}_{2}W_{1}W_{2} + \tilde{U}_{3}t + \tilde{U}_{4}tW_{2} + \hat{U}_{4}tW_{1}
+ \dot{U}_{4}tW_{1}W_{2} + \tilde{U}_{5}t^{2} + \dots),$$
(8.4.9)

where the functions \tilde{T}_i , \hat{T}_i , \tilde{T}_i , \tilde{S}_i , \hat{S}_i , \tilde{S}_i , \tilde{U}_i , \hat{U}_i and \tilde{U}_i are evaluated at (P, q, h).

As a consequence of (8.4.7) and (8.4.9), we have

$$\tilde{H}(P,Q) = \tilde{T}_1 + \tilde{T}_2 W_1 + \hat{T}_2 W_2 + \tilde{T}_2 W_1 W_2 + \tilde{T}_3 t
+ \tilde{T}_4 t W_1 + \hat{T}_4 t W_2 + \tilde{T}_4 t W_1 W_2 + \tilde{T}_5 t^2 + \dots,
\tilde{H}_1(P,Q) = \tilde{S}_1 + \tilde{S}_2 W_1 + \hat{S}_2 W_2 + \tilde{S}_2 W_1 W_2 + \tilde{S}_3 t
+ \tilde{S}_4 t W_1 + \hat{S}_4 t W_2 + \tilde{S}_4 t W_1 W_2 + \tilde{S}_5 t^2 + \dots,
\tilde{H}_2(P,Q) = \tilde{U}_1 + \tilde{U}_2 W_2 + \hat{U}_2 W_1 + \tilde{U}_2 W_1 W_2 + \tilde{U}_3 t
+ \tilde{U}_4 t W_2 + \hat{U}_4 t W_1 + \tilde{U}_4 t W_1 W_2 + \tilde{U}_5 t^2 + \dots$$
(8.4.12)

Expand H(P,Q) at (P,q) according to the formula of Wagner-Platen expansion in Stratonovich sense and the relation (8.4.3), and then let coefficients of terms of the same order of smallness on both sides of (8.4.10) be equal, we obtain

$$\begin{split} \tilde{T}_{1} &= \tilde{H}, \\ \tilde{T}_{2} &= \tilde{H}_{q} \tilde{H}_{1_{p}}, \\ \hat{T}_{2} &= \tilde{H}_{q} \tilde{H}_{2_{p}}, \\ \tilde{T}_{2} &= (\tilde{H}_{qq} \tilde{H}_{1_{p}} + \tilde{H}_{q} \tilde{H}_{1_{pq}}) \tilde{H}_{2_{p}} + (\tilde{H}_{qq} \tilde{H}_{2_{p}} + \tilde{H}_{q} \tilde{H}_{2_{pq}}) \tilde{H}_{1_{p}}, \\ \tilde{T}_{3} &= (\tilde{H}_{qq} \tilde{H}_{1_{p}} + \frac{1}{2} (\tilde{H}_{qq} \tilde{H}_{1_{p}} + \tilde{H}_{q} \tilde{H}_{1_{pq}}) \tilde{H}_{1_{p}} + \frac{1}{2} (\tilde{H}_{qq} \tilde{H}_{2_{p}} + \tilde{H}_{q} \tilde{H}_{2_{pq}}) \tilde{H}_{2_{p}}, \\ \vdots & (8.4.13) \end{split}$$

The same approach applied to (8.4.11) and (8.4.12) gives

$$\begin{split} \tilde{S}_{1} &= \tilde{H}_{1}, \\ \tilde{S}_{2} &= \tilde{H}_{1_{q}} \tilde{H}_{1_{p}}, \\ \hat{S}_{2} &= \tilde{H}_{1_{q}} \tilde{H}_{2_{p}}, \\ \tilde{S}_{2} &= (\tilde{H}_{1_{qq}} \tilde{H}_{1_{p}} + \tilde{H}_{1_{q}} \tilde{H}_{1_{pq}}) \tilde{H}_{2_{p}} + (\tilde{H}_{1_{qq}} \tilde{H}_{2_{p}} + \tilde{H}_{1_{q}} \tilde{H}_{2_{pq}}) \tilde{H}_{1_{p}}, \\ \tilde{S}_{3} &= \tilde{H}_{1_{q}} \tilde{H}_{p} + \frac{1}{2} (\tilde{H}_{1_{qq}} \tilde{H}_{1_{p}} + \tilde{H}_{1_{q}} \tilde{H}_{1_{pq}}) \tilde{H}_{1_{p}} + \frac{1}{2} (\tilde{H}_{1_{qq}} \tilde{H}_{2_{p}} + \tilde{H}_{1_{q}} \tilde{H}_{2_{pq}}) \tilde{H}_{2_{p}}, \\ \vdots & (8.4.14) \end{split}$$

and

$$\begin{split} \tilde{U}_{1} &= \tilde{H}_{2}, \\ \tilde{U}_{2} &= \tilde{H}_{2q} \tilde{H}_{1p}, \\ \hat{U}_{2} &= \tilde{H}_{2q} \tilde{H}_{2p}, \\ \hat{U}_{2} &= (\tilde{H}_{2qq} \tilde{H}_{1p} + \tilde{H}_{2q} \tilde{H}_{1pq}) \tilde{H}_{2p} + (\tilde{H}_{2qq} \tilde{H}_{2p} + \tilde{H}_{2q} \tilde{H}_{2pq}) \tilde{H}_{1p}, \\ \tilde{U}_{3} &= (\tilde{H}_{2q} \tilde{H}_{1p} + \frac{1}{2} (\tilde{H}_{2qq} \tilde{H}_{1p} + \tilde{H}_{2q} \tilde{H}_{1pq}) \tilde{H}_{1p} + \frac{1}{2} (\tilde{H}_{2qq} \tilde{H}_{2p} + \tilde{H}_{2q} \tilde{H}_{2pq}) \tilde{H}_{2p}, \\ \vdots & (8.4.15) \end{split}$$

respectively. As in the proof of Theorem 8.3, substitute (8.4.4)-(8.4.6) and (8.4.13)-(8.4.15) into the relation

$$\tilde{S}^{1}(P,q,h) = \bar{S}^{1}(P,q,h)$$
 (8.4.16)

with the two functions in this equation given in (8.4.8) and (8.4.2) respectively, and let coefficients of corresponding terms on both sides of (8.4.16) be equal, we get

$$\begin{array}{lll} H_1 &=& F_1, \\ H_2 &=& K_1, \\ \bar{H}_2 &=& F_2 - H_{1q} H_{1p}, \\ \dot{H}_2 &=& F_2 - H_{1q} H_{1p}, \\ \dot{H}_2 &=& K_2 - H_{2q} H_{1p}, \\ \dot{H}_3 &=& \bar{F}_2 - H_{1q} H_{2p}, \\ \dot{H}_3 &=& \bar{K}_2 - H_{2q} H_{2p}, \\ \dot{H}_3 &=& \bar{K}_2 - H_{2q} H_{2p}, \\ \dot{H}_4 &=& \bar{G}_2 - H_q H_{1p}, \\ \dot{H}_4 &=& \bar{G}_2 - H_q H_{1p}, \\ \dot{H}_4 &=& \bar{K}_2 - H_{2q} \bar{H}_{2p} - H_{1q} \bar{H}_{3p} - \bar{H}_{2q} H_{2p} - H_{1q} \hat{H}_{3p}, \\ &-& (H_{1qq} H_{1p} + H_{1q} H_{1pq}) H_{2p} - (H_{1qq} H_{2p} + H_{1q} H_{2pq}) H_{1p}, \\ \dot{H}_4 &=& \tilde{K}_2 - H_{2q} \bar{H}_{2p} - \hat{H}_{3q} H_{1p} - \hat{H}_{2q} H_{2p} - H_{2q} \hat{H}_{2p} \\ &-& (H_{2qq} H_{1p} + H_{2q} H_{1pq}) H_{2p} - (H_{2qq} H_{2p} + H_{2q} H_{2pq}) H_{1p}, \\ \bar{H}_5 &=& F_3 - \bar{H}_{2q} H_{1p} - H_{1q} \bar{H}_{2p} - \bar{H}_{3q} H_{2p} - \hat{H}_{2p} H_{1q} - H_{1q} H_{p} \\ &-& \frac{1}{2} (H_{1qq} H_{1p} + H_{1q} H_{1pq}) H_{1p} - \frac{1}{2} (H_{1qq} H_{2p} + H_{1q} H_{2pq}) H_{2p}, \\ \dot{H}_5 &=& K_3 - \hat{H}_{2q} H_{1p} - \bar{H}_{3p} H_{2q} - \hat{H}_{3p} H_{2p} - \hat{H}_{3p} H_{2q} - H_{2q} H_{p} \\ &-& \frac{1}{2} (H_{2qq} H_{1p} + H_{2q} H_{1pq}) H_{1p} - \frac{1}{2} (H_{2qq} H_{2p} + H_{2q} H_{2pq}) H_{2p}, \\ \dot{H}_5 &=& \tilde{G}_2 - H_{4q} H_{1p} - \bar{H}_{3p} H_{q} - H_{3q} H_{2p} - \hat{H}_{3p} H_{q} \\ &-& (H_{qq} H_{1p} + H_{q} H_{1pq}) H_{2p} - (H_{qq} H_{2p} + H_{q} H_{2pq}) H_{1p}, \\ \dot{H}_6 &=& G_3 - H_{3q} H_{1p} - \bar{H}_{2p} H_{q} - H_{4q} H_{2p} - \hat{H}_{2p} H_{q} - H_{q} H_{p} \\ &-& \frac{1}{2} (H_{qq} H_{1p} + H_{q} H_{1pq}) H_{1p} - \frac{1}{2} (H_{qq} H_{2p} + H_{q} H_{2pq}) H_{2p}, \\ \vdots , & \vdots , & (8.4.17) \\ \end{array}$$

from which the Hamiltonians \tilde{H} , \tilde{H}_1 and \tilde{H}_2 in (8.4.4)-(8.4.6) are determined explicitly. \square

Example 8.5. For the model of synchrotron oscillation (3.1.22)-(3.1.23)

$$dp = -\omega^2 \sin(q) dt - \sigma_1 \cos(q) \circ dW_1 - \sigma_2 \sin(q) \circ dW_2, \quad p(0) = p_0,$$

$$dq = pdt, \quad q(0) = q_0,$$

we have

$$H = -\omega^2 \cos(q) + \frac{p^2}{2}, \quad H_1 = \sigma_1 \sin(q), \quad H_2 = -\sigma_2 \cos(q).$$
 (8.4.18)

Now consider the symplectic method (6.1.43)-(6.1.44)

$$p_{n+1} = p_n - h\omega^2 sin(q_n) - \sigma_1 \cos(q_n) \Delta_n W_1 - \sigma_2 sin(q_n) \Delta_n W_2,$$

