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# Stochastic modified equations for symplectic methods applied to rough Hamiltonian systems

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We investigate stochastic modified equations to explain the mathematical mechanism of symplectic methods applied to rough Hamiltonian systems. The contribution of this paper is threefold. First, we construct a new type of stochastic modified equation. For symplectic methods applied to rough Hamiltonian systems, the associated stochastic modified equations are proved to have Hamiltonian formulations. Secondly, the pathwise convergence order of the truncated modified equation to the numerical method is obtained by techniques in rough path theory. Thirdly, if increments of noises are simulated by truncated random variables, we show that the error can be made exponentially small with respect to the time step size.

*Keywords*: stochastic modified equation; rough Hamiltonian system; symplectic method; rough path.

## 1. Introduction

In the study of a numerical method for a differential equation, the modified equation gives a lot of insights into the numerical method and is crucial in backward error analysis. For the stochastic differential equation (SDE) driven by a standard Brownian motion

$$\mathrm{d}Y_t = V(Y_t)\,\mathrm{d}W_t,$$

there exist various types of stochastic modified equations in different senses of convergence. In view of the weak convergence, adding a modified coefficient with powers of the time step size $h$ to the original SDE yields a modified equation of the form

$$\mathrm{d}\tilde{Y}_t = \left[V(\tilde{Y}_t) + \tilde{V}(\tilde{Y}_t)h^p\right]\mathrm{d}W_t, \tag{1.1}$$

which fits the numerical method to a higher weak order. The modified coefficient $\tilde{V}$ can be determined by the weak Taylor expansion (Shardlow, 2006) or by the expansion of the backward Kolmogorov equation (Zygalakis, 2011). As an application, the first-order integrated Euler method is proposed for the stochastic Langevin equation in Zygalakis (2011) to preserve the mean of a modified Hamiltonian. Another application of this kind of modified equations is to construct high weak order methods; see Abdulle *et al.* (2012) and Hong *et al.* (2017). The modification is also considered at the level of the Kolmogorov equation instead of at the level of the SDE. Given $\phi$, denote $u(t,x) = \mathbb{E}[\phi(Y_t(x))]$ and $(\mathscr{L}f)(x) = \frac{1}{2}\sum_{i,j}(VV^\top)_{ij}(x)\partial_{ij}f(x)$. The modified Kolmogorov equation for $\frac{\partial u}{\partial t} = \mathscr{L}u$ is

$$\frac{\partial \tilde{u}}{\partial t} = \left[\mathscr{L} + \mathscr{L}_1 h + \cdots + \mathscr{L}_N h^N\right]\tilde{u}$$

with $\mathscr{L}_l$ being some modified operators of order $2l+2$, $l = 1, \cdots, N$. Based on the modified Kolmogorov equation, Debussche & Faou (2012) proved that the numerical solution obtained by the Euler method for SDEs on the torus is exponentially mixing up to negligible terms. The results are extended to implicit methods for SDEs on $\mathbb{R}^m$ in Kopec (2015a,b); Anton (2019). With respect to strong convergence, using multiple Stratonovich integrals $J_{\alpha,t}$, Deng (2016) defined the modified equation

$$\mathrm{d}\tilde{Y}_t = \left[V(\tilde{Y}_t) + \sum_{\alpha} \tilde{V}_\alpha(\tilde{Y}_t)J_{\alpha,t}\right]\mathrm{d}W_t$$

for the Euler method, and the optimal truncation of the above series is studied.

Stochastic Hamiltonian systems are fundamental models in many physical and engineering sciences, such as the passive tracer model and the Kubo oscillator. The phase flow of a stochastic Hamiltonian system driven by standard Brownian motions preserves the symplectic structure almost surely and there has been a great amount of work about the construction of stochastic symplectic methods after the pioneering results in Milstein *et al.* (2002a,b). Lots of numerical simulations have shown that the stochastic symplectic methods are superior over long time computation to non-symplectic ones. From the perspective of the stochastic modified equation to investigate the superiority of the stochastic symplectic methods, it is natural to ask:

Problem 1.1 For a stochastic symplectic method applied to a stochastic Hamiltonian system, does there exist a stochastic modified equation that has a stochastic Hamiltonian formulation, such that its exact solution coincides with the numerical solution?

This problem is partially solved by Wang *et al.* (2016, 2018). As far as the weak convergence is concerned, for the case that the Hamiltonian functions associated to the diffusion parts do not depend on the generalized coordinate and momenta simultaneously, the modified equations in the form of (1.1) for stochastic symplectic methods are derived in Wang *et al.* (2016) via the generating function. These modified equations are perturbed stochastic Hamiltonian systems with respect to the original systems. In Wang *et al.* (2018), the modified coefficient in (1.1) is deduced for a symplectic splitting method applied to separable Hamiltonian systems with additive noises, and the flow of the corresponding modified equation preserves the symplectic structure.

With further researches on modeling random phenomenon, the stochastic signals are not necessarily semi-martingales or Markovian processes (Deya *et al.*, 2012; Friz & Riedel, 2014; Bayer *et al.*, 2016; Kelly, 2016; Liu & Tindel, 2019; Hu *et al.*, 2021), which motivates the study of SDEs driven by rough paths

$$\mathrm{d}Y_t = V(Y_t)\,\mathrm{d}X_t. \tag{1.2}$$

In particular, when the driving signals are standard Brownian motions, the solution of (1.2) is equivalent to that of the Stratonovich SDE, which is used to define the canonical formulation of stochastic

Hamiltonian systems driven by standard Brownian motions. In Hong *et al.* (2018), it is shown that the phase flow of a stochastic Hamiltonian system driven by rough paths also preserves the symplectic structure almost surely, and stochastic symplectic methods are proposed to inherit this property. In this article, we investigate the modified equations for stochastic symplectic methods applied to (1.2). Overcoming the difficulties caused by the non-differentiability and the low regularity of $X$, we propose a new type of stochastic modified equation

$$\mathrm{d}\tilde{y}_t = \Big[V(\tilde{y}_t) + \sum_{\alpha} \tilde{V}_\alpha(\tilde{y}_t)(X^1_{t_n,t_{n+1}})^{\alpha_1} \cdots (X^{\mathrm{d}}_{t_n,t_{n+1}})^{\alpha_{\mathrm{d}}}\Big]\,\mathrm{d}x^h_t, \quad t \in (t_n, t_{n+1}],\ t_n = nh,$$

which satisfies $\tilde{y}_{t_n} = Y^h_n$ with $Y^h_n$ being the numerical solution. Based on the Hermite polynomials, we prove that if a symplectic method is applied to a rough Hamiltonian system, then for any $\alpha$, there exists a Hamiltonian $\mathscr{H}_\alpha$ such that

$$\tilde{V}_\alpha = \mathbb{J}^{-1}\nabla\mathscr{H}_\alpha.$$

This implies that stochastic modified equations for symplectic methods are also stochastic Hamiltonian systems, and gives a positive answer to Problem 1.1.

Note that the coefficient of the stochastic modified equation is an infinite series. In order to obtain some rigorous estimates, we truncate the stochastic modified equation as

$$\mathrm{d}\tilde{y}^{\tilde{N}}_t = \Big[V(\tilde{y}^{\tilde{N}}_t) + \sum_{|\alpha|\leqslant\tilde{N}} \tilde{V}_\alpha(\tilde{y}^{\tilde{N}}_t)(X^1_{t_n,t_{n+1}})^{\alpha_1} \cdots (X^{\mathrm{d}}_{t_n,t_{n+1}})^{\alpha_{\mathrm{d}}}\Big]\,\mathrm{d}x^h_t, \quad t \in (t_n, t_{n+1}].$$

We further study the following two problems concerning the estimate between the numerical solution $Y^h_n$ given by a stochastic symplectic method and the exact solution $\tilde{y}^{\tilde{N}}_{t_n}$ of the corresponding truncated modified equation.

Problem 1.2 What is the convergence rate of the error between the numerical solution and the exact solution of the truncated modified equation?

Problem 1.3 Does there exist a truncation number $\tilde{N}$ such that the error is exponentially small with respect to the time step size?

Considering the nontrivial covariances of increments of $X$, we utilize the Itô–Lyons map in the rough path theory to obtain the pathwise convergence rate of the exact solution $\tilde{y}^{\tilde{N}}$ of truncated modified equation to the numerical solution $Y^h$, that is,

$$\sup_{1\leqslant n\leqslant N} \|\tilde{y}^{\tilde{N}}_{t_n} - Y^h_n\| \leqslant C(\omega)h^{\frac{\tilde{N}+1}{p}-1}, \quad a.s.,$$

where $\tilde{N}$ is the truncation number and $p$ depends on the regularity of the driving signal. This answers Problem 1.2. For Problem 1.3, we focus on the case of the standard Brownian motion where the increments of noises are simulated by truncated random variables proposed in Milstein *et al.* (2002a). Due to the lack of explicit expansion formulas of implicit numerical methods, we use the analytic assumption to estimate the numerical solution, the modified equation and the truncated modified equation, successively. Combining the estimates yields that there exists some truncation number $\tilde{N} = \tilde{N}(h)$ such that the one-step error is exponentially small with respect to the time step size:

$$\|\tilde{y}_{t_1}^{\tilde{N}} - Y_1^h\| \leqslant Ch\, e^{-h_0/h^{\frac{1}{2}-\epsilon}}.$$

The rest of this article is organized as follows. In Section 2, we introduce basic results in the rough path theory. In Section 3, for Problem 1.1, we illustrate the procedure in constructing stochastic modified equations and prove that stochastic modified equations associated to stochastic symplectic methods are Hamiltonian systems as well. In Section 4, we prove the pathwise convergence rate of the error between the numerical solution and the exact solution of the truncated modified equation, and obtain the exponential convergence for one-step error in the case of truncated Brownian increments, which answers Problems 1.2–1.3. Numerical experiments are presented in Section 5 to support theoretical results.

## 2. Preliminaries

In this section, we review the well-posedness of SDEs in the sense of the rough path theory; see, e.g., Lyons (1998); Friz & Victoir (2010).

Consider the SDE driven by multi-dimensional Gaussian signal

$$\begin{cases} \mathrm{d}Y_t = V_0(Y_t)\,\mathrm{d}t + \sum_{l=1}^{\mathrm{d}} V_l(Y_t)\,\mathrm{d}X_t^l, \quad t \in (0,T]; \\ Y_0 = z \in \mathbb{R}^m. \end{cases} \tag{2.1}$$

For a convenient notation involving the drift term, we define $V := (V_0, V_1, \cdots, V_{\mathrm{d}})$, $X_t^0 := t$, $X := (X^0, X^1, \cdots, X^{\mathrm{d}})$, and then an equivalent form of (2.1) is

$$\begin{cases} \mathrm{d}Y_t = V(Y_t)\,\mathrm{d}X_t, \quad t \in (0,T]; \\ Y_0 = z. \end{cases} \tag{2.2}$$

In this article, we focus on the case that the driving signal $X$ satisfies the following assumption.

ASSUMPTION 2.1 Let $X^l : [0,T] \to \mathbb{R}$, $l = 1, \cdots, \mathrm{d}$ be independent centered Gaussian processes with continuous sample paths. There exist some $\rho \in [1,2)$ and $K \in (0,+\infty)$ such that the covariance of $X$ satisfies

$$\sup_{\{t_k\},\{t_i\} \in \mathscr{D}([s,t])} \left( \sum_{t_k,t_i} \left| \mathbb{E}\big[X^l_{t_k,t_{k+1}} X^l_{t_i,t_{i+1}}\big] \right|^\rho \right)^{1/\rho} \leqslant K|t-s|^{1/\rho} \quad \forall\, 0 \leqslant s < t \leqslant T,$$

where $\mathscr{D}([s,t])$ denotes the set of all dissections of $[s,t]$ and $X^l_{t_k,t_{k+1}} := X^l_{t_{k+1}} - X^l_{t_k}$.

For instance, one can check that the fractional Brownian motion with Hurst parameter $H \in \left(\frac{1}{4}, \frac{1}{2}\right]$, whose covariance is $\mathbb{E}\big[|X^l_{s,t}|^2\big] = |t-s|^{2H}$, satisfies Assumption 2.1 with $\rho = \frac{1}{2H}$. Since the Hölder regularity for the trajectory of the fractional Brownian motion is not larger than $H$, the well-posedness of (2.2) fails to be established in the Riemann–Stieltjes integral sense. Hence, we interprete (2.2) in the rough path sense. To this end, we introduce some basic concepts in the rough path theory; see Friz & Victoir (2010) for more details.

Let $p \in [1, \infty)$ and $[p]$ be the integer part of $p$, i.e., $[p] \in \mathbb{N}_+$ with $p - 1 < [p] \leqslant p$. We denote by $\big(G^{[p]}(\mathbb{R}^{d+1}), \mathrm{d}\big)$ the free step-$[p]$ nilpotent Lie group of $\mathbb{R}^{d+1}$ equipped with the Carnot–Carathéodory metric (Friz & Victoir, 2010, Chap. 7). A continuous map $\mathbf{X} : [0, T] \to G^{[p]}(\mathbb{R}^{d+1}) \subset \bigoplus_{n=0}^{[p]} (\mathbb{R}^{d+1})^{\otimes n}$ is called $p$-rough path if

$$\|\mathbf{X}\|_{p\text{-}var;[0,T]} := \sup_{\{t_k\} \in \mathscr{D}([0,T])} \left( \sum_{t_k} \mathrm{d}(\mathbf{X}_{t_k}, \mathbf{X}_{t_{k+1}})^p \right)^{1/p} < \infty,$$

where $\mathscr{D}([0, T])$ is the set of dissections of $[0, T]$. Furthermore, we say that $\mathbf{X}$ is of Hölder-type if

$$\|\mathbf{X}\|_{\frac{1}{p}\text{-Höl};[0,T]} := \sup_{0 \leqslant s < t \leqslant T} \frac{\mathrm{d}(\mathbf{X}_s, \mathbf{X}_t)}{|t - s|^{1/p}} < \infty.$$

For example, if $x : [0, T] \to \mathbb{R}^{d+1}$ is a function of bounded variation and $x_0 = 0$, the corresponding rough path can be defined by $S_{[p]}(x) : [0, T] \to G^{[p]}(\mathbb{R}^{d+1})$ with

$$S_{[p]}(x)_t = \left( 1, \int_{0 \leqslant u_1 \leqslant t} \mathrm{d}x_{u_1}, \cdots, \int_{0 \leqslant u_1 < \cdots < u_{[p]} \leqslant t} \mathrm{d}x_{u_1} \otimes \cdots \otimes \mathrm{d}x_{u_{[p]}} \right).$$

It is a canonical lift for $x$ in the sense that the projection of $S_{[p]}(x)$ onto $\mathbb{R}^{d+1}$ coincides with $x$.