 $q_{n+1} = q_n + hp_{n+1},$

which is generated by

$$\bar{S}^{1}(P,q,h) = F_{1}W_{1}(h) + K_{1}W_{2}(h) + F_{2} \int_{0}^{h} W_{1} \circ dW_{1} + K_{2} \int_{0}^{h} W_{2} \circ dW_{2}
+ G_{1}h + \bar{F}_{2} \int_{0}^{h} W_{2} \circ dW_{1} + \bar{K}_{2} \int_{0}^{h} W_{1} \circ dW_{2}$$
(8.4.19)

via relation (5.1.9), where

$$G_1 = -\omega^2 \cos(q) + \frac{p^2}{2}, \quad F_1 = \sigma_1 \sin(q), \quad F_2 = \bar{F}_2 = 0,$$
 (8.4.20)

$$K_1 = -\sigma_2 \cos(q), \quad K_2 = \bar{K}_2 = 0.$$
 (8.4.21)

Substitute (8.4.18) and (8.4.20)-(8.4.21) into (8.4.17), we obtain

$$H_{1} = \sigma_{1}sin(q), \quad H_{2} = -\sigma_{2}\cos(q), \quad \bar{H}_{2} = 0,$$

$$\hat{H}_{2} = 0, \quad H = -\omega^{2}\cos(q) + \frac{p^{2}}{2}, \quad \bar{H}_{3} = 0,$$

$$\hat{H}_{3} = 0, \quad H_{3} = 0, \quad H_{4} = 0,$$

$$\bar{H}_{4} = 0, \quad \hat{H}_{4} = 0, \quad \bar{H}_{5} = -\sigma_{1}p\cos(q),$$

$$\hat{H}_{5} = -\sigma_{2}psin(q), \quad H_{5} = 0, \quad H_{6} = -p\omega^{2}sin(q),$$

$$\dots$$
(8.4.22)

Thus

$$\tilde{H} = -\omega^2 \cos(q) + \frac{p^2}{2} - h\omega^2 p \sin(q) + \dots,$$
 (8.4.23)

$$\tilde{H}_1 = \sigma_1 \sin(q) - h\sigma_1 p \cos(q) + \dots, \qquad (8.4.24)$$

$$\tilde{H}_2 = -\sigma_2 \cos(q) - h\sigma_2 p \sin(q) + \dots, \qquad (8.4.25)$$

and the truncated modified equation is

$$dy = J^{-1}\nabla \tilde{H}(y)dt + J^{-1}\nabla \tilde{H}_{1}(y) \circ dW_{1}(t) + J^{-1}\nabla \tilde{H}_{2}(y) \circ dW_{2}(t)$$

$$\approx \begin{pmatrix} h\omega^{2}p\cos(q) - \omega^{2}\sin(q) \\ p - h\omega^{2}\sin(q) \end{pmatrix} dt + \begin{pmatrix} -(\sigma_{1}\cos(q) + h\sigma_{1}p\sin(q)) \\ -h\sigma_{1}\cos(q) \end{pmatrix} \circ dW_{1}$$

$$+ \begin{pmatrix} h\sigma_{2}p\cos(q) - \sigma_{2}\sin(q) \\ -h\sigma_{2}\sin(q) \end{pmatrix} \circ dW_{2}, \tag{8.4.26}$$

which is also written as

$$dp = (h\omega^{2}p\cos(q) - \omega^{2}\sin(q))dt - (\sigma_{1}\cos(q) + h\sigma_{1}p\sin(q)) \circ dW_{1} + (h\sigma_{2}p\cos(q) - \sigma_{2}\sin(q)) \circ dW_{2}, p(0) = p_{0}, (8.4.27)$$

$$dq = (p - h\omega^{2}\sin(q))dt - h\sigma_{1}\cos(q) \circ dW_{1} - h\sigma_{2}\sin(q) \circ dW_{2}, q(0) = q_{0}.$$
 (8.4.28)

In numerical tests in Chapter 9, we simulate the solution of (8.4.27)-(8.4.28) by its symplectic Euler-Maruyama discretization

$$p_{n+1} = p_n + h^2 \omega^2 p_{n+1} \cos(q_n) - h\omega^2 \sin(q_n) - (\sigma_1 \cos(q_n) + h\sigma_1 p_{n+1} \sin(q_n)) \Delta_n W_1 + (h\sigma_2 p_{n+1} \cos(q_n) - \sigma_2 \sin(q_n)) \Delta_n W_2,$$
(8.4.29)
$$q_{n+1} = q_n + hp_{n+1} - h^2 \omega^2 \sin(q_n) - h\sigma_1 \cos(q_n) \Delta_n W_1 - h\sigma_2 \sin(q_n) \Delta_n W_2.$$
(8.4.30)

We realize it by fixed point iteration.

We can also use generating function $\bar{S}^3(u,v,h)$ with two noises to construct modified equation of a symplectic method with two noises. Assume that the symplectic method $\Phi_h: (p,q) \mapsto (P,Q)$ is generated by $\bar{S}^3(u,v,h)$ via relation (5.1.15)-(5.1.16)

$$P = p - \partial_2^T \bar{S}^3(u, v), \quad Q = q + \partial_1^T \bar{S}^3(u, v),$$

where $u = \frac{P+p}{2}$, $v = \frac{Q+q}{2}$. Then we can find as in Theorem 8.5 the modified equation of Φ_h , which is a stochastic Hamiltonian system, by using $\bar{S}^3(u,v,h)$.

Theorem 8.6. Given a stochastic Hamiltonian system with two noises (8.4.1)

$$dy = J^{-1}\nabla H(y)dt + J^{-1}\nabla H_1(y) \circ dW_1(t) + J^{-1}\nabla H_2(y) \circ dW_2(t),$$

where $y = \begin{pmatrix} p \\ q \end{pmatrix}$. Suppose that a symplectic method Φ_h has generating function

$$\bar{S}^{3}(u,v,h) = F_{1}(u,v)W_{1}(h) + K_{1}(u,v)W_{2}(h)
+ F_{2}(u,v) \int_{0}^{h} W_{1} \circ dW_{1} + K_{2}(u,v) \int_{0}^{h} W_{2} \circ dW_{2}
+ G_{1}(u,v)h + \bar{F}_{2}(u,v) \int_{0}^{h} W_{2} \circ dW_{1} + \bar{K}_{2}(u,v) \int_{0}^{h} W_{1} \circ dW_{2}
+ G_{2}(u,v) \int_{0}^{h} W_{1}ds + \bar{G}_{2}(u,v) \int_{0}^{h} W_{2}ds
+ \tilde{F}_{2}(u,v) \int_{0}^{h} W_{1}W_{2} \circ dW_{1} + \tilde{K}_{2}(u,v) \int_{0}^{h} W_{1}W_{2} \circ dW_{2}
+ F_{3}(u,v) \int_{0}^{h} s \circ dW_{1} + K_{3}(u,v) \int_{0}^{h} s \circ dW_{2}
+ \tilde{G}_{2}(u,v) \int_{0}^{h} W_{1}W_{2}ds + G_{3}(u,v) \int_{0}^{h} sds
+ \dots \qquad (8.4.31)$$

Then the modified equation of Φ_h is a stochastic Hamiltonian system with two noises

$$dy = J^{-1}\nabla \tilde{H}(y)dt + J^{-1}\nabla \tilde{H}_1(y) \circ dW_1(t) + J^{-1}\nabla \tilde{H}_2(y) \circ dW_2(t), \tag{8.4.32}$$

where

$$\begin{split} \tilde{H}(p,q) &= H(p,q) + H_3(p,q)W_1 + H_4(p,q)W_2 + H_5(p,q)W_1W_2 + H_6(p,q)h \\ &+ H_7(p,q)hW_1 + H_8(p,q)hW_2 + H_9(p,q)hW_1W_2 + H_{10}(p,q)h^2 + \dots, \\ & (8.4.33) \\ \tilde{H}_1(p,q) &= H_1(p,q) + \bar{H}_2(p,q)W_1 + \bar{H}_3(p,q)W_2 + \bar{H}_4(p,q)W_1W_2 + \bar{H}_5(p,q)h \\ &+ \bar{H}_6(p,q)hW_1 + \bar{H}_7(p,q)hW_2 + \bar{H}_8(p,q)hW_1W_2 + \bar{H}_9(p,q)h^2 + \dots, \\ & (8.4.34) \\ \tilde{H}_2(p,q) &= H_2(p,q) + \hat{H}_2(p,q)W_2 + \hat{H}_3(p,q)W_1 + \hat{H}_4(p,q)W_1W_2 + \hat{H}_5(p,q)h \\ &+ \hat{H}_6(p,q)hW_2 + \hat{H}_7(p,q)hW_1 + \hat{H}_8(p,q)hW_1W_2 + \hat{H}_9(p,q)h^2 + \dots. \end{split}$$

Proof. Suppose that the phase trajectory of the stochastic Hamiltonian system (8.4.32) is generated by the function $\tilde{S}^3(u,v,t)$ via relation (5.1.15)-(5.1.16). Thus according to Theorem 6.6, it is sufficient that $\tilde{S}^3(u,v,t)$ satisfies the following Hamilton-Jacobi equation with two noises:

$$\frac{\partial \tilde{S}^3}{\partial t} = \tilde{H}(P,Q) + \tilde{H}_1(P,Q)\dot{W}_1 + \tilde{H}_2(P,Q)\dot{W}_2, \quad \tilde{S}^3(u,v,0) = 0, \tag{8.4.36}$$

where $P = u - \frac{1}{2} \frac{\partial \tilde{S}^3}{\partial v}^T$, $Q = v + \frac{1}{2} \frac{\partial \tilde{S}^3}{\partial u}^T$. In order to solve the equation (8.4.36), let

$$\tilde{S}^{3}(u,v,t) = \tilde{S}_{1}(u,v,h)W_{1}(t) + \tilde{U}_{1}(u,v,h)W_{2}(t)
+ \tilde{S}_{2}(u,v,h) \int_{0}^{t} W_{1} \circ dW_{1} + \tilde{U}_{2}(u,v,h) \int_{0}^{t} W_{2} \circ dW_{2}
+ \tilde{T}_{1}(u,v,h)t + \hat{S}_{2}(u,v,h) \int_{0}^{t} W_{2} \circ dW_{1} + \hat{U}_{2}(u,v,h) \int_{0}^{t} W_{1} \circ dW_{2}
+ \tilde{T}_{2}(u,v,h) \int_{0}^{t} W_{1}ds + \hat{T}_{2}(u,v,h) \int_{0}^{t} W_{2}ds
+ \tilde{S}_{2}(u,v,h) \int_{0}^{t} W_{1}W_{2} \circ dW_{1} + \tilde{U}_{2}(u,v,h) \int_{0}^{t} W_{1}W_{2} \circ dW_{2}
+ \tilde{S}_{3}(u,v,h) \int_{0}^{t} s \circ dW_{1} + U_{3}(u,v,h) \int_{0}^{t} s \circ dW_{2}
+ \tilde{T}_{2}(u,v,h) \int_{0}^{t} W_{1}W_{2}ds + \tilde{T}_{3}(u,v,h) \int_{0}^{t} sds
+ \dots$$
(8.4.37)

Thus

$$\frac{\partial \tilde{S}^{3}}{\partial t} = \tilde{T}_{1} + \tilde{T}_{2}W_{1} + \hat{T}_{2}W_{2} + \tilde{T}_{2}W_{1}W_{2} + \tilde{T}_{3}t + \tilde{T}_{4}tW_{1} + \hat{T}_{4}tW_{2}
+ \tilde{T}_{4}tW_{1}W_{2} + \tilde{T}_{5}t^{2} + \dots
+ \dot{W}_{1}(\tilde{S}_{1} + \tilde{S}_{2}W_{1} + \hat{S}_{2}W_{2} + \tilde{S}_{2}W_{1}W_{2} + \tilde{S}_{3}t + \tilde{S}_{4}tW_{1} + \hat{S}_{4}tW_{2}
+ \dot{S}_{4}tW_{1}W_{2} + \tilde{S}_{5}t^{2} + \dots)
+ \dot{W}_{2}(\tilde{U}_{1} + \tilde{U}_{2}W_{2} + \hat{U}_{2}W_{1} + \check{U}_{2}W_{1}W_{2} + \tilde{U}_{3}t + \tilde{U}_{4}tW_{2} + \hat{U}_{4}tW_{1}
+ \dot{U}_{4}tW_{1}W_{2} + \tilde{U}_{5}t^{2} + \dots),$$
(8.4.38)

where the functions \tilde{T}_i , \hat{T}_i , \tilde{T}_i , \tilde{S}_i , \hat{S}_i , \hat{S}_i , \tilde{U}_i , \hat{U}_i and \tilde{U}_i are evaluated at (u, v, h).

(8.4.36) and (8.4.38) implies

$$\tilde{H}(P,Q) = \tilde{T}_1 + \tilde{T}_2 W_1 + \hat{T}_2 W_2 + \check{T}_2 W_1 W_2 + \tilde{T}_3 t
+ \tilde{T}_4 t W_1 + \hat{T}_4 t W_2 + \check{T}_4 t W_1 W_2 + \tilde{T}_5 t^2 + \dots,
\tilde{H}_1(P,Q) = \tilde{S}_1 + \tilde{S}_2 W_1 + \hat{S}_2 W_2 + \check{S}_2 W_1 W_2 + \tilde{S}_3 t
+ \tilde{S}_4 t W_1 + \hat{S}_4 t W_2 + \check{S}_4 t W_1 W_2 + \tilde{S}_5 t^2 + \dots,
\tilde{H}_2(P,Q) = \tilde{U}_1 + \tilde{U}_2 W_2 + \hat{U}_2 W_1 + \check{U}_2 W_1 W_2 + \tilde{U}_3 t
+ \tilde{U}_4 t W_2 + \hat{U}_4 t W_1 + \check{U}_4 t W_1 W_2 + \tilde{U}_5 t^2 + \dots$$
(8.4.41)

Expand $\tilde{H}(P,Q)$ at (u,v) according to the formula of Wagner-Platen expansion in Stratonovich sense and the relation (8.4.32), and then let coefficients of terms of the same order of smallness on both sides of (8.4.39) be equal, we obtain

$$\tilde{T}_{1} = \tilde{H},
\tilde{T}_{2} = \frac{1}{\sqrt{2}} (\tilde{H}_{v} \tilde{H}_{1_{u}} - \tilde{H}_{u} \tilde{H}_{1_{v}}),
\tilde{T}_{2} = \frac{1}{\sqrt{2}} (\tilde{H}_{v} \tilde{H}_{2_{u}} - \tilde{H}_{u} \tilde{H}_{2_{v}}),
\tilde{T}_{2} = \frac{1}{2} [\tilde{H}_{1v} (\tilde{H}_{uu} \tilde{H}_{2v} + \tilde{H}_{u} \tilde{H}_{2uv}) + \tilde{H}_{1u} (\tilde{H}_{vv} \tilde{H}_{2u} + \tilde{H}_{v} \tilde{H}_{2uv} - \tilde{H}_{uv} \tilde{H}_{2v} - \tilde{H}_{u} \tilde{H}_{2vv})
+ \tilde{H}_{2v} (\tilde{H}_{uu} \tilde{H}_{1v} + \tilde{H}_{u} \tilde{H}_{1uv}) + \tilde{H}_{1u} (\tilde{H}_{vv} \tilde{H}_{1u} + \tilde{H}_{v} \tilde{H}_{1uv} - \tilde{H}_{uv} \tilde{H}_{1v} - \tilde{H}_{u} \tilde{H}_{1vv})],
\tilde{T}_{3} = \frac{1}{2} [\tilde{H}_{v} \tilde{H}_{1u} - \tilde{H}_{u} \tilde{H}_{1v} + \tilde{H}_{1v} (\tilde{H}_{uu} \tilde{H}_{1v} + \tilde{H}_{u} \tilde{H}_{1uv}) + \tilde{H}_{1u} (\tilde{H}_{vv} \tilde{H}_{1u} + \tilde{H}_{v} \tilde{H}_{1uv})
- \tilde{H}_{uv} \tilde{H}_{1v} - \tilde{H}_{u} \tilde{H}_{1vv}) + \tilde{H}_{2v} (\tilde{H}_{uu} \tilde{H}_{2v} + \tilde{H}_{u} \tilde{H}_{2uv})
+ \tilde{H}_{2u} (\tilde{H}_{vv} \tilde{H}_{2u} + \tilde{H}_{v} \tilde{H}_{2uv} - \tilde{H}_{uv} \tilde{H}_{2v} - \tilde{H}_{u} \tilde{H}_{2vv})],
\dots$$
(8.4.42)

The same approach applied to $\tilde{H}_1(P,Q)$ and $\tilde{H}_2(P,Q)$ gives

$$\tilde{S}_{1} = \tilde{H}_{1},
\tilde{S}_{2} = \frac{1}{\sqrt{2}} (\tilde{H}_{1v} \tilde{H}_{1u} - \tilde{H}_{1u} \tilde{H}_{1v}) = 0,
\hat{S}_{2} = \frac{1}{\sqrt{2}} (\tilde{H}_{1v} \tilde{H}_{2u} - \tilde{H}_{1u} \tilde{H}_{2v}),
\tilde{S}_{2} = \frac{1}{2} [\tilde{H}_{1v} (\tilde{H}_{1uu} \tilde{H}_{2v} + \tilde{H}_{1u} \tilde{H}_{2uv}) + \tilde{H}_{1u} (\tilde{H}_{1vv} \tilde{H}_{2u} + \tilde{H}_{1v} \tilde{H}_{2uv} - \tilde{H}_{1uv} \tilde{H}_{2v} - \tilde{H}_{1u} \tilde{H}_{2vv})
+ \tilde{H}_{2v} (\tilde{H}_{1uu} \tilde{H}_{1v} + \tilde{H}_{1u} \tilde{H}_{1uv}) + \tilde{H}_{1u} (\tilde{H}_{1vv} \tilde{H}_{1u} + \tilde{H}_{1v} \tilde{H}_{1uv} - \tilde{H}_{1uv} \tilde{H}_{1v} - \tilde{H}_{1u} \tilde{H}_{1vv})],
\tilde{S}_{3} = \frac{1}{2} [\tilde{H}_{1v} \tilde{H}_{1u} - \tilde{H}_{1u} \tilde{H}_{1v} + \tilde{H}_{1v} (\tilde{H}_{1uu} \tilde{H}_{1v} + \tilde{H}_{1u} \tilde{H}_{1uv}) + \tilde{H}_{1u} (\tilde{H}_{1vv} \tilde{H}_{1u} + \tilde{H}_{1v} \tilde{H}_{1u}) + \tilde{H}_{1u} (\tilde{H}_{1vv} \tilde{H}_{1u} + \tilde{H}_{1v} \tilde{H}_{1uv})
- \tilde{H}_{1uv} \tilde{H}_{1v} - \tilde{H}_{1u} \tilde{H}_{1vv}) + \tilde{H}_{2v} (\tilde{H}_{1uu} \tilde{H}_{2v} + \tilde{H}_{1u} \tilde{H}_{2uv})
+ \tilde{H}_{2u} (\tilde{H}_{1vv} \tilde{H}_{2u} + \tilde{H}_{1v} \tilde{H}_{2uv} - \tilde{H}_{1uv} \tilde{H}_{2v} - \tilde{H}_{1u} \tilde{H}_{2vv})],
\dots,$$
(8.4.43)

and

$$\tilde{U}_{1} = \tilde{H}_{2},
\tilde{U}_{2} = \frac{1}{\sqrt{2}} (\tilde{H}_{2_{v}} \tilde{H}_{1_{u}} - \tilde{H}_{2_{u}} \tilde{H}_{1_{v}}),
\tilde{U}_{2} = \frac{1}{\sqrt{2}} (\tilde{H}_{2_{v}} \tilde{H}_{2_{u}} - \tilde{H}_{2_{u}} \tilde{H}_{2_{v}}) = 0,
\tilde{U}_{2} = \frac{1}{2} [\tilde{H}_{1_{v}} (\tilde{H}_{2_{uu}} \tilde{H}_{2_{v}} + \tilde{H}_{2_{u}} \tilde{H}_{2_{uv}}) + \tilde{H}_{1_{u}} (\tilde{H}_{2_{vv}} \tilde{H}_{2_{u}} + \tilde{H}_{2_{v}} \tilde{H}_{2_{uv}} - \tilde{H}_{2_{uv}} \tilde{H}_{2_{v}} - \tilde{H}_{2_{u}} \tilde{H}_{2_{vv}})
+ \tilde{H}_{2_{v}} (\tilde{H}_{2_{uu}} \tilde{H}_{1_{v}} + \tilde{H}_{2_{u}} \tilde{H}_{1_{uv}}) + \tilde{H}_{1_{u}} (\tilde{H}_{2_{vv}} \tilde{H}_{1_{u}} + \tilde{H}_{2_{v}} \tilde{H}_{1_{uv}} - \tilde{H}_{2_{uv}} \tilde{H}_{1_{v}} - \tilde{H}_{2_{u}} \tilde{H}_{1_{vv}})],
\tilde{U}_{3} = \frac{1}{2} [\tilde{H}_{2_{v}} \tilde{H}_{1_{u}} - \tilde{H}_{2_{u}} \tilde{H}_{1_{v}} + \tilde{H}_{1_{v}} (\tilde{H}_{2_{uu}} \tilde{H}_{1_{v}} + \tilde{H}_{2_{u}} \tilde{H}_{1_{uv}}) + \tilde{H}_{1_{u}} (\tilde{H}_{2_{vv}} \tilde{H}_{1_{u}} + \tilde{H}_{2_{v}} \tilde{H}_{1_{uv}})
- \tilde{H}_{2_{uv}} \tilde{H}_{1_{v}} - \tilde{H}_{2_{u}} \tilde{H}_{1_{vv}}) + \tilde{H}_{2_{v}} (\tilde{H}_{2_{uu}} \tilde{H}_{2_{v}} + \tilde{H}_{2_{u}} \tilde{H}_{2_{uv}})
+ \tilde{H}_{2_{u}} (\tilde{H}_{2_{vv}} \tilde{H}_{2_{u}} + \tilde{H}_{2_{-v}} \tilde{H}_{2_{uv}} - \tilde{H}_{2_{uv}} \tilde{H}_{2_{v}} - \tilde{H}_{2_{u}} \tilde{H}_{2_{vv}})],
\dots, (8.4.44)$$

respectively.