Moreover, the Gaussian process $X$ under Assumption 2.1 can be lifted to a Hölder-type $p$-rough path $\mathbf{X} \in G^{[p]}(\mathbb{R}^{d+1})$ for any $p > 2\rho$ (Friz & Victoir, 2010, Theorem 15.33), which is defined by the limit of $\{S_3(x^n)\}_{n=1}^{\infty}$ with $\{x^n\}_{n=1}^{\infty}$ being a sequence of piecewise linear or mollifier approximations to $X$. As a consequence, the well-posedness of (2.2) is given by that of the rough differential equation (RDE)

$$\begin{cases} \mathrm{d}Y_t = V(Y_t)\,\mathrm{d}\mathbf{X}_t, & t \in (0, T]; \\ Y_0 = z. \end{cases} \tag{2.3}$$

In the sequel, we introduce the definition of the solution of (2.3) and state the condition for the existence and uniqueness of the solution. Throughout the rest of this paper, we denote by $\|\cdot\|$ the Euclidean norm and by $C$ a generic constant which may be different from line to line.

Definition 2.2 (Friz & Victoir, 2010, Definition 10.17) Let $p \in [1, \infty)$ and $\mathbf{X}$ be a $p$-rough path. Suppose that there exists a sequence of functions $\{x^n\}_{n=1}^{\infty}$ of bounded variation taking values in $\mathbb{R}^{d+1}$ such that

$$\sup_{n \in \mathbb{N}} \|S_{[p]}(x^n)\|_{p\text{-}var;[0,T]} < \infty \quad \text{and} \quad \lim_{n \to \infty} \sup_{0 \leqslant s < t \leqslant T} \mathrm{d}\big(S_{[p]}(x^n)_{s,t}, \mathbf{X}_{s,t}\big) = 0,$$

where $S_{[p]}(x^n)_{s,t} := S_{[p]}(x^n)_s^{-1} \otimes S_{[p]}(x^n)_t$ and $\mathbf{X}_{s,t} := \mathbf{X}_s^{-1} \otimes \mathbf{X}_t$. Suppose in addition that $\{y^n\}_{n=1}^{\infty}$ are solutions of equations $\mathrm{d}y_t^n = V(y_t^n)\,\mathrm{d}x_t^n$, in the Riemann–Stieltjes integral sense, with the same initial value $z$ as in (2.3). If $y_t^n$ converges to $Y_t$ in the $L^{\infty}([0, T])$-norm, i.e.,

$$\lim_{n \to \infty} \sup_{0 \leqslant t \leqslant T} \|y_t^n - Y_t\| = 0,$$

then we call $Y_t$ a solution of (2.3).

DEFINITION 2.3 (Friz & Victoir, 2010, Definition 10.2) Let $\gamma > 0$, and $\lfloor\gamma\rfloor$ be the largest integer strictly smaller than $\gamma$, i.e., $\gamma - 1 \leqslant \lfloor\gamma\rfloor < \gamma$. We say that $V \in Lip^{\gamma}$, if $V : \mathbb{R}^m \to \mathbb{R}^{m\times d}$ is $\lfloor\gamma\rfloor$-times continuously differentiable and there exists some constant $C$ such that

$$\|D^k V(y)\| \leqslant C \quad \forall\, k = 0, \cdots, \lfloor\gamma\rfloor\ \forall\, y \in \mathbb{R}^m,$$
$$\|D^{\lfloor\gamma\rfloor} V(y_1) - D^{\lfloor\gamma\rfloor} V(y_2)\| \leqslant C\|y_1 - y_2\|^{\gamma-\lfloor\gamma\rfloor} \quad \forall\, y_1, y_2 \in \mathbb{R}^m,$$

where $D^k V$ denotes $k$th derivative of $V$. The smallest constant $C$ satisfying the above inequalities is denoted by $\|V\|_{Lip^{\gamma}}$.

LEMMA 2.4 (Friz & Victoir, 2010, Theorem 10.26 and Theorem 11.6) Let $p \in [1, \infty)$ and $\mathbf{X}$ be a $p$-rough path. If $V \in Lip^{\gamma}$ with $\gamma > p$, or $V$ is linear, then (2.3) has a unique solution. Additionally, the Jacobian $\frac{\partial Y_t}{\partial z}$ exists and satisfies the linear RDE

$$\begin{cases} \mathrm{d}\dfrac{\partial Y_t}{\partial z} = \displaystyle\sum_{l=0}^{\mathrm{d}} DV_l(Y_t)\frac{\partial Y_t}{\partial z}\,\mathrm{d}\mathbf{X}_t^l, \quad t \in (0, T]; \\ \dfrac{\partial Y_0}{\partial z} = \mathbb{I}_m \in \mathbb{R}^{m\times m}, \end{cases}$$

where $\mathbb{I}_m$ is the identity matrix.

REMARK 2.5 If $X$ is the standard Brownian motion, the solution $Y$ of (2.3) solves the corresponding Stratonovich SDE almost surely (Friz & Victoir, 2010, Theorem 17.3).

## 3. Construction of the stochastic modified equation

In this section, we investigate the formulation of stochastic modified equations associated to numerical methods for the SDE (2.1). In subsection 3.1, we construct a new stochastic modified equation and verify that the numerical solution to the original SDE solves exactly the proposed stochastic modified equation. In subsection 3.2, we prove that the stochastic modified equation preserves the symplectic conservation law if it is associated with a stochatic symplectic method for a rough Hamiltonian system. This answers Problem 1.1 proposed in the introduction.

### 3.1 *Construction of the stochastic modified equations for general methods*

Fix the time step size $h = T/N, N \in \mathbb{N}_+$. Let $Y_n^h$ be the numerical solution given by a numerical method, which is an approximation for $Y_{t_n}$, where $t_n = nh, n = 0, \cdots, N$. Our main assumption on the numerical method is as follows.

ASSUMPTION 3.1 The numerical solution $Y_{n+1}^h$ can be expanded as an infinite series of functions of $Y_n^h$:

$$Y_{n+1}^h = Y_n^h + \sum_{|\alpha|=1}^{\infty} \mathrm{d}_\alpha(Y_n^h) h^{\alpha_0} (X^1_{t_n,t_{n+1}})^{\alpha_1} \cdots (X^{\mathrm{d}}_{t_n,t_{n+1}})^{\alpha_{\mathrm{d}}}, \tag{3.1}$$

where $\alpha = (\alpha_0, \cdots, \alpha_{\mathrm{d}}) \in \mathbb{N}^{\mathrm{d}+1}$, $|\alpha| := \alpha_0 + \cdots + \alpha_{\mathrm{d}} \geqslant 1$ and $Y_0^h = z$. In addition, it holds that

$$\mathrm{d}_\alpha(y) = V_l(y), \quad |\alpha| = 1,\ \alpha_l = 1,\ l \in \{1, \cdots, \mathrm{d}\}. \tag{3.2}$$

Here, (3.1) is a formal series obtained by the Taylor expansion, which is used for deducing the formulation of stochastic modified equations. Since $\{Y_n^h\}_{n=1}^N$ is the numerical solution given by a numerical method, the coefficients $d_\alpha$ in the series are composed by $V$ and its derivatives. The specific conditions on $V$, which also imply conditions on $d_\alpha$, will be given in the theorems in the following sections. Moreover, (3.2) is a necessary condition to ensure that the numerical solution converges to the exact solution almost surely; see the convergence analysis in Corollary 9 of Friz & Riedel (2014) and in Theorems 5.2–5.3 of Hong *et al.* (2018). For convenience, in the rest of the article, we will denote $V_\alpha(y) := V_l(y)$ with $|\alpha| = 1, \alpha_l = 1$ and $l \in \{0, \cdots, \mathrm{d}\}$.

In Example 3.2, we take the Runge–Kutta (RK) method for an example to illustrate how to verify the expansion (3.1) for numerical solutions.

EXAMPLE 3.2 The $s$-stage RK method is defined by

$$\begin{cases} Y_{n+1,i}^h = Y_n^h + \sum_{j=1}^{s} a_{ij}\Big(V_0(Y_{n+1,j}^h)h + \sum_{l=1}^{\mathrm{d}} V_l(Y_{n+1,j}^h)X_{t_n,t_{n+1}}^l\Big), \\ Y_{n+1}^h = Y_n^h + \sum_{i=1}^{s} b_i\Big(V_0(Y_{n+1,i}^h)h + \sum_{l=1}^{\mathrm{d}} V_l(Y_{n+1,i}^h)X_{t_n,t_{n+1}}^l\Big). \end{cases} \tag{3.3}$$

Then the Taylor expansion produces that for $l = 0, \cdots, \mathrm{d}$,

$$\begin{aligned} &V_l(Y_{n+1,i}^h) \\ &= V_l(Y_n^h) + V_l'(Y_n^h)\Big(\sum_{j=1}^{s} a_{ij}\Big(V_0(Y_{n+1,j}^h)h + \sum_{l_1=1}^{\mathrm{d}} V_{l_1}(Y_{n+1,j}^h)X_{t_n,t_{n+1}}^{l_1}\Big)\Big) \\ &\quad + \frac{1}{2}V_l''(Y_n^h)\Big(\sum_{j=1}^{s} a_{ij}\Big(V_0(Y_{n+1,j}^h)h + \sum_{l_1=1}^{\mathrm{d}} V_{l_1}(Y_{n+1,j}^h)X_{t_n,t_{n+1}}^{l_1}\Big)\Big)^{\otimes 2} + \cdots \\ &= V_l(Y_n^h) + \sum_{j=1}^{s} a_{ij}V_l'(Y_n^h)\Big(V_0(Y_n^h)h + \sum_{l_1=1}^{\mathrm{d}} V_{l_1}(Y_n^h)X_{t_n,t_{n+1}}^{l_1}\Big) \\ &\quad + \sum_{j_1,j_2=1}^{s} a_{ij_1}a_{j_1j_2}V_l'(Y_n^h)V_0'(Y_n^h)\Big(V_0(Y_n^h)h + \sum_{l_1=1}^{\mathrm{d}} V_{l_1}(Y_n^h)X_{t_n,t_{n+1}}^{l_1}\Big)h \\ &\quad + \sum_{l_1=1}^{\mathrm{d}}\sum_{j_1,j_2=1}^{s} a_{ij_1}a_{j_1j_2}V_l'(Y_n^h)V_{l_1}'(Y_n^h)\Big(V_0(Y_n^h)h + \sum_{l_2=1}^{\mathrm{d}} V_{l_2}(Y_n^h)X_{t_n,t_{n+1}}^{l_2}\Big)X_{t_n,t_{n+1}}^{l_1} \\ &\quad + \frac{1}{2}\sum_{j_1,j_2=1}^{s} a_{ij_1}a_{ij_2}V_l''(Y_n^h)\Big(V_0(Y_n^h)h + \sum_{l_1=1}^{\mathrm{d}} V_{l_1}(Y_n^h)X_{t_n,t_{n+1}}^{l_1}\Big)\Big(V_0(Y_n^h)h + \sum_{l_2=1}^{\mathrm{d}} V_{l_2}(Y_n^h)X_{t_n,t_{n+1}}^{l_2}\Big) \\ &\quad + \cdots. \end{aligned}$$

Here $V_0'(y)V_0(y)$ is the derivative of $V_0(y)$ acting on $V_0(y)$, and $V_0''(y)V_0(y)V_0(y)$ is the second derivative of $V_0(y)$ acting $(V_0(y), V_0(y))$. Other operators are defined similarly. Substituting them into (3.3), we get

$$
\begin{aligned}
&Y_{n+1}^h\\
&= Y_n^h + \sum_{i=1}^{s} b_i \Bigg[ V_0(Y_n^h) + \sum_{j=1}^{s} a_{ij} V_0'(Y_n^h)\Big(V_0(Y_n^h)h + \sum_{l_1=1}^{\mathrm{d}} V_{l_1}(Y_n^h)X_{t_n,t_{n+1}}^{l_1}\Big)\\
&\quad + \sum_{j_1,j_2=1}^{s} a_{ij_1}a_{j_1j_2} V_0'(Y_n^h)V_0'(Y_n^h)\Big(V_0(Y_n^h)h + \sum_{l_1=1}^{\mathrm{d}} V_{l_1}(Y_n^h)X_{t_n,t_{n+1}}^{l_1}\Big)h\\
&\quad + \sum_{l_1=1}^{\mathrm{d}}\sum_{j_1,j_2=1}^{s} a_{ij_1}a_{j_1j_2} V_0'(Y_n^h)V_{l_1}'(Y_n^h)\Big(V_0(Y_n^h)h + \sum_{l_2=1}^{\mathrm{d}} V_{l_2}(Y_n^h)X_{t_n,t_{n+1}}^{l_2}\Big)X_{t_n,t_{n+1}}^{l_1}\\
&\quad + \frac{1}{2}\sum_{j_1,j_2=1}^{s} a_{ij_1}a_{ij_2} V_0''(Y_n^h)\Big(V_0(Y_n^h)h + \sum_{l_1=1}^{\mathrm{d}} V_{l_1}(Y_n^h)X_{t_n,t_{n+1}}^{l_1}\Big)\Big(V_0(Y_n^h)h + \sum_{l_2=1}^{\mathrm{d}} V_{l_2}(Y_n^h)X_{t_n,t_{n+1}}^{l_2}\Big)\Bigg]h\\
&\quad + \sum_{i=1}^{s}\sum_{l=1}^{\mathrm{d}} b_i \Bigg[ V_l(Y_n^h) + \sum_{j=1}^{s} a_{ij} V_l'(Y_n^h)\Big(V_0(Y_n^h)h + \sum_{l_1=1}^{\mathrm{d}} V_{l_1}(Y_n^h)X_{t_n,t_{n+1}}^{l_1}\Big)\\
&\quad + \sum_{j_1,j_2=1}^{s} a_{ij_1}a_{j_1j_2} V_l'(Y_n^h)V_0'(Y_n^h)\Big(V_0(Y_n^h)h + \sum_{l_1=1}^{\mathrm{d}} V_{l_1}(Y_n^h)X_{t_n,t_{n+1}}^{l_1}\Big)h\\
&\quad + \sum_{l_1=1}^{\mathrm{d}}\sum_{j_1,j_2=1}^{s} a_{ij_1}a_{j_1j_2} V_l'(Y_n^h)V_{l_1}'(Y_n^h)\Big(V_0(Y_n^h)h + \sum_{l_2=1}^{\mathrm{d}} V_{l_2}(Y_n^h)X_{t_n,t_{n+1}}^{l_2}\Big)X_{t_n,t_{n+1}}^{l_1}\\
&\quad + \frac{1}{2}\sum_{j_1,j_2=1}^{s} a_{ij_1}a_{ij_2} V_l''(Y_n^h)\Big(V_0(Y_n^h)h + \sum_{l_1=1}^{\mathrm{d}} V_{l_1}(Y_n^h)X_{t_n,t_{n+1}}^{l_1}\Big)\Big(V_0(Y_n^h)h + \sum_{l_2=1}^{\mathrm{d}} V_{l_2}(Y_n^h)X_{t_n,t_{n+1}}^{l_2}\Big)\Bigg]X_{t_n,t_{n+1}}^{l}\\
&\quad + \cdots,
\end{aligned}
$$

which satisfies the form of (3.1).

From Assumption 3.1, the increments of $X$ are utilized in numerical methods. Based on this observation, we combine with the piecewise approximation $x^h$ of $X$, which is given by

$$
x_t^{h,l} := X_{t_n}^l + \frac{t-t_n}{h} X_{t_n,t_{n+1}}^l, \quad t \in (t_n, t_{n+1}],\ n = 0, \cdots, N-1, \tag{3.4}
$$

to define the new stochatic modified equation as follows.

Definition 3.3 For $\alpha = (\alpha_0, \cdots, \alpha_{\mathrm{d}}) \in \mathbb{N}^{\mathrm{d}+1}$, denote

$$
\begin{aligned}
O_i^\alpha := \Big\{ &(k^{i,1}, \cdots, k^{i,i}) : k^{i,1}, \cdots, k^{i,i} \in \mathbb{N}^{\mathrm{d}+1},\ |k^{i,1}|, \cdots, |k^{i,i}| \geqslant 1,\\
&k_l^{i,1} + \cdots + k_l^{i,i} = \alpha_l, \quad l = 0, \cdots, \mathrm{d} \Big\}.
\end{aligned}
$$

The stochastic modified equation for a numerical method satisfying (3.1) is defined as an RDE

$$\begin{cases} \mathrm{d}\tilde{y}_t = \sum_{l=0}^{\mathrm{d}} \sum_{i(\alpha)=l} f_\alpha(\tilde{y}_t) h^{\alpha_0} (X^1_{t_n,t_{n+1}})^{\alpha_1} \cdots (X^l_{t_n,t_{n+1}})^{\alpha_l - 1} \cdots (X^{\mathrm{d}}_{t_n,t_{n+1}})^{\alpha_{\mathrm{d}}} \, \mathrm{d}x^{h,l}_t, \quad t \in (t_n, t_{n+1}]; \\ \tilde{y}_0 = z, \end{cases} \tag{3.5}$$

where $\tilde{y}$ is continuous on $[0, T]$, $i(\alpha)$ is denoted by

$$i(\alpha) = \min\{l : \alpha_l \geqslant 1, l = 0, \cdots, \mathrm{d}\} \in \{0, \cdots, \mathrm{d}\}, \tag{3.6}$$

and the coefficients $f_\alpha(y)$ are

$$\begin{cases} f_\alpha(y) = \mathrm{d}_\alpha(y), \quad |\alpha| = 1, \\ f_\alpha(y) = \mathrm{d}_\alpha(y) - \sum_{i=2}^{|\alpha|} \frac{1}{i!} \sum_{(k^{i,1}, \cdots, k^{i,i}) \in O^\alpha_i} (D_{k^{i,1}} \cdots D_{k^{i,i-1}} f_{k^{i,i}})(y), \quad |\alpha| \geqslant 2, \end{cases} \tag{3.7}$$

with $(D_{k^{i_1,i_2}} g)(y) := g'(y) f_{k^{i_1,i_2}}(y)$ for $k^{i_1,i_2} = (k^{i_1,i_2}_0, \cdots, k^{i_1,i_2}_{\mathrm{d}}) \in \mathbb{N}^{\mathrm{d}+1}$, $|k^{i_1,i_2}| \geqslant 1$.

REMARK 3.4 For a fixed time step size $h$, the driving signal $x^h$ is of bounded variation, then the stochastic modified equation is well defined in the Riemann–Stieltjes integral sense. It is emphasized that the 1-variation of $x^h$ is not uniformly bounded with respect to $h$ in general. Indeed, we only have that for $p > 2\rho$,

$$\sup_h \|S_{[p]}(x^h)\|_{p\text{-}var;[0,T]} < \infty$$

with $\rho$ given in Assumption 2.1; see Section 15.3.2 in Friz & Victoir (2010) for more details. In this sense, we call (3.5) an RDE.

REMARK 3.5 Recall the Wong–Zakai approximation of (2.2), i.e.,

$$\begin{cases} \mathrm{d}y^h_t = V(y^h_t)\, \mathrm{d}x^h_t = \sum_{l=0}^{\mathrm{d}} V_l(y^h_t)\, \mathrm{d}x^{h,l}_t, \quad t \in (0, T]; \\ y^h_0 = z. \end{cases}$$

The stochastic modified equation (3.5) associated with a numerical method under Assumption 3.1 is also a perturbation of the Wong–Zakai approximation of the original equation.

REMARK 3.6 The framework in this article about constructing the stochastic modified equation is also applicable for numerical methods with adaptive time step sizes.

EXAMPLE 3.7 Let $\mathrm{d}=1$. The modified Milstein scheme (see, e.g., Deya *et al.*, 2012) reads

$$Y_{n+1}^h = Y_n^h + V_0(Y_n^h)h + V_1(Y_n^h)X_{t_n,t_{n+1}}^1 + \frac{1}{2}V_1'(Y_n^h)V_1(Y_n^h)(X_{t_n,t_{n+1}}^1)^2,$$

which implies

$$\begin{aligned}
&\mathrm{d}_{(1,0)}(y) = V_0(y),\ \mathrm{d}_{(0,1)}(y) = V_1(y),\\
&\mathrm{d}_{(2,0)}(y) = \mathrm{d}_{(1,1)}(y) = 0,\ \mathrm{d}_{(0,2)}(y) = \frac{1}{2}V_1'(y)V_1(y),\\
&\mathrm{d}_\alpha(y) = 0, \quad |\alpha| \geqslant 3.
\end{aligned}$$

According to (3.7), the coefficients of the associated stochastic modified equations are

$$\begin{aligned}
|\alpha| = 1: \quad & f_{(1,0)}(y) = \mathrm{d}_{(1,0)}(y) = V_0(y),\\
& f_{(0,1)}(y) = \mathrm{d}_{(0,1)}(y) = V_1(y);\\
|\alpha| = 2: \quad & f_{(2,0)}(y) = \mathrm{d}_{(2,0)}(y) - \frac{1}{2!}\big(D_{(1,0)}f_{(1,0)}\big)(y) = -\frac{1}{2}V_0'(y)V_0(y),\\
& f_{(1,1)}(y) = \mathrm{d}_{(1,1)}(y) - \frac{1}{2!}\Big[\big(D_{(1,0)}f_{(0,1)}\big)(y) + \big(D_{(0,1)}f_{(1,0)}\big)(y)\Big]\\
&\qquad = -\frac{1}{2}\Big[V_1'(y)V_0(y) + V_0'(y)V_1(y)\Big],\\
& f_{(0,2)}(y) = \mathrm{d}_{(0,2)}(y) - \frac{1}{2!}\big(D_{(0,1)}f_{(0,1)}\big)(y)\\
&\qquad = \frac{1}{2}V_1'(y)V_1(y) - \frac{1}{2}V_1'(y)V_1(y) = 0;\\
|\alpha| \geqslant 3: \quad & \cdots
\end{aligned}$$

THEOREM 3.8 Suppose that $\tilde{y}$ is the solution of the stochastic modified equation (3.5) associated with a numerical method with numerical solution $Y^h$. Then we have

$$\tilde{y}_{t_n} = Y_n^h, \quad n = 0, \cdots, N.$$

*Proof.* Consider $t \in (t_n, t_{n+1}]$. Due to Definition 3.3, the stochastic modified equation can be written as

$$\mathrm{d}\tilde{y}_t = \sum_{|\alpha|=1}^{\infty} f_\alpha(\tilde{y}_t)h^{\alpha_0-1}(X_{t_n,t_{n+1}}^1)^{\alpha_1}\cdots(X_{t_n,t_{n+1}}^{\mathrm{d}})^{\alpha_{\mathrm{d}}}\,\mathrm{d}t.$$

Using the Taylor expansion and the chain rule, we have

$$
\begin{aligned}
&\tilde{y}_{t_{n+1}} \\
&\quad = \tilde{y}_{t_n} + \sum_{k=1}^{\infty} \frac{\mathrm{d}^k}{\mathrm{d}t^k}(\tilde{y}_t)\Big|_{t=t_n} \frac{h^k}{k!} \\
&\quad = \tilde{y}_{t_n} + \sum_{|\alpha|=1}^{\infty} f_\alpha(\tilde{y}_{t_n}) h^{\alpha_0} (X^1_{t_n,t_{n+1}})^{\alpha_1} \cdots (X^{\mathrm{d}}_{t_n,t_{n+1}})^{\alpha_{\mathrm{d}}} \\
&\qquad + \frac{1}{2!}\left[ \frac{\partial}{\partial y}\left( \sum_{|\alpha|=1}^{\infty} f_\alpha(y) h^{\alpha_0} (X^1_{t_n,t_{n+1}})^{\alpha_1} \cdots (X^{\mathrm{d}}_{t_n,t_{n+1}})^{\alpha_{\mathrm{d}}} \right)\Big|_{y=\tilde{y}_{t_n}} \right] \\
&\qquad \times \left( \sum_{|\alpha|=1}^{\infty} f_\alpha(\tilde{y}_{t_n}) h^{\alpha_0} (X^1_{t_n,t_{n+1}})^{\alpha_1} \cdots (X^{\mathrm{d}}_{t_n,t_{n+1}})^{\alpha_{\mathrm{d}}} \right) \\
&\qquad + \frac{1}{3!}\Bigg[ \frac{\partial}{\partial y}\Bigg(\Bigg( \frac{\partial}{\partial y}\Big( \sum_{|\alpha|=1}^{\infty} f_\alpha(y) h^{\alpha_0} (X^1_{t_n,t_{n+1}})^{\alpha_1} \cdots (X^{\mathrm{d}}_{t_n,t_{n+1}})^{\alpha_{\mathrm{d}}} \Big)\Bigg) \\
&\qquad \times \Big( \sum_{|\alpha|=1}^{\infty} f_\alpha(y) h^{\alpha_0} (X^1_{t_n,t_{n+1}})^{\alpha_1} \cdots (X^{\mathrm{d}}_{t_n,t_{n+1}})^{\alpha_{\mathrm{d}}} \Big)\Bigg)\Bigg|_{y=\tilde{y}_{t_n}} \Bigg] \\
&\qquad \times \left( \sum_{|\alpha|=1}^{\infty} f_\alpha(\tilde{y}_{t_n}) h^{\alpha_0} (X^1_{t_n,t_{n+1}})^{\alpha_1} \cdots (X^{\mathrm{d}}_{t_n,t_{n+1}})^{\alpha_{\mathrm{d}}} \right) + \cdots \\
&=: \tilde{y}_{t_n} + \sum_{|\alpha|=1}^{\infty} \tilde{f}_\alpha(\tilde{y}_{t_n}) h^{\alpha_0} (X^1_{t_n,t_{n+1}})^{\alpha_1} \cdots (X^{\mathrm{d}}_{t_n,t_{n+1}})^{\alpha_{\mathrm{d}}},
\end{aligned} \tag{3.8}
$$

where

$$
\begin{aligned}
&\tilde{f}_\alpha(y) = f_\alpha(y), \quad |\alpha| = 1, \\
&\tilde{f}_\alpha(y) = f_\alpha(y) + \sum_{i=2}^{|\alpha|} \frac{1}{i!} \sum_{(k^{i,1},\cdots,k^{i,i}) \in O_i^\alpha} (D_{k^{i,1}} \cdots D_{k^{i,i-1}} f_{k^{i,i}})(y), \quad |\alpha| \geqslant 2.
\end{aligned}
$$

Together with (3.7), we have

$$
\tilde{f}_\alpha(y) = d_\alpha(y) \quad \forall\, \alpha \in \mathbb{N}^{\mathrm{d}+1},\ |\alpha| \geqslant 1.
$$

Therefore, we obtain $\tilde{y}_{t_n} = Y_n^h$, for $n = 0, \cdots, N$. □

### 3.2 *Stochastic modified equation of stochastic symplectic method for stochastic Hamiltonian system*

We consider the stochastic Hamiltonian system in the rough path sense (rough Hamiltonian system for short):

$$\begin{cases} \mathrm{d}P_t = -\dfrac{\partial \mathscr{H}_0(P_t,Q_t)}{\partial Q_t}\,\mathrm{d}t - \sum_{l=1}^{\mathrm{d}} \dfrac{\partial \mathscr{H}_l(P_t,Q_t)}{\partial Q_t}\,\mathrm{d}X_t^l, & P_0 = p \in \mathbb{R}^m; \\ \mathrm{d}Q_t = \dfrac{\partial \mathscr{H}_0(P_t,Q_t)}{\partial P_t}\,\mathrm{d}t + \sum_{l=1}^{\mathrm{d}} \dfrac{\partial \mathscr{H}_l(P_t,Q_t)}{\partial P_t}\,\mathrm{d}X_t^l, & Q_0 = q \in \mathbb{R}^m. \end{cases} \tag{3.9}$$

One characteristic property of the rough Hamiltonian system is that its phase flow preserves the symplectic structure. Namely, the differential 2-form $\mathrm{d}P \wedge \mathrm{d}Q$ is invariant under the phase flow. Here the differential is made with respect to the initial value $(p, q)$, which is different from the formal time derivative in (3.9).

LEMMA 3.9 (Hong *et al.*, 2018, Theorem 3.1) The phase flow of the rough Hamiltonian system (3.9) preserves the symplectic structure, that is,

$$\mathrm{d}P \wedge \mathrm{d}Q = \mathrm{d}p \wedge \mathrm{d}q, \quad a.s.$$

Denote by $\mathbb{J}_{2m} := \begin{pmatrix} 0 & \mathbb{I}_m \\ -\mathbb{I}_m & 0 \end{pmatrix}$ the standard symplectic matrix. Letting $Y := (P^\top, Q^\top)^\top$, $z := (p^\top, q^\top)^\top$ and $V_l(y) := \mathbb{J}_{2m}^{-1} \nabla \mathscr{H}_l(y), l = 0, \cdots, \mathrm{d}$, we obtain a compact form as (2.2). Thus the stochastic modified equations in Definition 3.3 of numerical methods satisfying (3.1) for (3.9) are constructed. Moreover, based on Lemma 3.9, it is natural to perform symplectic methods which inherit the symplectic structure of the original rough Hamiltonian system, such as the symplectic RK methods in the next lemma.

LEMMA 3.10 (Hong *et al.*, 2018, Theorem 4.1) The $s$-stage RK method (3.3) inherits the symplectic structure of a rough Hamiltonian system, if the coefficients satisfy

$$a_{ij}b_i + a_{ji}b_j = b_ib_j \quad \forall\, i,j = 1, \cdots, s.$$

The following theorem reveals that the stochastic modified equation associated to a stochastic symplectic method is still a Hamiltonian system, which gives a positive answer to Problem 1.1 in the introduction. In the proof, since the vector field of the stochastic modified equation is a sum of random coefficients, we make use of the Hermite polynomial to separate each coefficient and then obtain the Hamiltonian formulation.