Substitute (8.4.42)-(8.4.44) and (8.4.33)-(8.4.35) into the relation

$$\tilde{S}^3(u,v,h) = \bar{S}^3(u,v,h),$$

and compares coefficients of terms with the same order of smallness on both sides of the equation, we obtain

$$H_{1} = F_{1},$$

$$H_{2} = K_{1},$$

$$\bar{H}_{2} = F_{2},$$

$$\hat{H}_{2} = K_{2} - \frac{1}{\sqrt{2}} (\tilde{H}_{2v} \tilde{H}_{1u} - \tilde{H}_{2u} \tilde{H}_{1v}),$$

$$H = G_{1},$$

$$\bar{H}_{3} = \bar{F}_{2} - \frac{1}{\sqrt{2}} (\tilde{H}_{1v} \tilde{H}_{2u} - \tilde{H}_{1u} \tilde{H}_{2v}),$$

$$\hat{H}_{3} = \bar{K}_{2},$$

$$H_{3} = G_{2} - \frac{1}{\sqrt{2}} (\tilde{H}_{v} \tilde{H}_{1u} - \tilde{H}_{u} \tilde{H}_{1v}),$$

$$H_{4} = \bar{G}_{2} - \frac{1}{\sqrt{2}} (\tilde{H}_{v} \tilde{H}_{2u} - \tilde{H}_{u} \tilde{H}_{2v}),$$

$$\vdots,$$

$$(8.4.45)$$

from which the Hamiltonians in (8.4.33)-(8.4.35) are determined explicitly.

Example 8.6. For the system with two additive noises (3.1.27)-(3.1.28)

$$dp = -qdt + \gamma \circ dW_2(t), \quad p(0) = p_0,$$

$$dq = pdt + \sigma \circ dW_1(t), \quad q(0) = q_0,$$

we have

$$H = \frac{1}{2}(p^2 + q^2), \quad H_1 = \sigma p, \quad H_2 = -\gamma q.$$

Its symplectic discretization (6.2.32)-(6.2.33)

$$p_{n+1} + \frac{h}{2}q_{n+1} = p_n - \frac{h}{2}q_n + \gamma \Delta_n W_2,$$

$$-\frac{h}{2}p_{n+1} + q_{n+1} = \frac{h}{2}p_n + q_n + \sigma \Delta_n W_1$$

is generated by

$$\bar{S}^{3}(u,v,h) = F_{1}W_{1} + K_{1}W_{2} + K_{2}\int_{0}^{h} W_{2} \circ dW_{2} + G_{1}h + \bar{F}_{2}\int_{0}^{h} W_{2} \circ dW_{1},$$

where

$$F_1 = \sigma u, \quad K_1 = -\gamma v, \quad F_2 = 0, \quad K_2 = -\frac{1}{\sqrt{2}}\sigma\gamma,$$

 $G_1 = \frac{1}{2}(u^2 + v^2), \quad \bar{F}_2 = \frac{1}{\sqrt{2}}\sigma\gamma, \quad \bar{K}_2 = 0.$

Thus, according to (8.4.45), we have

$$H_1 = \sigma u, \quad H_2 = -\gamma v, \quad \bar{H}_2 = 0, \quad \hat{H}_2 = 0,$$
 $H = \frac{1}{2}(u^2 + v^2), \quad \bar{H}_3 = 0, \quad \hat{H}_3 = 0,$
 $H_3 = -\frac{1}{\sqrt{2}}\sigma v, \quad H_4 = -\frac{1}{\sqrt{2}}\gamma u, \quad \dots$

$$(8.4.46)$$

Consequently, we get the following truncated Hamiltonians

$$\tilde{H}(u,v,h) \approx \frac{1}{2}(u^2+v^2) - \frac{1}{\sqrt{2}}\sigma v W_1(h) - \frac{1}{\sqrt{2}}\gamma u W_2(h),$$
 (8.4.47)

$$\tilde{H}_1(u, v, h) \approx \sigma u,$$
 (8.4.48)

$$\tilde{H}_2(u, v, h) \approx -\gamma v,$$
 (8.4.49)

which implies that the truncated modified equation is

$$dy = J^{-1}\nabla \tilde{H}(y)dt + J^{-1}\nabla \tilde{H}_{1}(y) \circ dW_{1} + J^{-1}\nabla \tilde{H}_{2}(y) \circ dW_{2}$$

$$\approx \left(\frac{\sigma}{\sqrt{2}}W_{1}(h) - q \atop p - \frac{\gamma}{\sqrt{2}}W_{2}(h)\right)dt + \left(\begin{array}{c}0\\\sigma\end{array}\right) \circ dW_{1} + \left(\begin{array}{c}\gamma\\0\end{array}\right) \circ dW_{2}. \tag{8.4.50}$$

With initial value (p_0, q_0) , (8.4.50) can also be written as

$$dp = \left(\frac{\sigma}{\sqrt{2}}W_1(h) - q\right)dt + \gamma \circ dW_2, \quad p(0) = p_0,$$
 (8.4.51)

$$dq = (p - \frac{\gamma}{\sqrt{2}}W_2(h))dt + \sigma \circ dW_1, \quad q(0) = q_0.$$
 (8.4.52)

We simulate the modified equation (8.4.51)-(8.4.52) in Chapter 9 by its midpoint discretization

$$p_{n+1} + \frac{h}{2}q_{n+1} = p_n - \frac{h}{2}q_n + \frac{h}{\sqrt{2}}\sigma\Delta_n W_1 + \gamma\Delta_n W_2,$$
 (8.4.53)

$$-\frac{h}{2}p_{n+1} + q_{n+1} = \frac{h}{2}P_n + q_n - \frac{h}{\sqrt{2}}\gamma\Delta_n W_2 + \sigma\Delta_n W_1.$$
 (8.4.54)

Chapter 9

Numerical Tests

In this chapter, numerical tests are performed on the schemes produced in the previous chapters via variational integrators and generating functions, in order to observe their effect of simulating stochastic Hamiltonian systems. As test systems the linear stochastic oscillator (3.1.7)-(3.1.8), the Kubo oscillator (3.1.16)-(3.1.17), the model of synchrotron oscillations (3.1.22)-(3.1.23), and the system with two additive noises (3.1.27)-(3.1.28) are considered. Numerical tests are also performed to compare sample trajectories of some stochastic symplectic methods and their modified equations constructed via generating functions.

9.1 A Linear Stochastic Oscillator

For convenience, we write the equation of the linear stochastic oscillator (3.1.7)-(3.1.8) once again.

$$dy = -xdt + \sigma dW, \quad y(0) = 0,$$
 (9.1.1)

$$dx = ydt, x(0) = 1. (9.1.2)$$

The scheme (5.3.27)-(5.3.28) generated by $\bar{S}^1(P,q,t)$

$$x_{n+1} = x_n + hy_{n+1},$$

$$y_{n+1} = y_n - hx_n + \sigma \Delta W_n,$$

is the symplectic Euler-Maruyama method and of mean-square order of convergence 1. We check by numerical tests its ability of preserving the linear growth property of the second moment (3.1.14) and the oscillation property of the oscillator given in Proposition 3.8.

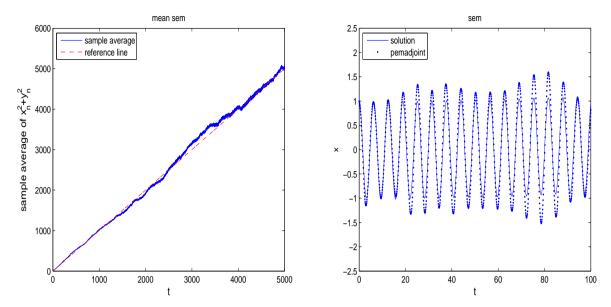


Figure 1.1: Linear growth of second moment.

Figure 1.2: Oscillation property of x.

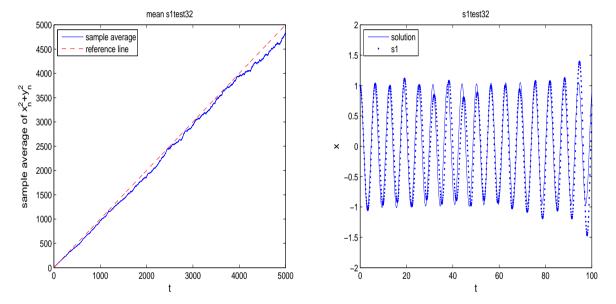


Figure 1.3: Linear growth of second moment.

Figure 1.4: Oscillation property of x.

Figure 1.1 shows linear growth of second moment of the numerical solution arising from scheme (5.3.27)-(5.3.28), where we take $\sigma = 1$, $t \in [0, 5000]$, and step size h = 0.2. The second moment $\mathbb{E}(x_n^2 + y_n^2)$ of the numerical solution is approximated by taking sample average of 500 sample trajectories produced by the numerical scheme. The reference line (dashed) has slope 1.

In Figure 1.2, the solid curve simulates the solution x given in (3.1.13) with $x_0 = 1$ and $\sigma = 0.1$. The step size in simulating the integral in solution (3.1.13) is $\Delta s = 0.001$. The dotted curve is numerical x created by scheme (5.3.27)-(5.3.28), where the step size is h = 0.1, and $t \in [0, 100]$.

Consider the scheme (5.3.32)-(5.3.33) with mean-square order $\frac{3}{2}$ produced by \bar{S}^1

$$y_n = y_{n+1} + hx_n - \sigma \Delta W_n + \frac{h^2}{2} y_{n+1},$$

$$x_{n+1} = x_n + hy_{n+1} - \sigma \int_0^h s \circ dW + \frac{h^2}{2} x_n.$$

The linear growth property of the second moment of the numerical solution given by the scheme (5.3.32)-(5.3.33) is illustrated in Figure 1.3, and its oscillation property in Figure 1.4. The solid curve in Figure 1.3 and the dotted one in Figure 1.4 are from the numerical solution, as in Figure 1.1 and 1.2. The data for Figure 1.3 and 1.4 are the same as that for Figure 1.1 and 1.2 respectively.

The scheme (5.4.22)-(5.4.23) is the midpoint rule

$$x_{n+1} = x_n + h \frac{y_n + y_{n+1}}{2},$$

 $y_{n+1} = y_n - h \frac{x_n + x_{n+1}}{2} + \sigma \Delta W_n,$

which is generated by \bar{S}^3 , and also by the variational integrator as given in Example 4.2. This method is of mean-square order 1 according to the construction of \bar{S}^3 .