THEOREM 3.11 Assume that $V$ is bounded with bounded derivatives up to any order, and that there exist a constant $\varsigma > 1/2$ and a function $L : [0, T] \to (0, +\infty)$ such that

$$\lim_{h\to 0} h^{-1/\varsigma}\mathbb{E}\big\|X_t - X_{t+h}\big\|^2 = L(t). \tag{3.10}$$

If $Y_1^h(z)$, the one-step numerical solution, is given by applying a symplectic method satisfying Assumption 3.1 to (3.9), then the associated stochastic modified equation (3.5) is a Hamiltonian system. More precisely, for any $f_\alpha : \mathbb{R}^{2m} \to \mathbb{R}^{2m}$ in (3.5), there exists a Hamiltonian $\mathscr{H}_\alpha : \mathbb{R}^{2m} \to \mathbb{R}$ such that

$$f_\alpha(y) = \mathbb{J}_{2m}^{-1} \nabla \mathscr{H}_\alpha(y). \tag{3.11}$$

*Proof.* By $\varsigma > 1/2$, we have $1/2\varsigma < 1$. For $\alpha \in \mathbb{N}^{\mathrm{d}+1}$, define $\theta(\alpha) := \alpha_0 + \frac{\alpha_1+\cdots+\alpha_{\mathrm{d}}}{2\varsigma}$. Define a set $S := \{x : x = m + \frac{k}{2\varsigma}, m, k \in \mathbb{N}\}$. We sequence the elements in $S$ and denote them by $\theta_0, \theta_1, \theta_2, \cdots$, such that $\theta_n < \theta_{n+1}$. Then for any $\alpha$, there exits an integer $n$ such that $\theta(\alpha) = \theta_n$.

From condition (3.2), we have immediately that (3.11) holds for $\alpha$ with $\theta(\alpha) = \theta_1$. For $r \in \mathbb{N}_+$, assume by induction that for any $\alpha$ such that $\theta(\alpha) \leqslant \theta_r$, (3.11) holds. By Assumption 3.1, the expansion of the one-step numerical solution is

$$Y_1^h(z) = z + \sum_{|\alpha|=1}^{\infty} d_\alpha(z) h^{\alpha_0} (X_{t_0,t_1}^1)^{\alpha_1} \cdots (X_{t_0,t_1}^{\mathrm{d}})^{\alpha_{\mathrm{d}}}.$$

Consider the following equation:

$$\mathrm{d}\tilde{y}_t^r = \sum_{\theta(\alpha)=\theta_1}^{\theta_r} f_\alpha(\tilde{y}_t^r) h^{\alpha_0-1} (X_{t_n,t_{n+1}}^1)^{\alpha_1} \cdots (X_{t_n,t_{n+1}}^{\mathrm{d}})^{\alpha_{\mathrm{d}}}\, \mathrm{d}t, \quad \tilde{y}_0^r = z, \ \ t \in (0, t_1].$$

Denote by $\pi^r(z)_t$ the flow of the above equation. By the Taylor expansion and the chain rule, similar approach to calculating (3.8) leads to

$$\pi^r(z)_h = z + \sum_{|\alpha|=1}^{\infty} f_\alpha^r(z) h^{\alpha_0} (X_{t_0,t_1}^1)^{\alpha_1} \cdots (X_{t_0,t_1}^{\mathrm{d}})^{\alpha_{\mathrm{d}}},$$

where $f_\alpha^r$ is determined by $f_{\alpha'}$ with $|\alpha'| \leqslant |\alpha|$. Comparing the above expansion with (3.1), we have from the recursion (3.7) that for all $\alpha$ such that $\theta(\alpha) \leqslant \theta_r$,

$$\mathrm{d}_\alpha(z) - f_\alpha^r(z) = 0;$$

for all $\alpha$ such that $\theta(\alpha) = \theta_{r+1}$,

$$\mathrm{d}_\alpha(z) - f_\alpha^r(z) = f_\alpha.$$

Based on the assumption that $V$ and its derivatives are bounded, we have $\left\|Y_1^h(z)\right\|_{L^p(\Omega)} \leqslant C$ for $p \geqslant 1$. Moreover, since the coefficients $\{f_\alpha\}$ and $\{f_\alpha^r\}$ are determined by $V$ and its derivatives, we obtain the boundedness of $\{f_\alpha\}$ and $\{f_\alpha^r\}$, which yields $\left\|\pi^r(z)_t\right\|_{L^p(\Omega)} \leqslant C$. Then there exists a random variable $R_{r+2}$ such that

$$Y_1^h(z) = \pi^r(z)_h + \sum_{\theta(\alpha)=\theta_{r+1}} f_\alpha(z) h^{\alpha_0} (X_{t_0,t_1}^1)^{\alpha_1} \cdots (X_{t_0,t_1}^{\mathrm{d}})^{\alpha_{\mathrm{d}}} + R_{r+2}, \quad a.s.,$$

where the leading term of $R_{r+2}$ involves $h^{\alpha_0}(X^1_{t_0,t_1})^{\alpha_1}\cdots(X^{\mathrm{d}}_{t_0,t_1})^{\alpha_{\mathrm{d}}}$ with $\alpha_0+\frac{\alpha_1+\cdots+\alpha_{\mathrm{d}}}{2\varsigma}=\theta_{r+2}$, which gives $\|R_{r+2}\|_{L^p(\Omega)}\leqslant Ch^{\theta_{r+2}}$. Taking the derivatives of $\pi^r(z)_h$ and $Y^h_1(z)$ with respect to $z$, we deduce that the Jacobians satisfy

$$\frac{\partial\pi^r(z)_h}{\partial z}=\mathbb{I}_{2m}+R_h,\quad a.s.,$$
$$\frac{\partial Y^h_1(z)}{\partial z}=\frac{\partial\pi^r(z)_h}{\partial z}+\sum_{\theta(\alpha)=\theta_{r+1}}f'_\alpha(z)h^{\alpha_0}(X^1_{t_0,t_1})^{\alpha_1}\cdots(X^{\mathrm{d}}_{t_0,t_1})^{\alpha_{\mathrm{d}}}+\frac{\partial R_{r+2}}{\partial z},\quad a.s.,$$

where $f'_\alpha(z):=\frac{\partial f_\alpha(z)}{\partial z}$. Since the leading term of $R_h$ involves $h^{\alpha_0}(X^1_{t_0,t_1})^{\alpha_1}\cdots(X^{\mathrm{d}}_{t_0,t_1})^{\alpha_{\mathrm{d}}}$ with $\alpha_0+\frac{\alpha_1+\cdots+\alpha_{\mathrm{d}}}{2\varsigma}=\theta_1$, and the leading term of $\frac{\partial R_{r+2}}{\partial z}$ involves $h^{\alpha_0}(X^1_{t_0,t_1})^{\alpha_1}\cdots(X^{\mathrm{d}}_{t_0,t_1})^{\alpha_{\mathrm{d}}}$ with $\alpha_0+\frac{\alpha_1+\cdots+\alpha_{\mathrm{d}}}{2\varsigma}=\theta_{r+2}$, we get $\|R_h\|_{L^p(\Omega)}\leqslant C(p)h^{\theta_1}$ and $\left\|\frac{\partial R_{r+2}}{\partial z}\right\|_{L^p(\Omega)}\leqslant C(p)h^{\theta_{r+2}}$. The definition of the symplectic method means

$$\mathbb{J}_{2m}=\Big(\frac{\partial Y^h_1(z)}{\partial z}\Big)^\top\mathbb{J}_{2m}\,\frac{\partial Y^h_1(z)}{\partial z},\quad a.s.$$

Substituting the expressions of the Jacobians into the above equality, we obtain

$$\begin{aligned}\mathbb{J}_{2m}=&\Big(\frac{\partial\pi^r(z)_h}{\partial z}\Big)^\top\mathbb{J}_{2m}\,\frac{\partial\pi^r(z)_h}{\partial z}+\sum_{\theta(\alpha)=\theta_{r+1}}\mathbb{J}_{2m}f'_\alpha(z)h^{\alpha_0}(X^1_{t_0,t_1})^{\alpha_1}\cdots(X^{\mathrm{d}}_{t_0,t_1})^{\alpha_{\mathrm{d}}}\\&+\sum_{\theta(\alpha)=\theta_{r+1}}f'_\alpha(z)^\top\mathbb{J}_{2m}\,h^{\alpha_0}(X^1_{t_0,t_1})^{\alpha_1}\cdots(X^{\mathrm{d}}_{t_0,t_1})^{\alpha_{\mathrm{d}}}+R,\quad a.s.,\end{aligned}$$

where $\|R\|_{L^p(\Omega)}\leqslant C(p)h^{\theta_{r+2}}$, due to the leading term of $R$ involving $h^{\alpha_0}(X^1_{t_0,t_1})^{\alpha_1}\cdots(X^{\mathrm{d}}_{t_0,t_1})^{\alpha_{\mathrm{d}}}$ with $\alpha_0+\frac{\alpha_1+\cdots+\alpha_{\mathrm{d}}}{2\varsigma}=\theta_{r+2}$. The induction assumption implies

$$\mathbb{J}_{2m}=\Big(\frac{\partial\pi^r(z)_h}{\partial z}\Big)^\top\mathbb{J}_{2m}\,\frac{\partial\pi^r(z)_h}{\partial z},\quad a.s.,$$

which provides

$$\sum_{\theta(\alpha)=\theta_{r+1}}\Big(\mathbb{J}_{2m}f'_\alpha(z)+f'_\alpha(z)^\top\mathbb{J}_{2m}\Big)h^{-\frac{\alpha_1+\cdots+\alpha_{\mathrm{d}}}{2\varsigma}}(X^1_{t_0,t_1})^{\alpha_1}\cdots(X^{\mathrm{d}}_{t_0,t_1})^{\alpha_{\mathrm{d}}}=-h^{-\theta_{r+1}}R,\quad a.s.$$

The assumption (3.10) implies that for $l=1,\cdots,\mathrm{d}$, there exists a function $M:[0,T]\times(0,+\infty)\to(0,+\infty)$ such that

$$X^l_{t_0,t_1}=h^{\frac{1}{2\varsigma}}M^{\frac{1}{2}}(t_0,h)\xi_{h,l},\quad\lim_{h\to0}M(t,h)=L(t),$$

where $\xi_{h,l}$, $l = 1, \cdots, \mathrm{d}$, are independent and identically distributed standard normal random variables. Letting $h$ tend to 0 and using the fact $L(t) > 0$ and

$$\lim_{h\to 0} \left\| h^{-\theta_{r+1}} R \right\|_{L^2(\Omega)} = 0,$$

we have that

$$\sum_{\theta(\alpha)=\theta_{r+1}} \left( \mathbb{J}_{2m} f'_\alpha(z) + f'_\alpha(z)^\top \mathbb{J}_{2m} \right) \xi_1^{\alpha_1} \cdots \xi_{\mathrm{d}}^{\alpha_{\mathrm{d}}} = 0, \quad a.s., \tag{3.12}$$

where $\xi_l$, $l = 1, \cdots, \mathrm{d}$, are independent and identically distributed standard normal random variables. In Theorem 1.6 of Gautschi (2004), it is proved that there exists a unique monic orthogonal polynomial sequence $\{p_k(x)\}_{k=1}^\infty$ with respect to the measure induced by $\xi_1$, i.e., the Hermite polynomials. This means that for any $k \in \mathbb{N}_+$, we have

$$x^k = p_k(x) + \sum_{j<k} a_j p_j(x).$$

Then we rewrite (3.12) as

$$\begin{aligned} 0 = &\sum_{\theta(\alpha)=\theta_{r+1}} \left( \mathbb{J}_{2m} f'_\alpha(z) + f'_\alpha(z)^\top \mathbb{J}_{2m} \right) \\ &\times \Big( p_{\alpha_1}(\xi_1) + \sum_{k_1<\alpha_1} a_{k_1} p_{k_1}(\xi_1) \Big) \cdots \Big( p_{\alpha_{\mathrm{d}}}(\xi_{\mathrm{d}}) + \sum_{k_{\mathrm{d}}<\alpha_{\mathrm{d}}} a_{k_{\mathrm{d}}} p_{k_{\mathrm{d}}}(\xi_{\mathrm{d}}) \Big). \end{aligned}$$

Recall that $\theta(\alpha) = \alpha_0 + \frac{\alpha_1+\cdots+\alpha_{\mathrm{d}}}{2\varsigma}$. We denote $G$ the integer part of $2\varsigma\theta_{r+1}$. We decomposite the summation above by

$$\begin{aligned} 0 = &\sum_{\theta(\alpha)=\theta_{r+1},\alpha_1+\cdots+\alpha_{\mathrm{d}}=G} \left( \mathbb{J}_{2m} f'_\alpha(z) + f'_\alpha(z)^\top \mathbb{J}_{2m} \right) \\ &\times \Big( p_{\alpha_1}(\xi_1) + \sum_{k_1<\alpha_1} a_{k_1} p_{k_1}(\xi_1) \Big) \cdots \Big( p_{\alpha_{\mathrm{d}}}(\xi_{\mathrm{d}}) + \sum_{k_{\mathrm{d}}<\alpha_{\mathrm{d}}} a_{k_{\mathrm{d}}} p_{k_{\mathrm{d}}}(\xi_{\mathrm{d}}) \Big) \\ &+ \sum_{\theta(\alpha)=\theta_{r+1},\alpha_1+\cdots+\alpha_{\mathrm{d}}\leqslant G-1} \left( \mathbb{J}_{2m} f'_\alpha(z) + f'_\alpha(z)^\top \mathbb{J}_{2m} \right) \\ &\times \Big( p_{\alpha_1}(\xi_1) + \sum_{k_1<\alpha_1} a_{k_1} p_{k_1}(\xi_1) \Big) \cdots \Big( p_{\alpha_{\mathrm{d}}}(\xi_{\mathrm{d}}) + \sum_{k_{\mathrm{d}}<\alpha_{\mathrm{d}}} a_{k_{\mathrm{d}}} p_{k_{\mathrm{d}}}(\xi_{\mathrm{d}}) \Big) \\ = &\sum_{\theta(\alpha)=\theta_{r+1},\alpha_1+\cdots+\alpha_{\mathrm{d}}=G} \left( \mathbb{J}_{2m} f'_\alpha(z) + f'_\alpha(z)^\top \mathbb{J}_{2m} \right) p_{\alpha_1}(\xi_1) \cdots p_{\alpha_{\mathrm{d}}}(\xi_{\mathrm{d}}) \\ &+ \sum_{\theta(\alpha)=\theta_{r+1},k_1+\cdots+k_{\mathrm{d}}\leqslant G-1} g_{k_1,\cdots,k_{\mathrm{d}}}(z) p_{k_1}(\xi_1) \cdots p_{k_{\mathrm{d}}}(\xi_{\mathrm{d}}), \quad a.s., \end{aligned}$$

where the last line in the above equality collects the polynomials with degree lower than $G$. For any $\alpha$ satisfying $\theta_{r+1}$ and $\alpha_1 + \cdots + \alpha_{\mathrm{d}} = G$, multiplying the above equation by $p_{\alpha_1}(\xi_1) \cdots p_{\alpha_{\mathrm{d}}}(\xi_{\mathrm{d}})$ and taking the expectation, we deduce from the independence of $\xi_1, \cdots, \xi_{\mathrm{d}}$ and the orthogonality of $\{p_k(x)\}_{k=1}^{\infty}$ that

$$\mathbb{J}_{2m} f'_\alpha(z) + f'_\alpha(z)^\top \mathbb{J}_{2m} = 0.$$

Plugging it into (3.12) and rewriting it as before, we have

$$\begin{aligned} 0 = & \sum_{\theta(\alpha)=\theta_{r+1}, \alpha_1+\cdots+\alpha_{\mathrm{d}}=G-1} \left(\mathbb{J}_{2m} f'_\alpha(z) + f'_\alpha(z)^\top \mathbb{J}_{2m}\right) p_{\alpha_1}(\xi_1)\cdots p_{\alpha_{\mathrm{d}}}(\xi_{\mathrm{d}}) \\ & + \sum_{\theta(\alpha)=\theta_{r+1}, k_1+\cdots+k_{\mathrm{d}}\leqslant G-2} \tilde{g}_{k_1,\cdots,k_{\mathrm{d}}}(z) p_{k_1}(\xi_1)\cdots p_{k_{\mathrm{d}}}(\xi_{\mathrm{d}}), \quad a.s. \end{aligned}$$

Similarly, we have for any $\alpha$ satisfying $\theta_{r+1}$ and $\alpha_1 + \cdots + \alpha_{\mathrm{d}} = G - 1$, $\mathbb{J}_{2m} f'_\alpha(z) + f'_\alpha(z)^\top \mathbb{J}_{2m} = 0$. Repeatedly using previous arguments, we have $\mathbb{J}_{2m} f'_\alpha(z) + f'_\alpha(z)^\top \mathbb{J}_{2m} = 0$ for any $\alpha$ satisfying $\theta_{r+1}$. Combining with the fact $\mathbb{J}_{2m}^\top = -\mathbb{J}_{2m}$, we obtain $\mathbb{J}_{2m} f'_\alpha(z) - (\mathbb{J}_{2m} f'_\alpha(z))^\top = 0$, i.e., $\mathbb{J}_{2m} f'_\alpha(z)$ is symmetric. Then the statement (3.11) follows from the integrability lemma (Hairer *et al.*, 2006, Lemma 2.7 in Chap. VI). □

Remark 3.12 Based on Assumption 2.1, we have $\|X_{t_n,t_{n+1}}\|_{L^2(\Omega)} \leqslant K h^{1/2\rho}$, $1 \leqslant \rho < 2$, which is an upper bound for the regularity of the noise. In the proof of Theorem 3.11, we use the assumption (3.10) to characterize the regularity of the noise more precisely, which is satisfied by a large class of Gaussian processes used in the rough path theory. For example, for the fractional Brownian motion, the constant $\varsigma = \frac{1}{2H}$ and $L(t) \equiv 1$ in (3.10). In particular, $\varsigma = 1$ and $L(t) \equiv 1$ when the noise is the standard Brownian motion.