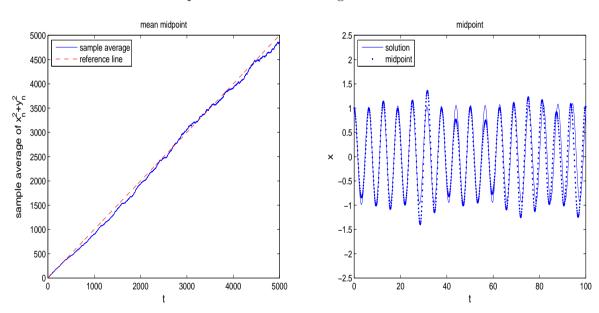


Figure 1.5: Linear growth of second moment.

Figure 1.6: Oscillation property of x.

Data and settings for Figure 1.5 and 1.6 are the same as that for Figure 1.3 and 1.4 respectively.

Scheme (5.4.25)-(5.4.26)

$$x_{n+1} = x_n + h \frac{y_n + y_{n+1}}{2} - \frac{\sigma}{2} \int_0^h s \circ dW + \frac{\sigma}{\sqrt{2}} \int_0^h W ds,$$

$$y_{n+1} = y_n - h \frac{x_n + x_{n+1}}{2} + \sigma \Delta W_n.$$

is produced by \bar{S}^3 with mean-square order $\frac{3}{2}$.

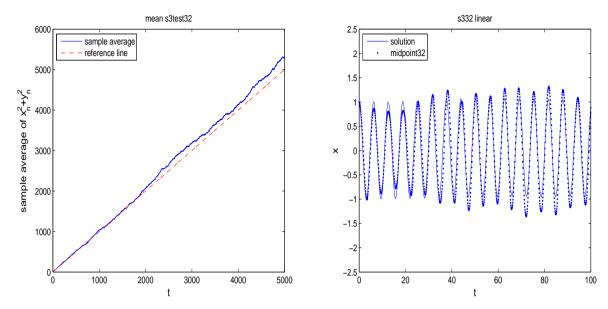


Figure 1.7: Linear growth of second moment.

Figure 1.8: Oscillation property of x.

Data and settings for Figure 1.7 and 1.8 are the same as that for Figure 1.5 and 1.6 respectively.

9.2 Kubo Oscillator

For the Kubo oscillator (3.1.16)-(3.1.17) with given initial values

$$dp = -aqdt - \sigma q \circ dW(t), \qquad p(0) = 1,$$

$$dq = apdt + \sigma p \circ dW(t), \qquad q(0) = 0,$$

 \bar{S}^1 generates the scheme (5.3.42)-(5.3.43)

$$p_{n+1} = p_n - ahq_n - \frac{h}{2}\sigma^2 p_{n+1} - \sigma q_n \Delta W_n,$$

$$q_{n+1} = q_n + ahp_{n+1} + \frac{h}{2}\sigma^2 q_n + \sigma p_{n+1} \Delta W_n,$$

which is of mean-square order 1, and also given by Milstein et. al. in [29]. A method of mean-square order $\frac{3}{2}$ generated by \vec{S}^1 is scheme (5.3.46)

$$-(ah + \frac{h^2}{2}a\sigma^2 + \sigma\Delta W_n + \sigma^3 \int_0^h s \circ dW)p_{n+1} + q_{n+1} = (1 + \frac{h\sigma^2}{2} + \frac{h^2a^2}{2} + a\sigma h\Delta W_n)q_n,$$

$$(1 + \frac{h\sigma^2}{2} + \frac{h^2a^2}{2} + a\sigma h\Delta W_n)p_{n+1} = p_n - (ah + \sigma\Delta W_n)q_n.$$

As indicated by (3.1.21), the phase trajectory of Kubo oscillator is a circle centered at the origin and with radius $\sqrt{p_0^2 + q_0^2}$, which is 1 in our discussion here. Figure 2.1 and 2.2 below show the phase trajectories of the numerical solutions arising from scheme (5.3.42)-(5.3.43) and (5.3.46) respectively.

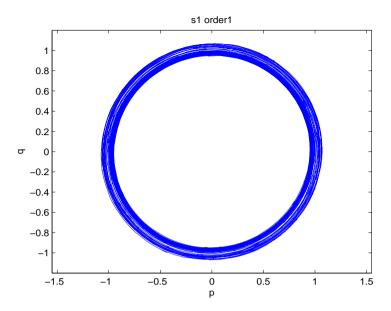


Figure 2.1: Phase trajectory of (5.3.42)-(5.3.43).

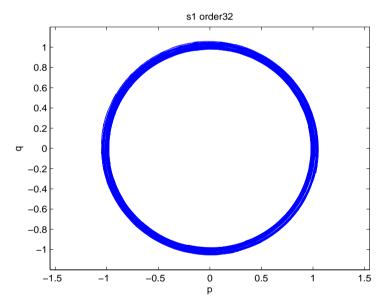


Figure 2.2: Phase trajectory of (5.3.46).

It is clear that the method of mean-square order $\frac{3}{2}$ simulates phase trajectory better than that of order 1. We take $a=2, \sigma=0.3, t\in[0,200]$, and step size h=0.02 in the two tests above, where ΔW_n in the schemes are truncated according to (3.2.13) with k=2.

Applying generating function \bar{S}^3 to the Kubo oscillator, we obtain scheme (5.4.31)-(5.4.32)

$$\begin{array}{rcl} p_{n+1} & = & p_n - ah\frac{q_n + q_{n+1}}{2} - \sigma\frac{q_n + q_{n+1}}{2}\Delta W_n, \\ \\ q_{n+1} & = & q_n + ah\frac{p_n + p_{n+1}}{2} + \sigma\frac{p_n + p_{n+1}}{2}\Delta W_n, \end{array}$$

which is also given by Milstein et. al. in [29], and of mean-square order 1. A method of mean-square order $\frac{3}{2}$ produced by \bar{S}^3 is scheme (5.4.34)-(5.4.35)

$$p_{n+1} = p_n - (ah + \sigma \Delta W_n + \frac{ah^2\sigma^2}{4} + \frac{\sigma^3}{2} \int_0^h s \circ dW) \frac{q_n + q_{n+1}}{2},$$

$$q_{n+1} = q_n + (ah + \sigma \Delta W_n - \frac{ah^2\sigma^2}{4} - \frac{\sigma^3}{2} \int_0^h s \circ dW) \frac{p_n + p_{n+1}}{2}.$$

The phase trajectories arising from (5.4.31)-(5.4.32) and (5.4.34)-(5.4.35) are shown in Figure 2.3 and 2.4 respectively.

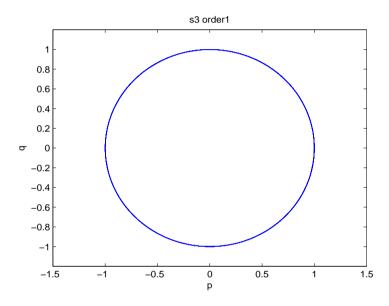


Figure 2.3: Phase trajectory of (5.4.31)-(5.4.32).

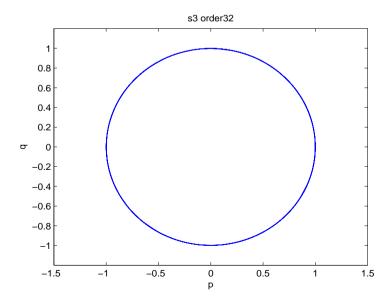


Figure 2.4: Phase trajectory of (5.4.34)-(5.4.35).

Both of the two schemes reproduce phase trajectory of the Kubo oscillator with high accuracy. The advantage of applying \bar{S}^3 instead of \bar{S}^1 to the simulation of Kubo oscillator is clear.

9.3 A Model of Synchrotron Oscillations

For the model of synchrotron oscillations (3.1.22)-(3.1.23)

$$dp = -\omega^2 \sin(q) dt - \sigma_1 \cos(q) \circ dW_1 - \sigma_2 \sin(q) \circ dW_2,$$

$$dq = p dt,$$

Milstein et. al. proposed in [29] the symplectic scheme

$$p_{n+1} = p_n - h\omega^2 \sin(q_{n+1}) - \sigma_1 \cos(q_{n+1}) \Delta_n W_1 - \sigma_2 \sin(q_{n+1}) \Delta_n W_2, \quad (9.3.1)$$

$$q_{n+1} = q_n + hp_n, \quad (9.3.2)$$

which is of mean-square order 1. It is also shown that this scheme simulates the sample trajectory of the model with high accuracy. In the following tests, we use the sample trajectory created by it as reference.

Applying \bar{S}^1 , we have constructed scheme (6.1.43)-(6.1.44)

$$p_{n+1} = p_n - h\omega^2 \sin(q_n) - \sigma_1 \cos(q_n) \Delta_n W_1 - \sigma_2 \sin(q_n) \Delta_n W_2,$$

 $q_{n+1} = q_n + hp_{n+1},$

which is the adjoint method of (9.3.1)-(9.3.2), and of mean-square order 1. The scheme (6.1.49)-(6.1.50)

$$p_{n+1} = p_n - h\omega^2 \sin(q_n) - \frac{h^2}{2}\omega^2 p_{n+1}\cos(q_n) - \sigma_1 \cos(q_n)\Delta_n W_1$$

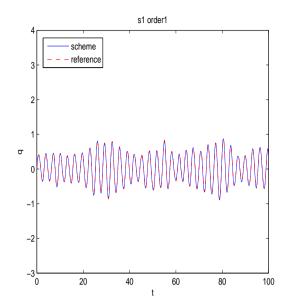
$$+ \sigma_1 p_{n+1}\sin(q_n) \int_0^h s \circ dW_1(s) - \sigma_2 \sin(q_n)\Delta_n W_2$$

$$- \sigma_2 p_{n+1}\cos(q_n) \int_0^h s \circ dW_2(s),$$

$$q_{n+1} = q_n + hp_{n+1} + \frac{h^2}{2}\omega^2 \sin(q_n) + \sigma_1 \cos(q_n) \int_0^h s \circ dW_1(s)$$

$$+ \sigma_2 \sin(q_n) \int_0^h s \circ dW_2(s)$$

generated by \bar{S}^1 is of mean-square order $\frac{3}{2}$. Figure 3.1 and 3.2 below illustrate comparison between sample trajectory of the approximated solution and that of numerical solution created by method (6.1.43)-(6.1.44) and (6.1.49)-(6.1.50) respectively.



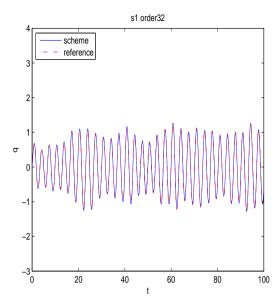


Figure 3.1: Sample trajectory of (6.1.43)-(6.1.44).

Figure 3.2: Sample trajectory of (6.1.49)-(6.1.50).

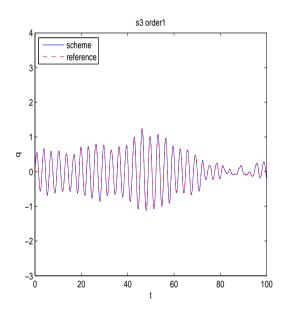


Figure 3.3: Sample trajectory of (6.2.27)-(6.2.28).

Solid curves in Figure 3.1 and 3.2 are sample trajectories created by method (6.1.43)-(6.1.44) and (6.1.49)-(6.1.50), dash-dotted ones are produced by (9.3.1)-(9.3.2) as reference. They coincide visually in both figures above. We take $\sigma_1 = 0.2$, $\sigma_2 = 0.1$, $\omega = 2$, $t \in [0, 100]$ and step size h = 0.02. ΔW_n is truncated according to (3.2.13) with k = 2.

 \bar{S}^3 generates the scheme (6.2.27)-(6.2.28)

$$p_{n+1} = p_n - \sin(\frac{q_n + q_{n+1}}{2})(\omega^2 h + \sigma_2 \Delta_n W_2) - \cos(\frac{q_n + q_{n+1}}{2})\sigma_1 \Delta_n W_1,$$

$$q_{n+1} = q_n + h \frac{p_n + p_{n+1}}{2}$$

for the model system, which is of mean-square order 1. A sample trajectory produced by it is shown in Figure 3.3. Data and settings for Figure 3.3 coincide with those for Figure 3.1 and 3.2. Note that the scheme (6.2.27)-(6.2.28) is implicit. Substituting (6.2.28) into (6.2.27), we then applied fixed point iteration to solving p_{n+1} , the convergence of which requires

$$h < \frac{4}{|c_1| + |c_2|},\tag{9.3.3}$$

where

$$c_1 = h\omega^2 + \sigma_2 \Delta_n W_2, \qquad c_2 = \sigma_1 \Delta_n W_1.$$
 (9.3.4)

Thus we make truncation on $\Delta_n W_1$ and $\Delta_n W_2$, and to check whether (9.3.3) is satisfied. If not, let $|c_1| + |c_2| = \frac{4}{nh}$, where n is times of fixed point iteration.

9.4 A System with Two Additive Noises

For the system with two additive noises (3.1.27)-(3.1.28)

$$dp = -qdt + \gamma \circ dW_2(t), \qquad p(0) = 0,$$

$$dq = pdt + \sigma \circ dW_1(t), \qquad q(0) = 0,$$

we have constructed generating function \bar{S}^1 , which is given in (6.1.54) and generates via relation (5.1.9) the symplectic Euler-Maruyama method (6.1.51)-(6.1.52)

$$p_{n+1} = p_n - hq_n + \gamma \Delta_n W_2,$$

 $q_{n+1} = q_n + hp_{n+1} + \sigma \Delta_n W_1.$

This method is of mean-square order 1. Figure 4.1 illustrates the oscillation of the numerical q produced by (6.1.51)-(6.1.52) and the exact q given by (3.1.29). The method of mean-square order $\frac{3}{2}$, i.e., the scheme (6.1.57)-(6.1.58)

$$p_{n+1} = p_n + \gamma \Delta_n W_2 - \sigma \int_0^h W_1(s) ds - q_n h - \frac{h^2}{2} p_{n+1},$$

$$q_{n+1} = q_n + \sigma \Delta_n W_1 - \gamma \int_0^h s \circ dW_2(s) + p_{n+1} h + \frac{h^2}{2} q_n$$

is generated by the function \bar{S}^1 in (6.1.56). Figure 4.2 shows oscillation of numerical q produced by (6.1.57)-(6.1.58), and exact q by solution formula (3.1.29).

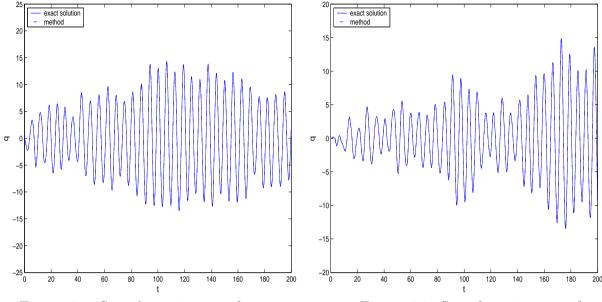


Figure 4.1: Sample trajectory of (6.1.51)-(6.1.52).

Figure 4.2: Sample trajectory of (6.1.57)-(6.1.58).

In Figures 4.1 and 4.2, exact q are presented by solid line, and numerical ones by dash-dotted line. They coincide visually in both figures. Data for the two tests are $\gamma=1$, $\sigma=0,\,t\in[0,200]$, and the step size is h=0.02.

The generating function \bar{S}^3 in (6.2.31) generates via relation (5.1.15)-(5.1.16) the numerical scheme (6.2.32)-(6.2.33)

$$p_{n+1} + \frac{h}{2}q_{n+1} = p_n - \frac{h}{2}q_n + \gamma \Delta_n W_2,$$

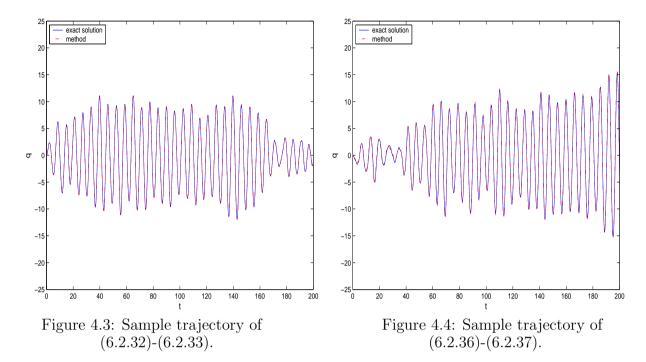
$$-\frac{h}{2}p_{n+1} + q_{n+1} = \frac{h}{2}p_n + q_n + \sigma \Delta_n W_1,$$

which is of mean-square order 1. Figure 4.3 compares behavior of q created by the numerical method (6.2.32)-(6.2.33) and the exact solution formula (3.1.29). A method of mean-square order $\frac{3}{2}$ is given in (6.2.36)-(6.2.37)

$$p_{n+1} + \frac{h}{2}q_{n+1} = p_n - \frac{h}{2}q_n + \gamma \Delta_n W_2 - \frac{\sigma}{\sqrt{2}} \int_0^h W_1(s) ds + \frac{\sigma}{2} \int_0^h s \circ dW_1(s),$$

$$-\frac{h}{2}p_{n+1} + q_{n+1} = \frac{h}{2}p_n + q_n + \sigma \Delta_n W_1 + \frac{\gamma}{\sqrt{2}} \int_0^h W_2(s) ds - \frac{\gamma}{2} \int_0^h s \circ dW_2(s),$$

which is generated by the generating function \bar{S}^3 in (6.2.35). We show in Figure 4.4 the oscillation of the numerical q produced by (6.2.36)-(6.2.37) and that of the exact q given by (3.1.29).



In Figures 4.3 and 4.4, the solid curves are the exact q, and the dash-dotted curves the numerical one. We see no difference between them in both figures, which shows good behavior of the numerical solutions produced by (6.2.32)-(6.2.33) and (6.2.36)-(6.2.37). Data for creating the two figures are same with that for Figures 4.1 and 4.2.

9.5 Modified Equations

Modified equations can be constructed by applying generating function of a symplectic method, which is studied in Chapter 8. We illustrate through numerical tests the trajectories of numerical solutions and their modified equations constructed by generating functions.

Example 9.1. Consider the linear stochastic oscillator (3.1.7)-(3.1.8)

$$dy = -xdt + \sigma \circ dW(t), \quad y(0) = y_0,$$

$$dx = ydt, \quad x(0) = x_0.$$

For the symplectic Euler-Maruyama method (5.3.27)-(5.3.28)

$$x_{n+1} = x_n + hy_{n+1},$$

$$y_{n+1} = y_n - hx_n + \sigma \Delta W_n,$$

Example 8.1 gives its modified equation (8.2.26)-(8.2.27)

$$dy = (hy - x)dt + \sigma \circ dW(t), \qquad y(0) = y_0,$$

$$dx = (y - hx)dt + \sigma h \circ dW(t), \quad x(0) = x_0,$$

which is obtained through using generating function \bar{S}^1 in (8.2.20) with (8.2.21) for the method (5.3.27)-(5.3.28). In order to simulate the solution of the modified equation, we

use its symplectic Euler-Maruyama discretization (8.2.30)

$$\left(\begin{array}{c} x_{n+1} \\ y_{n+1} \end{array} \right) = \left(\begin{array}{cc} \frac{-h^4 + 3h^2 - 1}{h^2 - 1} & \frac{-h}{h^2 - 1} \\ \frac{h}{h^2 - 1} & \frac{-1}{h^2 - 1} \end{array} \right) \left(\begin{array}{c} x_n \\ y_n \end{array} \right) + \left(\begin{array}{c} \frac{\sigma h^3 - 2\sigma h}{h^2 - 1} \\ \frac{-\sigma}{h^2 - 1} \end{array} \right) \Delta W_n.$$

Figure 5.1 shows oscillation of x of the exact solution, the method (5.3.27)-(5.3.28), and the modified equation (8.2.26)-(8.2.27), which are presented with solid, dashed, and broken curves respectively.

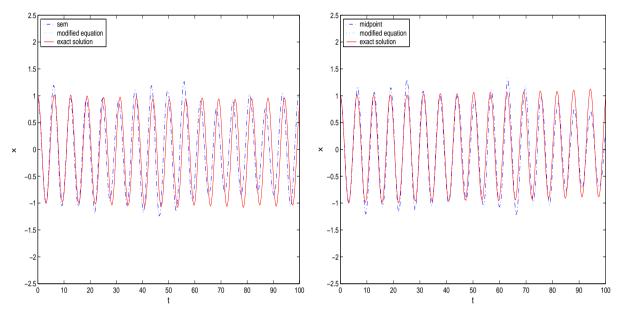


Fig. 5.1: Sample trajectories of exact solution of (3.1.7)-(3.1.8), method (5.3.27)-(5.3.28) and its modified equation (8.2.26)-(8.2.27).

We can see from Figure 5.1 that the sample trajectory of the method (5.3.27)-(5.3.28) coincides visually with the approximated sample trajectory of its modified equation (8.2.26)-(8.2.27).

 \bar{S}^3 in (8.3.18) with (8.3.19) generates via relation (5.1.15)-(5.1.16) the midpoint rule (5.4.22)-(5.4.23)

$$x_{n+1} = x_n + h \frac{y_n + y_{n+1}}{2},$$

 $y_{n+1} = y_n - h \frac{x_n + x_{n+1}}{2} + \sigma \Delta W_n$

for the linear stochastic oscillator (3.1.7)-(3.1.8). The truncated modified equation of the method (5.4.22)-(5.4.23) is constructed by applying \bar{S}^3 in (8.3.18) with (8.3.19), which is given in (8.3.24)-(8.3.25)

$$\begin{array}{rcl} dy & = & -xdt + \sigma \circ dW, \\ dx & = & (y + \frac{\sigma}{\sqrt{2}}W(h))dt + \frac{\sigma}{2}h \circ dW, \end{array}$$

sample trajectory of which is simulated by its midpoint discretization (8.3.26)-(8.3.27). Figure 5.2 compares oscillation of x of exact solution, numerical method (5.4.22)-(5.4.23),

and its truncated modified equation (8.3.24)-(8.3.25), which are presented with solid, dashed, and broken curves respectively. Trajectory of the method coincides with that of its modified equation. Data for creating Figures 5.1 and 5.2 are $x_0 = 1$, $y_0 = 0$, $\sigma = 0.1$, $t \in [0, 100]$, and the step size is h = 0.1.