Remark 3.13 For the weak convergent symplectic method which approximates $X^l_{t_n,t_{n+1}}$ by $\varsigma_{ln}\sqrt{h}$ with the random variable $\varsigma_{ln}$ defined through $\mathbb{P}(\varsigma_{ln} = \pm 1) = \frac{1}{2}$, such as the method studied in Anton (2019), one can construct the stochastic modified equation by regarding $X^l_{t_n,t_{n+1}}$ as $\varsigma_{ln}\sqrt{h}$. Further, since the formulation of the coefficients $\{f_\alpha\}$ of the stochastic modified equation does not rely on the simulation of the noise, the proof above also leads to $f_\alpha(y) = \mathbb{J}_{2m}^{-1}\nabla\mathscr{H}_\alpha(y)$.

Remark 3.14 Theorems 3.8–3.11 show that the numerical solution given by a rough symplectic method applied to a rough Hamiltonian system exactly solves another rough Hamiltonian system. For non-symplectic methods, the associated modified equations are not Hamiltonian systems in general. This explains the superiority of rough symplectic methods over long time computation to non-symplectic ones in numerical simulations presented in Section 5.

## 4. Convergence analysis

In this section, we consider the $\tilde{N}$-truncated modified equation ($\tilde{N} \geqslant 1$)

$$\begin{cases} \mathrm{d}\tilde{y}^{\tilde{N}}_t = \displaystyle\sum_{l=0}^{\mathrm{d}} \sum_{i(\alpha)=l}^{1\leqslant|\alpha|\leqslant\tilde{N}} f_\alpha(\tilde{y}^{\tilde{N}}_t) h^{\alpha_0} (X^1_{t_n,t_{n+1}})^{\alpha_1} \cdots (X^l_{t_n,t_{n+1}})^{\alpha_l - 1} \cdots (X^{\mathrm{d}}_{t_n,t_{n+1}})^{\alpha_{\mathrm{d}}} \, \mathrm{d}x^{h,l}_t, \quad t \in (t_n, t_{n+1}]; \\ \tilde{y}^{\tilde{N}}_0 = z, \end{cases} \tag{4.1}$$

where $f_\alpha$ is given by (3.7), $|\alpha| = 1, \cdots, \tilde{N}$. We remark that Theorem 3.11 also implies the symplecticity of the $\tilde{N}$-truncated modified equation associated with a symplectic method applied to a rough Hamiltonian system. Therefore, taking $\tilde{N}$ as an index, we obtain a family of stochastic modified equations with Hamiltonian formulations.

In subsection 4.1, we give the convergence analysis on the error between $Y_n^h$ and $\tilde{y}_{t_n}^{\tilde{N}}$ for the case that $X$ is a general Gaussian rough path satisfying Assumption 2.1, which answers Problem 1.2. Here the rough path theory is essential since

$$\sup_h \|x^h\|_{1\text{-}var;[0,T]} = \infty, \quad \sup_h \|S_{[p]}(x^h)\|_{p\text{-}var;[0,T]} < \infty, \quad p > 2\rho.$$

As for Problem 1.3, we focus on the case that $X$ is the standard Brownian motion and the increments are simulated by bounded Gaussian random variables. We optimize $\tilde{N}$ such that the error is exponentially small with respect to $h$, in subsection 4.2.

REMARK 4.1 For the forward error analysis, that is, the estimate for the difference between the numerical solution $Y_n^h$ and the exact solution $Y_{t_n}$ of the original stochastic equation (2.1), we refer to Hong *et al.* (2018), Bayer *et al.* (2016) and Friz & Riedel (2014), and the references therein.

### 4.1 *The general rough case*

THEOREM 4.2 Under Assumption 2.1, if $V$ is bounded with bounded derivatives up order $\tilde{N}$, then for any $p > 2\rho$, there exists a random variable $C(\omega) = C(\omega, p, \|V\|_{Lip^{\tilde{N}}}, \tilde{N})$ such that

$$\|\tilde{y}_{t_1}^{\tilde{N}} - Y_1^h\| \leqslant C(\omega) h^{\frac{\tilde{N}+1}{p}}, \quad a.s.,$$

where $\tilde{y}^{\tilde{N}}$ is the solution of (4.1) and $Y_1^h$ is defined by a numerical method satisfying (3.1).

*Proof.* Consider the expansion

$$\tilde{y}_h^{\tilde{N}} = z + \sum_{|\alpha|=1}^{\infty} f_\alpha^{\tilde{N}}(z) h^{\alpha_0} (X_{t_0,t_1}^1)^{\alpha_1} \cdots (X_{t_0,t_1}^{\mathrm{d}})^{\alpha_{\mathrm{d}}}.$$

Fix $p > 2\rho \geqslant 2$. Since the recursion (3.7) implies $f_\alpha^{\tilde{N}} = \tilde{f}_\alpha = d_\alpha$ with $1 \leqslant |\alpha| \leqslant \tilde{N}$, and Assumption 2.1 produces $\|X\|_{\frac{1}{p}\text{-Höl};[t_0,t_1]} < \infty$, we deduce from the Taylor expansion that the leading term of the error between $\tilde{y}_{t_1}^{\tilde{N}}$ and $Y_1^h$ is involved with $h^{\alpha_0}(X_{t_0,t_1}^1)^{\alpha_1} \cdots (X_{t_0,t_1}^{\mathrm{d}})^{\alpha_{\mathrm{d}}}$, where $\alpha_0 = 0$ and $\alpha_1 \cdots + \alpha_{\mathrm{d}} = \tilde{N} + 1$. Hence,

$$\|\tilde{y}_{t_1}^{\tilde{N}} - Y_1^h\| \leqslant C(\omega, p, \|V\|_{Lip^{\tilde{N}}}, \tilde{N}) h^{\frac{\tilde{N}+1}{p}}.$$

□

Theorem 4.3 Under Assumption 2.1, if $V \in Lip^{\tilde{N}-1+\gamma}$ with $\gamma > 2\rho$ and $\tilde{N} > 2\rho - 1$, then for any $p \in (2\rho, \gamma)$, there exists a random variable $C(\omega) = C(\omega, p, \gamma, \|V\|_{Lip^{\tilde{N}-1+\gamma}}, \tilde{N}, T)$ such that

$$\sup_{1\leqslant n\leqslant N} \|\tilde{y}_{t_n}^{\tilde{N}} - Y_n^h\| \leqslant C(\omega) h^{\frac{\tilde{N}+1}{p}-1}, \quad a.s.,$$

where $\tilde{y}^{\tilde{N}}$ is the solution of (4.1) and $Y_n^h$ is defined by a numerical method satisfying (3.1).

*Proof.* Denoting by $\pi(t_0, y_0, x^h)_t$ the flow of (4.1), which initiates from $y_0$ at time $t_0$, we have

$$\begin{aligned}\|Y_k^h - \tilde{y}_{t_k}^{\tilde{N}}\| &= \|\pi(t_k, Y_k^h, x^h)_{t_k} - \pi(t_0, Y_0^h, x^h)_{t_k}\| \\ &\leqslant \sum_{s=1}^{k} \|\pi(t_s, Y_s^h, x^h)_{t_k} - \pi(t_{s-1}, Y_{s-1}^h, x^h)_{t_k}\|, \quad 1 \leqslant k \leqslant N.\end{aligned}$$

Due to the Lipschitz continuity of the Itô–Lyons map (Friz & Victoir, 2010, Theorem 10.26), we get

$$\begin{aligned}&\|\pi(t_s, Y_s^h, x^h)_{t_k} - \pi(t_{s-1}, Y_{s-1}^h, x^h)_{t_k}\| \\ &\quad = \|\pi(t_{k-1}, \pi(t_s, Y_s^h, x^h)_{t_{k-1}}, x^h)_{t_k} - \pi(t_{k-1}, \pi(t_{s-1}, Y_{s-1}^h, x^h)_{t_{k-1}}, x^h)_{t_k}\| \\ &\quad \leqslant C \exp\{C\bar{\nu}^p \|S_{[p]}(x^h)(\omega)\|_{p\text{-}var;[t_{k-1},t_k]}^p\} \|\pi(t_s, Y_s^h, x^h)_{t_{k-1}} - \pi(t_{s-1}, Y_{s-1}^h, x^h)_{t_{k-1}}\|,\end{aligned}$$

where $C := C(p, \gamma)$ and $\bar{\nu} := \bar{\nu}(\|X\|_{\frac{1}{p}\text{-Höl};[0,T]}(\omega), \|V\|_{Lip^{\tilde{N}-1+\gamma}}, \tilde{N})$. From

$$\|S_{[p]}(x^h)(\omega)\|_{p\text{-}var;[u_1,u_2]}^p + \|S_{[p]}(x^h)(\omega)\|_{p\text{-}var;[u_2,u_3]}^p \leqslant \|S_{[p]}(x^h)(\omega)\|_{p\text{-}var;[u_1,u_3]}^p,$$

it yields that

$$\begin{aligned}&\|\pi(t_s, Y_s^h, x^h)_{t_k} - \pi(t_{s-1}, Y_{s-1}^h, x^h)_{t_k}\| \\ &\quad \leqslant C \exp\{C\bar{\nu}^p \|S_{[p]}(x^h)(\omega)\|_{p\text{-}var;[t_s,t_k]}^p\} \|\pi(t_s, Y_s^h, x^h)_{t_s} - \pi(t_{s-1}, Y_{s-1}^h, x^h)_{t_s}\| \\ &\quad \leqslant C \exp\{C\bar{\nu}^p \|S_{[p]}(x^h)(\omega)\|_{p\text{-}var;[0,T]}^p\} \|Y_s^h - \pi(t_{s-1}, Y_{s-1}^h, x^h)_{t_s}\|, \quad 1 \leqslant s \leqslant k.\end{aligned}$$

It follows from Theorem 15.33 in Friz & Victoir (2010) that

$$\lim_{h\to 0} \|S_{[p]}(x^h)(\omega)\|_{p\text{-}var;[0,T]} = \|\mathbf{X}(\omega)\|_{p\text{-}var;[0,T]}, \quad a.s.,$$

which yields

$$\sup_{h>0} \|S_{[p]}(x^h)(\omega)\|^p_{p\text{-}var;[0,T]} < \infty, \quad a.s.$$

According to Assumption 2.1 and Definition 2.3, $V \in Lip^{\tilde{N}-1+\gamma}$ with $\gamma > 2\rho > 1$ leads to that $V$ is bounded with bounded derivatives up order $\tilde{N}$. Then we derive by Theorem 4.2 that

$$\begin{aligned}\|Y^h_k - \tilde{y}^{\tilde{N}}_{t_k}\| &\leqslant \sum_{s=1}^{k} C\exp\{C\bar{\nu}^p \|S_{[p]}(x^h)(\omega)\|^p_{p\text{-}var;[0,T]}\}\|Y^h_s - \pi(t_{s-1}, Y^h_{s-1}, x^h)_{t_s}\| \\ &\leqslant C(\omega, p, \gamma, \|V\|_{Lip^{\tilde{N}-1+\gamma}}, \tilde{N}, T)h^{\frac{\tilde{N}+1}{p}-1}\end{aligned}$$

due to $\gamma > 2\rho \geqslant 2$. □

In the case of additive noises, the terms satisfying $|\alpha| \geqslant 2$ and $\alpha_0 = 0$ will include the derivatives of the diffusion coefficients, which are zero. Then (3.1) in Assumption 3.1 on the numerical method degenerates to

$$\begin{aligned}Y^h_{n+1} = Y^h_n &+ \sum_{|\alpha|=1} \mathrm{d}_\alpha(Y^h_n)h^{\alpha_0}(X^1_{t_n,t_{n+1}})^{\alpha_1}\cdots(X^{\mathrm{d}}_{t_n,t_{n+1}})^{\alpha_{\mathrm{d}}} \\ &+ \sum_{|\alpha|\geqslant 2, \alpha_0 \geqslant 1}^{\infty} \mathrm{d}_\alpha(Y^h_n)h^{\alpha_0}(X^1_{t_n,t_{n+1}})^{\alpha_1}\cdots(X^{\mathrm{d}}_{t_n,t_{n+1}})^{\alpha_{\mathrm{d}}}. \end{aligned} \tag{4.2}$$

Consequently, the convergence rate of the error between $Y^h_n$ and $\tilde{y}^{\tilde{N}}_{t_n}$ increases, which is stated in the following theorem.

THEOREM 4.4 Let Assumption 2.1 hold and $V_i(y) \equiv \sigma_i \in \mathbb{R}^m$, $i = 1, \cdots, \mathrm{d}$. If $V_0 \in Lip^{\tilde{N}-1+\gamma}$ with $\gamma > 2\rho$, then for any $p \in (2\rho, \gamma)$, there exists a random variable $C(\omega) = C(\omega, p, \|V\|_{Lip^{\tilde{N}}}, \tilde{N})$ such that

$$\sup_{1\leqslant n\leqslant N} \|\tilde{y}^{\tilde{N}}_{t_n} - Y^h_n\| \leqslant C(\omega)h^{\frac{\tilde{N}}{p}}, \quad a.s.,$$

where $\tilde{y}^{\tilde{N}}$ is the solution of (4.1) and $Y^h_n$ is defined by a numerical method satisfying (4.2).