Example 9.2. For the Kubo oscillator (3.1.16)-(3.1.17)

$$dp = -aqdt - \sigma q \circ dW(t), \quad p(0) = p_0,$$

$$dq = apdt + \sigma p \circ dW(t), \quad q(0) = q_0,$$

 \bar{S}^1 in (5.3.45) generates via relation (5.1.9) the symplectic scheme (5.3.46)

$$-(ah + \frac{h^2}{2}a\sigma^2 + \sigma\Delta W_n + \sigma^3 \int_0^h s \circ dW)p_{n+1} + q_{n+1} = (1 + \frac{h\sigma^2}{2} + \frac{h^2a^2}{2} + a\sigma h\Delta W_n)q_n,$$

$$(1 + \frac{h\sigma^2}{2} + \frac{h^2a^2}{2} + a\sigma h\Delta W_n)p_{n+1} = p_n - (ah + \sigma\Delta W_n)q_n,$$

which is of mean-square order $\frac{3}{2}$. Its truncated modified equation is deduced based on \bar{S}^1 , and given in (8.2.36)-(8.2.37)

$$dp = -aqdt + (\frac{h}{2}\sigma^3p^2 - \sigma q) \circ dW, \quad p(0) = p_0,$$

$$dq = apdt + (\sigma p - h\sigma^3pq) \circ dW, \quad q(0) = q_0.$$

Figure 5.3 contributes to comparison between sample trajectory of the numerical method (5.3.46) and its truncated modified equation (8.2.36)-(8.2.37), where we use the symplectic Euler-Maruyama discretization (8.2.38)-(8.2.39) to simulate the sample trajectory of (8.2.36)-(8.2.37). Fixed point iteration is performed in realizing (8.2.38)-(8.2.39). Dashed and solid curves represent trajectory of method and its modified equation respectively. It is found that the sample trajectories coincide very well.

Figures 5.4 and 5.5 are approximated phase trajectories of the method (5.3.46) and its modified equation (8.2.36)-(8.2.37), respectively. Data for Figures 5.3-5.5 are $p_0=1$, $q_0=0, a=2, \sigma=0.3, t\in[0,100]$, and the step size is h=0.01. Number of iterations in each step in realizing (8.2.38)-(8.2.39) is n=100, and ΔW_n is truncated according to (3.2.13) with k=2.

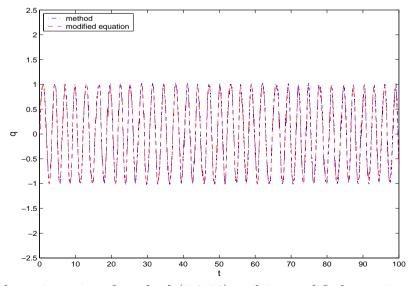


Figure 5.3: Sample trajectories of method (5.3.46) and its modified equation (8.2.36)-(8.2.37).

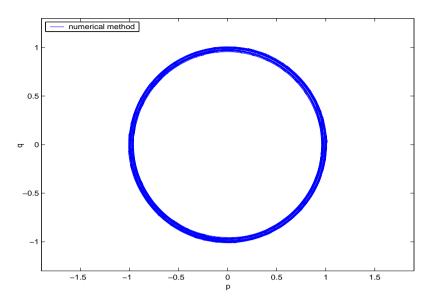


Figure 5.4: Phase trajectory of method (5.3.46).

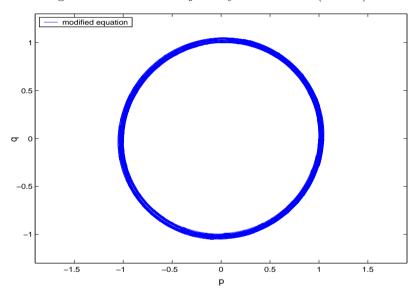


Figure 5.5: Phase trajectory of modified equation (8.2.26)-(8.2.27).

 \bar{S}^3 in (8.3.30) with (8.3.31) generates via relation (5.1.15)-(5.1.16) the midpoint rule (5.4.31)-(5.4.32)

$$p_{n+1} = p_n - ah \frac{q_n + q_{n+1}}{2} - \sigma \frac{q_n + q_{n+1}}{2} \Delta W_n,$$

$$q_{n+1} = q_n + ah \frac{p_n + p_{n+1}}{2} + \sigma \frac{p_n + p_{n+1}}{2} \Delta W_n$$

for the Kubo oscillator (3.1.16)-(3.1.17). Its truncated modified equation is (8.3.36)-(8.3.37)

$$dp = \left(\frac{ha\sigma^2q}{2} - aq\right)dt + \left(\frac{h\sigma^3q}{2} - \sigma q\right) \circ dW, \quad p(0) = p_0,$$

$$dq = \left(ap + \frac{ha\sigma^2p}{2}\right)dt + \left(\sigma p + \frac{h\sigma^3p}{2}\right) \circ dW, \quad q(0) = q_0,$$

which we use midpoint discretization (8.3.38) to simulate. Figure 5.6 gives a sample trajectory of method (5.4.31)-(5.4.32) (solid), and its modified equation (8.3.36)-(8.3.37) (dashed).

Figures 5.7 and 5.8 are phase trajectories of the method (5.4.31)-(5.4.32) and its modified equation (8.3.36)-(8.3.37), respectively. The two seem to have little difference. Data for Figure 5.6 are $p_0 = 1$, $q_0 = 0$, a = 2, $\sigma = 0.3$, $t \in [0, 100]$, and the step size is h = 0.1. Truncation of ΔW_n is the same with that for creating Figures 5.3-5.5. For Figures 5.7 and 5.8, we choose $t \in [0, 200]$, and the other data are the same with that for Figure 5.6.

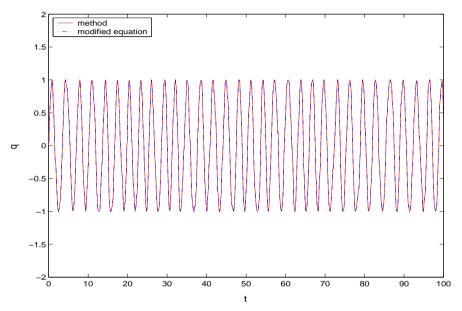


Fig. 5.6: Sample trajectories of method (5.4.31)-(5.4.32) and its modified equation (8.3.36)-(8.3.37).

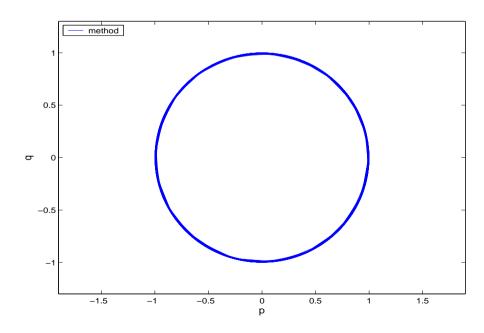


Figure 5.7: Phase trajectory of method (5.4.31)-(5.4.32).

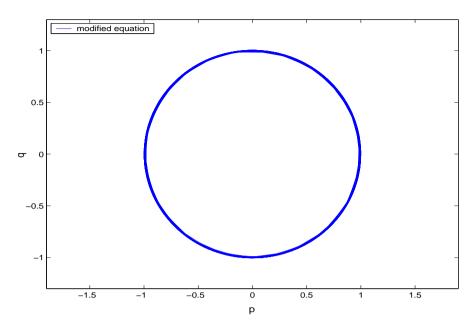


Figure 5.8: Phase trajectory of modified equation (8.3.36)-(8.3.37).

Example 9.3. The method with two noises (6.1.43)-(6.1.44)

$$p_{n+1} = p_n - h\omega^2 sin(q_n) - \sigma_1 \cos(q_n) \Delta_n W_1 - \sigma_2 sin(q_n) \Delta_n W_2,$$

 $q_{n+1} = q_n + hp_{n+1}$

is a symplectic discretization of the model of synchrotron oscillations (3.1.22)-(3.1.23)

$$dp = -\omega^2 \sin(q) dt - \sigma_1 \cos(q) \circ dW_1 - \sigma_2 \sin(q) \circ dW_2,$$

$$dq = pdt.$$

 \bar{S}^1 in (6.1.42) generates via relation (5.1.9) the numerical scheme (6.1.43)-(6.1.44). It is derived in Chapter 8 that the truncated modified equation of method (6.1.43)-(6.1.44) is (8.4.27)-(8.4.28)

$$dp = (h\omega^{2}p\cos(q) - \omega^{2}\sin(q))dt - (\sigma_{1}\cos(q) + h\sigma_{1}p\sin(q)) \circ dW_{1} + (h\sigma_{2}p\cos(q) - \sigma_{2}\sin(q)) \circ dW_{2}, p(0) = p_{0}, dq = (p - h\omega^{2}\sin(q))dt - h\sigma_{1}\cos(q) \circ dW_{1} - h\sigma_{2}\sin(q) \circ dW_{2}, q(0) = q_{0}.$$

Figure 5.9 shows sample trajectories of method (6.1.43)-(6.1.44) (dashed) and its modified equation (8.4.27)-(8.4.28) (solid) which is simulated by its symplectic Euler-Maruyama discretization (8.4.29)-(8.4.30). We use fixed point iteration to realize (8.4.29)-(8.4.30). Data for Figure 5.9 is $p_0 = 1$, $q_0 = 0$, $\sigma_1 = 0.2$, $\sigma_2 = 0.1$, $\omega = 2$, $t \in [0, 100]$, and the step size is h = 0.05. Number of iterations in each step in realizing (8.4.29)-(8.4.30) is n = 100, and ΔW_n is truncated according to (3.2.13) with k = 2.

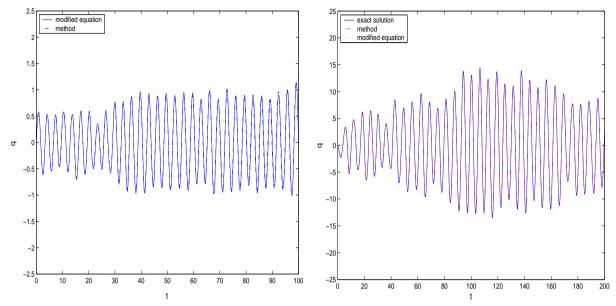


Fig. 5.9: Sample trajectories of method (6.1.43)-(6.1.44) and its modified equation (8.4.27)-(8.4.28).