*Proof.* Combining (4.2) with (3.7), we have that the leading term of the local error between $\tilde{y}^{\tilde{N}}_{t_1}$ and $Y^h_1$ is involved with $h^{\alpha_0}(X^1_{t_0,t_1})^{\alpha_1}\cdots(X^{\mathrm{d}}_{t_0,t_1})^{\alpha_{\mathrm{d}}}$, where $\alpha_0 = 1$ and $\alpha_1 \cdots + \alpha_{\mathrm{d}} = \tilde{N}$. Then

$$\|\tilde{y}^{\tilde{N}}_{t_1} - Y^h_1\| \leqslant C(\omega)h^{\frac{\tilde{N}}{p}+1}, \quad a.s.,$$

from which we conclude the result by using the same arguments as in the proof of Theorem 4.3. □

### 4.2 *The standard Brownian case*

In the previous subsection, we prove that the error between the numerical solution and the exact solution of the truncated modified equation is bounded by a polynomial function with respect to the time step size $h$ by fixing the truncation number $\tilde{N}$. To further study the convergence analysis, we show in this subsection that by fixing the time step size $h$, there exists a truncation number $\tilde{N}$ such that the error can be made exponentially small. In this sense, we call it the best truncation number. We deal with the case that $X^l$, $l = 1, \cdots, \mathrm{d}$ are independent standard Brownian motions. In this case, we simulate the increments $X^l_{t_n,t_{n+1}}$ by

$$\Delta_{n+1,l} := \zeta_{n+1,l}\sqrt{h} \tag{4.3}$$

with

$$\zeta_{n+1,l} := \begin{cases} \xi_{n+1,l}, & |\xi_{n+1,l}| \leqslant A_h, \\ A_h, & \xi_{n+1,l} > A_h, \\ -A_h, & \xi_{n+1,l} < -A_h. \end{cases}$$

Here $\xi_{n+1,l}$, $n = 0, 1, \cdots, N-1$, $l = 1, \cdots, \mathrm{d}$, are independent Gaussian normal random variables, and $A_h = \sqrt{4|\ln h|}$. Similar to Assumption 3.1, we assume that the expansion of the numerical solution is

$$Y^h_{n+1} = Y^h_n + \sum_{|\alpha|=1}^{\infty} d_\alpha(Y^h_n) h^{\alpha_0} \Delta^{\alpha_1}_{n+1,1} \cdots \Delta^{\alpha_{\mathrm{d}}}_{n+1,\mathrm{d}}.$$

For convenience, we illustrate our idea by the RK method

$$\begin{cases} Y^h_{n+1,i} = Y^h_n + \sum_{j=1}^{s} a_{ij}\left(V_0(Y^h_{n+1,j})h + \sum_{l=1}^{\mathrm{d}} V_l(Y^h_{n+1,j})\Delta_{n+1,l}\right), \\ Y^h_{n+1} = Y^h_n + \sum_{i=1}^{s} b_i\left(V_0(Y^h_{n+1,i})h + \sum_{l=1}^{\mathrm{d}} V_l(Y^h_{n+1,i})\Delta_{n+1,l}\right). \end{cases} \tag{4.4}$$

We also stress that the procedure does not rely on the special structure of RK methods and is available for a large class of numerical methods.

To fit this case into the previous analysis, it suffices to prove that the process $\bar{x}^h = (\bar{x}^{h,1}, \cdots, \bar{x}^{h,\mathrm{d}})$ defined by

$$\bar{x}^{h,l}_t := \bar{x}^{h,l}_{t_n} + \frac{t - t_n}{h}\Delta_{n+1,l} \quad \forall\, t \in (t_n, t_{n+1}],\ \ l = 1, \cdots, \mathrm{d},\ \ n = 0, \cdots, N-1,$$

can be lifted to a $p$-rough path with $[p] = 2$ almost surely, as a counterpart of the process (3.4).

PROPOSITION 4.5 Let $2 < p < 3$. Then it holds that there exists some random variable $C(\omega) := C(\omega, p, T)$ independent of $h$ such that

$$\left\| S_2(\bar{x}^h(\omega)) \right\|_{p\text{-}var;[0,T]} \leqslant C(\omega), \quad a.s.$$

*Proof.* Let $t_{i-1} < s < t_i < t_j < t < t_{j+1}$. Since for any $m \in \mathbb{N}_+$, $\mathbb{E}\left[\Delta^{2m}_{1,1}\right] \leqslant (2m-1)!!\,h^m$ and $\mathbb{E}\left[\Delta^{2m-1}_{1,1}\right] = 0$, we have

$$\mathbb{E}\left[\left|\int_s^{t_i} \mathrm{d}\bar{x}^{h,l}_{u_1}\right|^{2m}\right] = \mathbb{E}\left[\left(\frac{t_i - s}{h}\Delta_{i,l}\right)^{2m}\right] \leqslant \left(\frac{t_i - s}{h}\right)^{2m} \mathbb{E}\left[\Delta^{2m}_{1,1}\right] \leqslant C|t_i - s|^m,$$

$$\mathbb{E}\left[\left|\int_{t_j}^{t} \mathrm{d}\bar{x}^{h,l}_{u_1}\right|^{2m}\right] = \mathbb{E}\left[\left(\frac{t - t_j}{h}\Delta_{j+1,l}\right)^{2m}\right] \leqslant \left(\frac{t - t_j}{h}\right)^{2m} \mathbb{E}\left[\Delta^{2m}_{1,1}\right] \leqslant C|t - t_j|^m,$$

and

$$
\begin{aligned}
\mathbb{E}\left[\left|\int_{t_i}^{t_j} \mathrm{d}\bar{x}_{u_1}^{h,l}\right|^{2m}\right] &= \mathbb{E}\left[\left(\sum_{k=i+1}^{j} \Delta_{k,l}\right)^{2m}\right] \\
&= \sum_{\beta_{i+1}+\cdots+\beta_j=2m,\ \beta_{i+1},\cdots,\beta_j \text{ are even}} C_{2m}^{\beta_{i+1}} C_{2m-\beta_{i+1}}^{\beta_{i+2}} \cdots C_{2m-\beta_{i+1}-\cdots-\beta_{j-1}}^{\beta_j} \mathbb{E}\Big[\Delta_{i+1,l}^{\beta_{i+1}} \cdots \Delta_{j,l}^{\beta_j}\Big] \\
&\leqslant \sum_{\beta_{i+1}+\cdots+\beta_j=2m,\ \beta_{i+1},\cdots,\beta_j \text{ are even}} (2m)!\, \mathbb{E}\left[\Delta_{i+1,l}^{\beta_{i+1}}\right] \cdots \mathbb{E}\left[\Delta_{j,l}^{\beta_j}\right] \\
&\leqslant \#\Big\{(\beta_{i+1},\cdots,\beta_j):\ \beta_{i+1}+\cdots+\beta_j = 2m,\ \beta_{i+1},\cdots,\beta_j \text{ are even}\Big\}(2m)!\,(2m-1)!!\,h^m \\
&\leqslant (j-i)^m (2m)!\,(2m-1)!!\,h^m \leqslant C|t_j - t_i|^m.
\end{aligned}
$$

Here, $C_n^m$ denotes the combinatorial number and $\#\mathscr{O}$ gives the number of elements in the set $\mathscr{O}$. Combining the above estimates, we obtain

$$
\mathbb{E}\left[\left|\int_{s}^{t} \mathrm{d}\bar{x}_{u_1}^{h,l}\right|^{2m}\right] \leqslant C\left\{\mathbb{E}\left[\left|\int_{s}^{t_i} \mathrm{d}\bar{x}_{u_1}^{h,l}\right|^{2m}\right] + \mathbb{E}\left[\left|\int_{t_i}^{t_j} \mathrm{d}\bar{x}_{u_1}^{h,l}\right|^{2m}\right] + \mathbb{E}\left[\left|\int_{t_j}^{t} \mathrm{d}\bar{x}_{u_1}^{h,l}\right|^{2m}\right]\right\} \leqslant C|t-s|^m.
$$

For an iterated integral, let $t_{i-1} < s < t_i < t_j < t < t_{j+1}$ and $l_1, l_2 \in \{1,\cdots,\mathrm{d}\}$. If $l_1 \neq l_2$, then the definition of $\bar{x}$ and the independence of $\Delta_{k_1,l_1}$ and $\Delta_{k_2,l_2}$ lead to

$$
\begin{aligned}
&\mathbb{E}\left[\left|\int_{t_i}^{t_j}\int_{t_i}^{u_1} \mathrm{d}\bar{x}_{u_2}^{h,l_1}\mathrm{d}\bar{x}_{u_1}^{h,l_2}\right|^{2m}\right] \\
&= \mathbb{E}\left[\left|\sum_{k=i+1}^{j}\sum_{l=i+1}^{k-1} \Delta_{k,l_1}\Delta_{l,l_2} + \sum_{k=i+1}^{j} \frac{1}{2}\Delta_{k,l_1}\Delta_{k,l_2}\right|^{2m}\right] \\
&\leqslant \sum_{\beta_{i+1}+\cdots+\beta_j=2m,\ \beta_{i+1},\cdots,\beta_j \text{ are even}} C_{2m}^{\beta_{i+1}} C_{2m-\beta_{i+1}}^{\beta_{i+2}} \cdots C_{2m-\beta_{i+1}-\cdots-\beta_{j-1}}^{\beta_j} \mathbb{E}\Big[\Delta_{i+1,l_1}^{\beta_{i+1}} \cdots \Delta_{j,l_1}^{\beta_j}\Big] \\
&\quad\times \sum_{\gamma_{i+1}+\cdots+\gamma_j=2m,\ \gamma_{i+1},\cdots,\gamma_j \text{ are even}} C_{2m}^{\gamma_{i+1}} C_{2m-\gamma_{i+1}}^{\gamma_{i+2}} \cdots C_{2m-\gamma_{i+1}-\cdots-\gamma_{j-1}}^{\gamma_j} \mathbb{E}\Big[\Delta_{i+1,l_2}^{\gamma_{i+1}} \cdots \Delta_{j,l_2}^{\gamma_j}\Big] \\
&\leqslant \Big((j-i)^m (2m)!\,(2m-1)!!\,h^m\Big)^2 \leqslant C|t_j - t_i|^{2m}.
\end{aligned}
$$

If $l_1 = l_2$, then

$$
\begin{aligned}
&\mathbb{E}\left[\left|\int_{t_i}^{t_j}\int_{t_i}^{u_1} \mathrm{d}\bar{x}_{u_2}^{h,l_1}\,\mathrm{d}\bar{x}_{u_1}^{h,l_2}\right|^{2m}\right] \\
&= \mathbb{E}\left[\left|\sum_{k=i+1}^{j}\sum_{l=i+1}^{k-1} \Delta_{k,l_1}\Delta_{l,l_1} + \sum_{k=i+1}^{j}\frac{1}{2}\Delta_{k,l_1}^2\right|^{2m}\right] \\
&\leqslant \sum_{\beta_{i+1}+\cdots+\beta_j=4m,\ \beta_{i+1},\cdots,\beta_j \text{ are even}} C_{4m}^{\beta_{i+1}} C_{4m-\beta_{i+1}}^{\beta_{i+2}} \cdots C_{4m-\beta_{i+1}-\cdots-\beta_{j-1}}^{\beta_j}\,\mathbb{E}\Big[\Delta_{i+1,l_1}^{\beta_{i+1}} \cdots \Delta_{j,l_1}^{\beta_j}\Big] \\
&\leqslant \#\Big\{(\beta_{i+1},\cdots,\beta_j):\ \beta_{i+1}+\cdots+\beta_j = 4m,\ \beta_{i+1 i+1},\cdots,\beta_j \text{ are even}\Big\}(4m)!\,\mathbb{E}\Big[\Delta_{i+1,l_1}^{\beta_{i+1}}\Big]\cdots\mathbb{E}\Big[\Delta_{j,l_1}^{\beta_j}\Big] \\
&\leqslant (j-i)^{2m}(4m)!\,(4m-1)!!\,h^{2m} \leqslant C|t_j - t_i|^{2m}.
\end{aligned}
$$

Besides,

$$
\begin{aligned}
\mathbb{E}\left[\left|\int_{t_i}^{t_j}\int_{s}^{t_i} \mathrm{d}\bar{x}_{u_2}^{h,l_1}\,\mathrm{d}\bar{x}_{u_1}^{h,l_2}\right|^{2m}\right] &\leqslant \left(\frac{t_i - s}{h}\right)^{2m}\mathbb{E}\left[\Delta_{1,1}^{2m}\right]\mathbb{E}\left[\left|\int_{t_i}^{t_j}\mathrm{d}\bar{x}_{u_1}^{h,l}\right|^{2m}\right] \leqslant C|t_i - s|^m |t_j - t_i|^m, \\
\mathbb{E}\left[\left|\int_{s}^{t_i}\int_{s}^{u_1} \mathrm{d}\bar{x}_{u_2}^{h,l_1}\,\mathrm{d}\bar{x}_{u_1}^{h,l_2}\right|^{2m}\right] &\leqslant \left(\frac{t_i - s}{h}\right)^{4m}\left(\mathbb{E}\left[\Delta_{1,1}^{2m}\right]\right)^2 \leqslant C|t_i - s|^{2m}.
\end{aligned}
$$

Similarly, it holds that

$$
\mathbb{E}\left[\left|\int_{t_j}^{t}\int_{s}^{u_1} \mathrm{d}\bar{x}_{u_2}^{h,l_1}\,\mathrm{d}\bar{x}_{u_1}^{h,l_2}\right|^{2m}\right] \leqslant C|t - t_j|^m |t_j - s|^m + C|t - t_j|^{2m}.
$$

Therefore, we obtain

$$
\mathbb{E}\left[\left|\int_{s}^{t}\int_{s}^{u_1} \mathrm{d}\bar{x}_{u_2}^{h,l_1}\,\mathrm{d}\bar{x}_{u_1}^{h,l_2}\right|^{2m}\right] \leqslant C|t - s|^{2m}.
$$

For any $p$ such that $2 < p < 3$, i.e., $\frac{1}{3} < \frac{1}{p} < \frac{1}{2}$, choose $q = 4m$ sufficiently large with $m \in \mathbb{N}_+$ such that $\left(\frac{1}{2} - \frac{1}{q}\right) - \frac{1}{q} > \frac{1}{p}$. By the Besov–Hölder embedding theorem (Friz & Victoir, 2010, Corollary A.2), we get

$$
\left\|S_2(\bar{x}^h)\right\|^q_{\left(\left(\frac{1}{2}-\frac{1}{q}\right)-\frac{1}{q}\right)\text{-Höl};[0,T]} \leqslant C(q)\int_0^T\int_0^T \frac{\left|\mathrm{d}(S_2(\bar{x}^h)_s, S_2(\bar{x}^h)_t)\right|^q}{|t - s|^{1+q\left(\frac{1}{2}-\frac{1}{q}\right)}}\,\mathrm{d}s\,\mathrm{d}t,
$$

where

$$d(S_2(\bar{x}^h)_s, S_2(\bar{x}^h)_t) \leqslant C \max\left\{\left|\int_s^t d\bar{x}_{u_1}^{h,l}\right|, \left|\int_s^t \int_s^{u_1} d\bar{x}_{u_2}^{h,l_1} d\bar{x}_{u_1}^{h,l_2}\right|^{\frac{1}{2}}\right\}$$
$$\leqslant C\left(\left|\int_s^t d\bar{x}_{u_1}^{h,l}\right| + \left|\int_s^t \int_s^{u_1} d\bar{x}_{u_2}^{h,l_1} d\bar{x}_{u_1}^{h,l_2}\right|^{\frac{1}{2}}\right).$$