Fig. 5.10: Sample trajectories of exact solution (3.1.29), method (6.2.32)-(6.2.33) and its modified equation (8.4.51)-(8.4.52).

Example 9.4. For the system with two additive noises (3.1.27)-(3.1.28)

$$dq = pdt + \sigma \circ dW_1(t), \qquad q(0) = q_0,$$

$$dp = -qdt + \gamma \circ dW_2(t), \qquad p(0) = p_0,$$

generating function \bar{S}^3 in (6.2.31) generates via relation (5.1.15)-(5.1.16) the numerical scheme (6.2.32)-(6.2.33)

$$p_{n+1} + \frac{h}{2}q_{n+1} = p_n - \frac{h}{2}q_n + \gamma \Delta_n W_2,$$

$$-\frac{h}{2}p_{n+1} + q_{n+1} = \frac{h}{2}p_n + q_n + \sigma \Delta_n W_1.$$

Its truncated modified equation is derived as (8.4.51)-(8.4.52)

$$dp = (\frac{\sigma}{\sqrt{2}}W_1(h) - q)dt + \gamma \circ dW_2, \quad p(0) = p_0,$$

$$dq = (p - \frac{\gamma}{\sqrt{2}}W_2(h))dt + \sigma \circ dW_1, \quad q(0) = q_0.$$

We use its midpoint discretization (8.4.53)-(8.4.54) to simulate (8.4.51)-(8.4.52). In Figure 5.10, sample trajectories of the exact solution (3.1.29) (solid), method (6.2.32)-(6.2.33) (dashed) and its modified equation (8.4.51)-(8.4.52) (broken) are sketched for comparison. They coincide visually. Data for Figure 5.10 are $p_0 = q_0 = 0$, $\sigma = 0$, $\gamma = 1$, $t \in [0, 200]$, and the step size is h = 0.02.

Conclusion. Through numerical tests on schemes produced by variational integrator and generating functions, we find that these schemes are efficient and provide numerical solutions preserving symplecticity, as well as other structures of underlying stochastic

Hamiltonian systems. Sample trajectories of methods and their stochastic modified equations coincide well, which shows rationality of the construction of stochastic modified equations via generating functions. All these give support to our theories of stochastic variational integrators and generating functions.

Bibliography

- [1] V.I. Arnold, Mathematical Methods of Classical Mechanics, Springer-Verlag New York, Inc., 1978.
- [2] J.M. Bismut, *Mécanique Aléatoire*, Lecture Notes in Math. 866, Springer, Berlin, 1981.
- [3] R.A. Carmona, B. Rozovskii, *Stochastic Partial Differential Equations: Six Perspectives*, Mathematical Surveys and Monographs, Volume **64**, American Mathematical Society, 1999.
- [4] G. Da Prato, L. Tubaro, Stochastic Partial Differential Equations and Applications, Marcel Dekker, Inc., New York · Basel, 2002.
- [5] I.M. Davies, On the Stochastic Lagrangian and a New Derivation of the Schrödinger Equation, J. Phys. A: Math. Gen. 22, 1989, 3199-3203.
- [6] L.C. Evans, An Introduction to Stochastic Differential Equations, Version 1.2, Department of Mathematics, UC Berkeley.
- [7] K. Feng, On Difference Schemes and Symplectic Geometry, Proceedings of the 5-th Intern. Symposium on Differential Geometry & Differential Equations, August 1984, Beijing, 1985, 42-58.
- [8] K. Feng, Difference Schemes for Hamiltonian Formalism and Symplectic Geometry, J. Comp. Math. 4, 279-289, 1986.
- [9] K. Feng, H.M. Wu, M.-Z. Qin, D.L. Wang, Construction of Canonical Difference Schemes For Hamiltonian Formalism via Generating Functions, J Comp Math. 7 (1), 1989, 71-96.
- [10] Gastão S.F. Frederico, Delfim F.M. Torres, Nonconservative Noether's Theorem in Optimal Control, Proceedings of the 13th IFAC Workshop on Applications of Optimisation, IFAC Publication, Elsevier Ltd, Oxford, UK., 2006.
- [11] F. Guerra, L.M. Morato, Quantization of Dynamical Systems and Stochastic Control Theory, Physical Review D, Volume 27, 8, 1983, 1774-1786.
- [12] E. Hairer, C. Lubich, G. Wanner, *Geometric Numerical Integration*, Springer-Verlag Berlin Heidelberg, 2002.
- [13] D.J. Higham, An Algorithmic Introduction to Numerical Simulation of Stochastic Differential Equations, SIAM Rev. 43, No. 3, 2001, 525-546.

142 BIBLIOGRAPHY

[14] J. Hong, R. Scherer, L. Wang, Midpoint Rule for a Linear Stochastic Oscillator with Additive Noise, Neural, Parallel, and Scientific Computing, 14, No. 1, 2006, 1-12.

- [15] J. Hong, R. Scherer, L. Wang, Predictor-Corrector Methods for a Linear Stochastic Oscillator with Additive Noise, Mathematical and Computer Modelling, 2007, doi:10.1016/j.mcm.2006.12.009.
- [16] P.E. Klöden, A Brief Overview of Numerical Methods for Stochastic Differential Equations, Conferenza tenuta il giorno 25 Maggio 2001.
- [17] P.E. Klöden, E. Platen, Numerical Solution of Stochastic Differential Equations, Springer-Verlag Berlin Heidelberg, 1992.
- [18] Z. Li, Stochastic Differential Equations, April 8, 2004.
- [19] M.I. Loffredo, L.M. Morato, Lagrangian Variational Principle in Stochastic Mechanics: Gauge Structure and Stability, J. Math. Phys. **30** (2), 1989, 354-360.
- [20] R. MacKay, Some Aspects of the Dynamics of Hamiltonian Systems, in: D.S. Broomhead & A. Iserles, eds., The Dynamics of Numerics and the Numerics of Dynamics, Clarendon Press, Oxford, 1992, 137-193.
- [21] X. Mao, Stochastic Differential Equations and Applications, Horwood, Chichester, 1997.
- [22] L. Markus, A. Weerasinghe, *Stochastic Oscillators*, J. Differential Equations **71** (2), 1988, 288-314.
- [23] J.E. Marsden, T.Ratiu, *Introduction to Mechanics and Symmetry*, Texts in Applied Mathematics **Vol. 17**, Springer-Verlag, 1994.
- [24] J.E. Marsden, M. West, Discrete Mechanics and Variational Integrators, Acta Numerica 10, 2001, 1-158.
- [25] G.N. Milstein, Numerical Integration of Stochastic Differential Equations, Kluwer Academic Publishers, 1995.
- [26] G.N. Milstein, YU.M. Repin, M.V. Tretyakov, Symplectic Methods for Hamiltonian Systems with Additive Noise, Preprint 640, Weierstraß-Institut für Angewandte Analysis und Stochastik, Berlin, Germany, 2001.
- [27] G.N. Milstein, YU.M. Repin, M.V. Tretyakov, Mean-Square Symplectic Method for Hamiltoian Systems with Multiplicative Noise, Preprint 670, Weierstraß-Institut für Angewandte Analysis und Stochastik, Berlin, Germany, 2001.
- [28] G.N. Milstein, YU.M. Repin, M.V. Tretyakov, Symplectic Integration of Hamiltonian Systems with Additive Noise, SIAM J. Numer. Anal., Vol. 39, No. 6, 2002, 2066-2088.
- [29] G.N. Milstein, YU.M. Repin, M.V. Tretyakov, Numerical Methods for Stochastic Systems Preserving Symplectic Structure, SIAM J. Numer. Anal., Vol. 40, No. 4, 2002, 1583-1604.

BIBLIOGRAPHY 143

[30] T. Misawa, On Stochastic Hamiltonian Mechanics for Diffusion Processes, IL NUOVO CIMENTO, Vol. 91 B, 11 Gennajo 1986, 1-24.

- [31] T. Misawa, Canonical Stochastic Dynamical Systems, J. Math. Phys., 28 (11), 1987.
- [32] T. Misawa, A Stochastic Hamilton-Jacobi Theory in Stochastic Hamiltonian Mechanics for Diffusion Processes, IL NUOVO CIMENTO, Vol. 99 B, N. 2, 11 Giugno 1987.
- [33] T. Misawa, Energy Conservative Stochastic Difference Scheme for Stochastic Hamilton Dynamical Systems, Japan Journal of Industrial and Applied Mathematics, Vol. 17, No. 1, 2000, 119-128.
- [34] S. Morita, T. Ohtsuka, Semi-Natural Motion Generation Based on Hamilton's Principle, SICE Annual Conference, Fukui University, Japan, 2003.
- [35] E. Nelson, Phys. Rev., **150**, 1966, 1079.
- [36] E. Nelson, *Dynamical Theories of Brownian Motion*, Mathematical Notes, Princeton University Press, 1967.
- [37] E. Nelson, *Quantum Fluctuations*, Princeton Series in Physics, Princeton University Press, 1985.
- [38] A. Recati, Non Conservative Systems from a Generalized Hamilton's Principle, Lecture Notes: Mathematical Methods for Physics II: Some Notes on Variational Principle, Lagrangian and Hamiltonian Formalism, 2, Institut für Theoretische Physik, Universität Innsbruck, http://bozon.uibk.ac.at/~arecati/notestalks.html/.
- [39] R.D. Ruth, A Canonical Integration Technique, IEEE Trans. Nuclear Science, 1983, NS-30: 2669-2671.
- [40] H. Schurz, The Invariance of Asymptotic Laws of Linear Stochastic Systems under Discretization, ZAMM· Z. Angew. Math. Mech. 79, 6, 1999, 375-382.
- [41] A.H. Strømmen Melbø, D.J. Higham, Numerical Simulation of a Linear Stochastic Oscillator with Additive Noise, Appl. Numer. Math., 51, No. 1, 2004, 89-99.
- [42] F.T. Tveter, Deriving the Hamilton Equations of Motion for a Nonconservative System Using a Variational Principle, Journal of Mathematical Physics, Volume 39, No. 3, 1998.
- [43] R. de Vogelaere, Methods of Integration which Preserve the Contact Transformation Property of the Hamiltonian Equations, Report No. 4, Dept. Math., Univ. of Notre Dame, Notre Dame, Ind., 1956.
- [44] W. Wagner, E. Platen, Approximation of Itô Integral Equations, Preprint ZIMM, Akad. Wissenschaft. DDR, Berlin, 1978.
- [45] J.M. Wendlandt, J.E. Marsden, Mechanical Integrators Derived from a Discrete Variational Principle, Physica D 106, 1997, 223-246.
- [46] J. Yeh, Stochastic Processes and the Wiener Integral, Marcel Dekker, Inc., New York, 1973.

144 BIBLIOGRAPHY

[47] J.-C. Zambrini, Maupertuis' Principle of Least Action in Stochastic Calculus of Variations, J. Math. Phys., 25, 5, 1984, 1314-1322.

[48] J.-C. Zambrini, Stochastic Dynamics: A Review of Stochastic Calculus of Variations, Int. J. Theor. Phys., 24, 1985, 277-327.