Taking the expectation on both sides, we obtain

$$\mathbb{E}\left[\left\|S_2(\bar{x}^h)\right\|^q_{(\frac{1}{2}-\frac{1}{q}-\frac{1}{q})\text{-Höl};[0,T]}\right] \leqslant C(q)\int_0^T\int_0^T \frac{\mathbb{E}\left[\left|d(S_2(\bar{x}^h)_s, S_2(\bar{x}^h)_t)\right|^q\right]}{|t-s|^{\frac{q}{2}}} ds\, dt$$
$$\leqslant C(q)\int_0^T\int_0^T \frac{\mathbb{E}\left[\left|\int_s^t d\bar{x}_{u_1}^{h,l}\right|^q + \left|\int_s^t\int_s^{u_1} d\bar{x}_{u_2}^{h,l_1} d\bar{x}_{u_1}^{h,l_2}\right|^{\frac{q}{2}}\right]}{|t-s|^{\frac{q}{2}}} ds\, dt$$
$$\leqslant C(q)T^2.$$

This yields that $\bar{x}^h$ can be lifted to a $p$-rough path almost surely, and that there exists some random variable $C(\omega)$ independent of $h$ such that

$$\left\|S_2(\bar{x}^h(\omega))\right\|_{p\text{-}var;[0,T]} \leqslant C\left\|S_2(\bar{x}^h)(\omega)\right\|_{\frac{1}{p}\text{-Höl};[0,T]} \leqslant C(\omega,p,T), \quad a.s.$$

With the help of Proposition 4.5, the associated modified equation here is

$$\begin{cases} d\tilde{y}_t = \sum_{l=0}^{\mathrm{d}} \sum_{i(\alpha)=l} f_\alpha(\tilde{y}_t) h^{\alpha_0} \Delta_{n+1,1}^{\alpha_1} \cdots \Delta_{n+1,l}^{\alpha_l-1} \cdots \Delta_{n+1,\mathrm{d}}^{\alpha_{\mathrm{d}}} d\bar{x}_t^{h,l}, \quad t \in (t_n, t_{n+1}]; \\ \tilde{y}_0 = z, \end{cases} \tag{4.5}$$

and the $\tilde{N}$-truncated modified equation is

$$\begin{cases} d\tilde{y}_t^{\tilde{N}} = \sum_{l=0}^{\mathrm{d}} \sum_{i(\alpha)=l}^{1\leqslant|\alpha|\leqslant\tilde{N}} f_\alpha(\tilde{y}_t^{\tilde{N}}) h^{\alpha_0} \Delta_{n+1,1}^{\alpha_1} \cdots \Delta_{n+1,l}^{\alpha_l-1} \cdots \Delta_{n+1,\mathrm{d}}^{\alpha_{\mathrm{d}}} d\bar{x}_t^{h,l}, \quad t \in (t_n, t_{n+1}]; \\ \tilde{y}_0^{\tilde{N}} = z. \end{cases} \tag{4.6}$$

We obtain that there exists some truncated number $\tilde{N} = \tilde{N}(h)$ such that the local error is exponentially small with respect to the time step size $h$, which answers Problem 1.3. Included in the appendix, the proof combines estimates for coefficients of the truncated increments, the numerical solution, the modified equation and the truncated modified equation such that the temporal regularity of increments of the Brownian motion is unfolded in the result (4.7). □

Theorem 4.6 Assume that there exist positive constants $R, M$ such that $V_l$, $l = 0, 1, \cdots, \mathrm{d}$ are analytic on a neighbourhood of the closed ball

$$B_{2R}(z) := \left\{ y \in \mathbb{C}^m : \|y - z\| \leqslant 2R \right\}$$

with

$$\|V_l(y)\| \leqslant M \quad \forall\, y \in B_{2R}(z).$$

Then for any $\epsilon \in (0, \frac{1}{2})$, there exist constants $C = C(\epsilon, R, M)$, $\tau = \tau(\epsilon, R, M)$ and $h_0 = h_0(R, M)$ such that for any $h \in (0, \tau)$, there exists a truncation number $\tilde{N} = \tilde{N}(\epsilon, R, M, h)$ satisfying

$$\|\tilde{y}^{\tilde{N}}_{t_1} - Y^h_1\| \leqslant C h e^{-h_0/h^{\frac{1}{2}-\epsilon}}, \tag{4.7}$$

where $\tilde{y}^{\tilde{N}}_{t_1}$ is the solution of (4.6) and $Y^h_1$ is defined by the one-step numerical method (4.4).

Remark 4.7 We remark that in the backward error analysis of the deterministic Hamiltonian system, the result that the error between the numerical solution and the exact solution of the corresponding modified equation is exponentially small leads to the near conservation of the energy of the original Hamiltonian system with symplectic methods over an exponentially long time interval. The key lies in the conservation of the energy (resp. modified energy) of the original Hamiltonian system (resp. the modified equation); see Hairer *et al.* (2006). However, in the stochastic case, the stochastic Hamiltonian system does not have the energy conservation law in general, not to mention the stochastic modified equation. Even for a special case (e.g., $V_l = C_l V_0$ with $C_l$ a constant, $l = 1, \cdots, \mathrm{d}$ in (2.1)) where the stochastic system has the energy conservation law, the modified equation associated to a symplectic method does not have the energy conservation law in general. Therefore, the long-term conservation of the energy by the stochastic symplectic methods is still an open problem.

## 5. Numerical experiments

Numerical experiments are carried out based on three rough Hamiltonian systems in this section. Based on Examples 5.1–5.2, we verify the convergence orders proved in Theorems 4.3–4.4 for multiplicative and additive cases, accordingly. In Example 5.3, which is a linear system with the energy conservation law, we present the long time behavior of several numerical methods and the corresponding modified equations.

Example 5.1

$$\begin{cases} \mathrm{d}P_t = \sin(P_t)\sin(Q_t)\,\mathrm{d}t - \cos(Q_t)\,\mathrm{d}X^2_t, & P_0 = p, \\ \mathrm{d}Q_t = \cos(P_t)\cos(Q_t)\,\mathrm{d}t - \sin(P_t)\,\mathrm{d}X^1_t, & Q_0 = q, \end{cases}$$

where $X^1$ and $X^2$ are independent fractional Brownian motions with Hurst parameter $H \in (1/4, 1/2]$. The Hamiltonians are

$$\mathscr{H}_0(P_t, Q_t) = \sin(P_t)\cos(Q_t), \quad \mathscr{H}_1(P_t, Q_t) = \cos(P_t), \quad \mathscr{H}_2(P_t, Q_t) = \sin(Q_t).$$

EXAMPLE 5.2 (flow driven by the Taylor–Green velocity field (Wang *et al.*, 2018, Corollary 4.3))

$$\begin{cases} \mathrm{d}P_t = -\sin(Q_t)\,\mathrm{d}t + \sqrt{2}\sigma\,\mathrm{d}X_t^1, & P_0 = p, \\ \mathrm{d}Q_t = \sin(P_t)\,\mathrm{d}t + \sqrt{2}\sigma\,\mathrm{d}X_t^2, & Q_0 = q, \end{cases}$$

where $X^1$ and $X^2$ are independent fractional Brownian motions with Hurst parameter $H \in (1/4, 1/2]$. The Hamiltonians are

$$\mathscr{H}_0(P_t, Q_t) = -\cos(P_t) - \cos(Q_t), \quad \mathscr{H}_1(P_t, Q_t) = -\sqrt{2}\sigma Q_t, \quad \mathscr{H}_2(P_t, Q_t) = \sqrt{2}\sigma P_t.$$

We consider the midpoint scheme

$$Y_{n+1}^h = Y_n^h + V\left(\frac{Y_n^h + Y_{n+1}^h}{2}\right) X_{t_n, t_{n+1}}, \tag{5.1}$$

whose 2-truncated and 4-truncated modified equations are defined via the following formulas for the coefficients:

$$\begin{aligned} |\alpha| = 1: &\quad f_\alpha(y) = V_\alpha(y); \\ |\alpha| = 2: &\quad f_\alpha(y) = 0; \\ |\alpha| = 3: &\quad f_\alpha(y) = \sum_{\alpha_1+\alpha_2+\alpha_3=\alpha} \left[ -\frac{1}{24} V''_{\alpha_3}(y) V_{\alpha_2}(y) V_{\alpha_1}(y) + \frac{1}{12} V'_{\alpha_3}(y) V'_{\alpha_2}(y) V_{\alpha_1}(y) \right]; \\ |\alpha| = 4: &\quad f_\alpha(y) = 0. \end{aligned}$$

To investigate the error between the numerical solution and the exact solution of the associated $\tilde{N}$-truncated modified equation, we apply the midpoint scheme to Example 5.1 with the initial datum $(p, q) = (1, 0)$ and the time interval $[0, T] = [0, 1]$. Figure 1 plots the mean-square error $\|Y_N^h - \tilde{y}_T^{\tilde{N}}\|_{L^2(\Omega)}$, where $\tilde{N} = 2, 4$, the time step sizes are $h = 2^{-i}$, $i = 4, 5, 6, 7, 8$, and the Hurst parameters are $H = 0.4, 0.45, 0.5$. For each time step size $h$, the 'exact' solution of a truncated modified equation is simulated by using the midpoint scheme to this modified equation with a tiny step size $\delta = 2^{-12}$. The increments of the fractional Brownian motions are simulated by the method introduced in Wood & Chan (1994), which exploits the efficiency of the fast Fourier transform. The expectation is approximated by 200 sample trajectories. The convergence orders are showed to be $3H-1$ and $5H-1$ for the cases $\tilde{N} = 2$ and $\tilde{N} = 4$, respectively. According to Proposition 15.5 in Friz & Victoir (2010), the fractional Brownian motion satisfies Assumption 2.1 with $\rho = \frac{1}{2H}$. For a sufficiently small $\epsilon > 0$, we take $p = \frac{1}{H} + \epsilon > 2\rho$ and $\gamma = \frac{1}{H} + 2\epsilon > p$ in Theorem 4.3 and then the theoretical estimate for the multiplicative case is supported by the numerical result. In Example 5.2, we take $p = 1$, $q = 0$, $\sigma = 2$ and $T = 1$, and choose $H = 0.3, 0.4, 0.5$. Figure 2 presents that the convergence orders for the cases $\tilde{N} = 2$ and $\tilde{N} = 4$ are $2H$ and $4H$, respectively. With $p = \frac{1}{H} + \epsilon$ and $\gamma = \frac{1}{H} + 2\epsilon$, the estimate for the additive case in Theorem 4.4 is verified. Furthermore, one can find out that the numerical solution is closer to the exact solution of the 4-truncated modified equation than that of the 2-truncated modified equation.

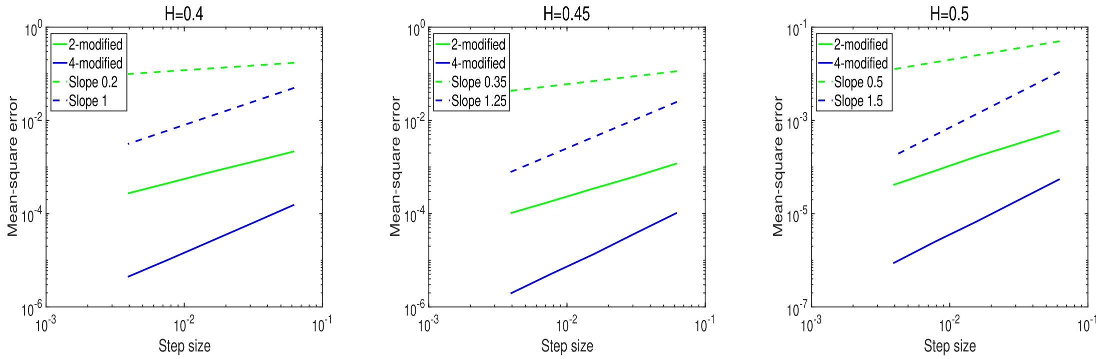



FIG. 1. Mean-square error vs. Step size for Example 5.1.

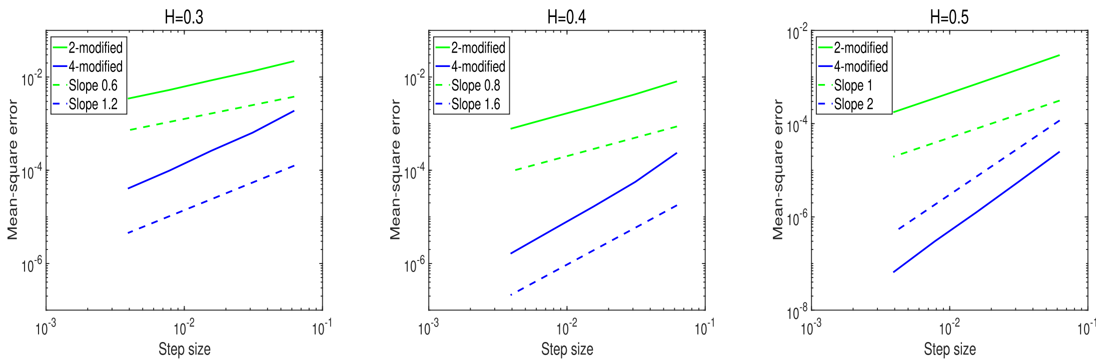



FIG. 2. Mean-square error vs. Step size for Example 5.2.

EXAMPLE 5.3 (Kubo oscillator in Hong *et al.* (2018))

$$\begin{cases} dP_t = -aQ_t\,dt - \sigma \sum_{i=1}^{2} Q_t\,dX_t^i, & P_0 = p, \\ dQ_t = aP_t\,dt + \sigma \sum_{i=1}^{2} P_t\,dX_t^i, & Q_0 = q, \end{cases}$$

where $X^1$ and $X^2$ are independent standard Brownian motions. The Hamiltonians satisfy

$$\frac{2}{a}\mathscr{H}_0(P_t, Q_t) = \frac{2}{\sigma}\mathscr{H}_1(P_t, Q_t) = \frac{2}{\sigma}\mathscr{H}_2(P_t, Q_t) = P_t^2 + Q_t^2.$$

Note that $\mathscr{H}(P_t, Q_t) = P_t^2 + Q_t^2$ is an invariant. The exact solution reads

$$\begin{cases} P_t = p\cos\left(at + \sigma\sum_{i=1}^{2} X_t^i\right) - q\sin\left(at + \sigma\sum_{i=1}^{2} X_t^i\right), \\ Q_t = q\cos\left(at + \sigma\sum_{i=1}^{2} X_t^i\right) + p\sin\left(at + \sigma\sum_{i=1}^{2} X_t^i\right). \end{cases}$$

We compare the midpoint scheme (5.1), which is symplectic and energy-preserving, with the following two numerical methods. One is an explicit RK method defined by

$$Y_{n+1}^h = Y_n^h + V\left(Y_n^h + \frac{1}{2}V(Y_n^h)X_{t_n,t_{n+1}}\right)X_{t_n,t_{n+1}}, \tag{5.2}$$

which is neither symplectic nor energy-preserving. The associated 2-truncated and 4-truncated modified equations are defined through the formulas for the coefficients:

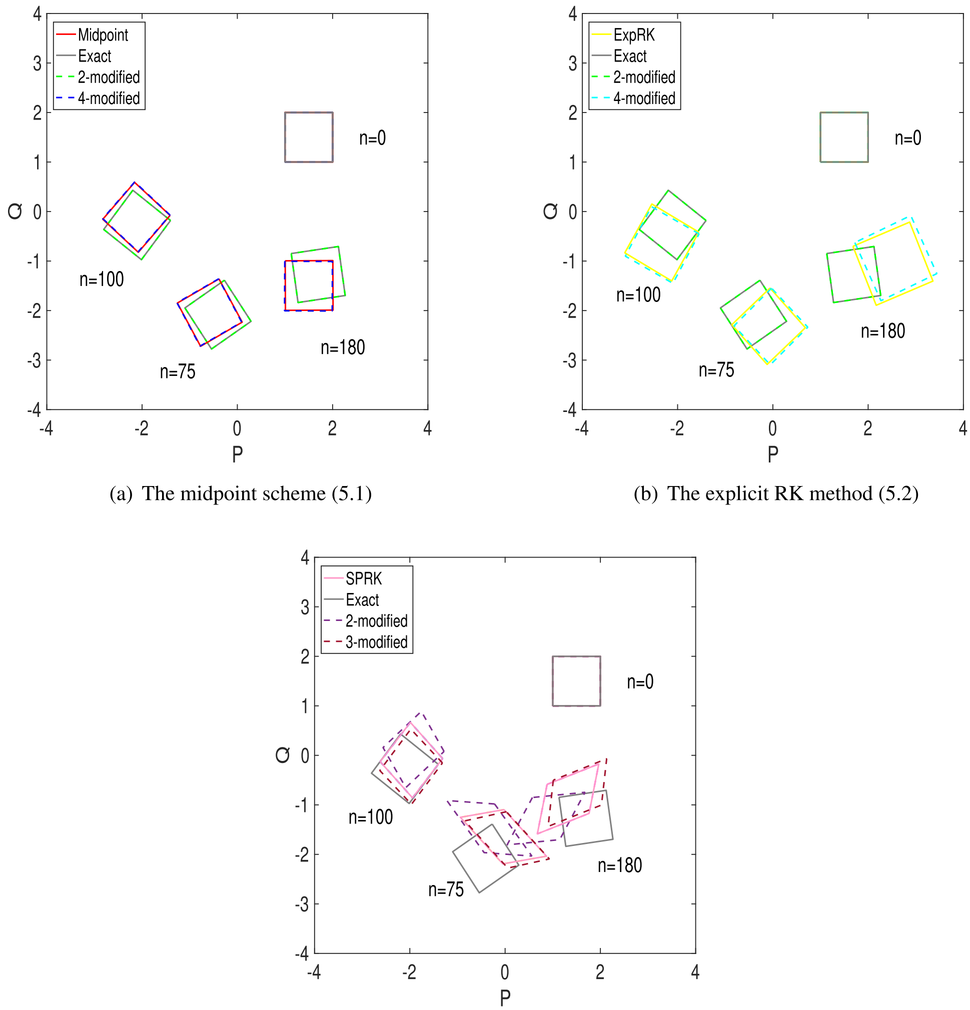
$$\begin{aligned} |\alpha| = 1: \quad & f_\alpha(y) = V_\alpha(y); \quad |\alpha| = 2: \quad f_\alpha(y) = 0; \\ |\alpha| = 3: \quad & f_\alpha(y) = \sum_{\alpha_1+\alpha_2+\alpha_3=\alpha}\left[-\frac{1}{24}V''_{\alpha_3}(y)V_{\alpha_2}(y)V_{\alpha_1}(y) - \frac{1}{6}V'_{\alpha_3}(y)V'_{\alpha_2}(y)V_{\alpha_1}(y)\right]; \\ |\alpha| = 4: \quad & f_\alpha(y) = \sum_{\alpha_1+\alpha_2+\alpha_3+\alpha_4=\alpha}\left[\frac{1}{12}V'_{\alpha_4}V''_{\alpha_3}(y)V_{\alpha_2}(y)V_{\alpha_1}(y) + \frac{1}{8}V'_{\alpha_4}(y)V'_{\alpha_3}(y)V'_{\alpha_2}(y)V_{\alpha_1}(y)\right]. \end{aligned}$$

Another one is a symplectic partitioned RK method which is not energy-preserving. Applying it to Example 5.3 leads to

$$\begin{cases} P_{n+1}^h = P_n^h - aQ_n^h h - \sigma^2 P_{n+1}^h h - \sigma\sum_{i=1}^{2} Q_n^h X_{t_n,t_{n+1}}^i, \\ Q_{n+1}^h = Q_n^h + aP_{n+1}^h h + \sigma^2 Q_n^h h + \sigma\sum_{i=1}^{2} P_{n+1}^h X_{t_n,t_{n+1}}^i; \end{cases} \tag{5.3}$$

see also Section 5.1 in Milstein *et al.* (2002a). The coefficients of the associated modified equations for $1 \leqslant |\alpha| \leqslant 3$ are calculated as follows. Denote $y = (y^1, y^2)^\top \in \mathbb{R}^2$, then

$$\begin{aligned} |\alpha| = 1: \quad & f_{(1,0,0)}(y) = \begin{pmatrix} -\sigma^2 & -a \\ a & \sigma^2 \end{pmatrix}\begin{pmatrix} y^1 \\ y^2 \end{pmatrix}, \\ & f_{(0,1,0)}(y) = f_{(0,0,1)}(y) = \begin{pmatrix} 0 & -\sigma \\ \sigma & 0 \end{pmatrix}\begin{pmatrix} y^1 \\ y^2 \end{pmatrix}; \\ |\alpha| = 2: \quad & f_{(2,0,0)}(y) = \begin{pmatrix} \frac{\sigma^4}{2} + \frac{a^2}{2} & a\sigma^2 \\ -a\sigma^2 & -\frac{\sigma^4}{2} - \frac{a^2}{2} \end{pmatrix}\begin{pmatrix} y^1 \\ y^2 \end{pmatrix}, \end{aligned}$$

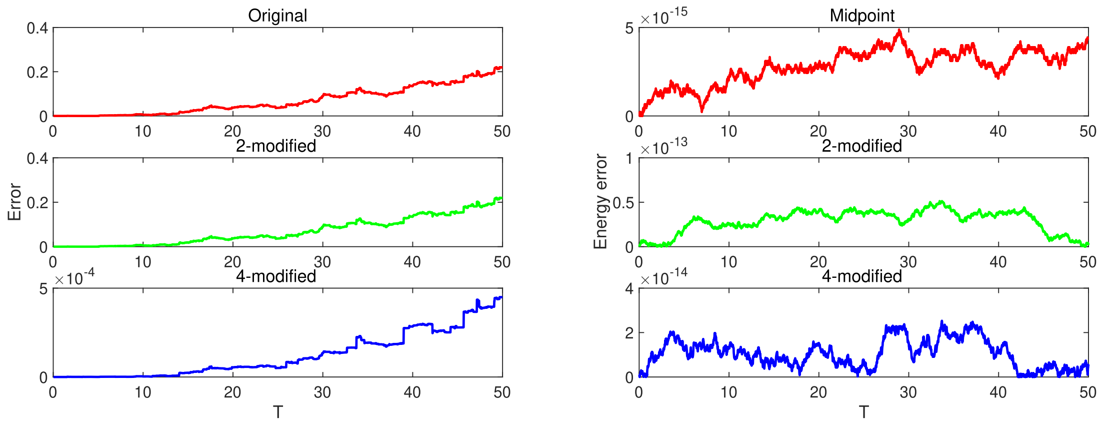



(a) The midpoint scheme (5.1) (b) The explicit RK method (5.2)

(c) The symplectic partitioned RK method (5.3)

FIG. 3. Evolution of domains in the phase plane.

$$f_{(0,1,1)}(y) = \begin{pmatrix} \sigma^2 & 0 \\ 0 & -\sigma^2 \end{pmatrix} \begin{pmatrix} y^1 \\ y^2 \end{pmatrix},$$
$$f_{(1,1,0)}(y) = f_{(1,0,1)}(y) = \begin{pmatrix} a\sigma & \sigma^3 \\ -\sigma^3 & -a\sigma \end{pmatrix} \begin{pmatrix} y^1 \\ y^2 \end{pmatrix},$$
$$f_{(0,2,0)}(y) = f_{(0,0,2)}(y) = \begin{pmatrix} \frac{\sigma^2}{2} & 0 \\ 0 & -\frac{\sigma^2}{2} \end{pmatrix} \begin{pmatrix} y^1 \\ y^2 \end{pmatrix};$$




(a) Error for one trajectory (b) Energy error for one trajectory

FIG. 4. The midpoint scheme (5.1).

$$|\alpha| = 3: \quad f_{(3,0,0)}(y) = \begin{pmatrix} -\frac{\sigma^6}{3} - \frac{2a^2\sigma^2}{3} & -\frac{5a\sigma^4}{6} - \frac{a^3}{6} \\ \frac{5a\sigma^4}{6} + \frac{a^3}{6} & \frac{\sigma^6}{3} + \frac{2a^2\sigma^2}{3} \end{pmatrix} \begin{pmatrix} y^1 \\ y^2 \end{pmatrix},$$

$$f_{(1,1,1)}(y) = \begin{pmatrix} -\frac{4\sigma^4}{3} & -a\sigma^2 \\ a\sigma^2 & \frac{4\sigma^4}{3} \end{pmatrix} \begin{pmatrix} y^1 \\ y^2 \end{pmatrix},$$

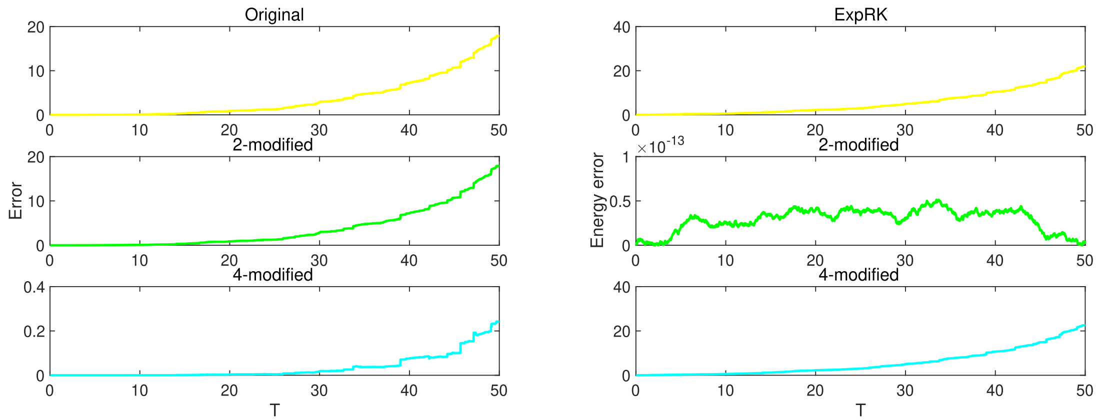
$$f_{(1,2,0)}(y) = f_{(1,0,2)}(y) = \begin{pmatrix} -\sigma^4 & -\frac{2a\sigma^2}{3} \\ \frac{2a\sigma^2}{3} & \sigma^4 \end{pmatrix} \begin{pmatrix} y^1 \\ y^2 \end{pmatrix},$$

$$f_{(0,2,1)}(y) = f_{(0,1,2)}(y) = \begin{pmatrix} 0 & -\frac{\sigma^3}{2} \\ \frac{\sigma^3}{2} & 0 \end{pmatrix} \begin{pmatrix} y^1 \\ y^2 \end{pmatrix},$$

$$f_{(2,1,0)}(y) = f_{(2,0,1)}(y) = \begin{pmatrix} -\frac{4a\sigma^3}{3} & -\frac{5\sigma^5}{6} - \frac{a^2\sigma}{2} \\ \frac{5\sigma^5}{6} + \frac{a^2\sigma}{2} & \frac{4a\sigma^3}{3} \end{pmatrix} \begin{pmatrix} y^1 \\ y^2 \end{pmatrix},$$

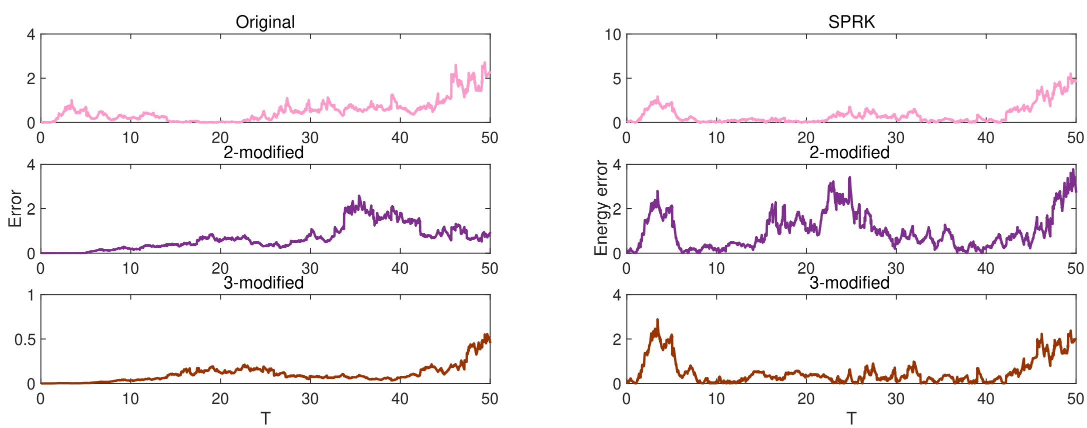
$$f_{(0,3,0)}(y) = f_{(0,0,3)}(y) = \begin{pmatrix} 0 & -\frac{\sigma^3}{6} \\ \frac{\sigma^3}{6} & 0 \end{pmatrix} \begin{pmatrix} y^1 \\ y^2 \end{pmatrix}.$$

We set $a = 1$, $\sigma = 0.9$, $T = 20$, $N = 10 \times 2^6$ (i.e., $h = \frac{T}{N} = 0.0313$). We present the evolution of domains under the flow of $Y_n^h(z)$, $Y_{t_n}(z)$ and $\tilde{y}_{t_n}^{\tilde{N}}(z)$ with $n = 0, 75, 100, 180$, for one realization of Example 5.3 in Figure 3. For the methods (5.1)-(5.2), the truncation numbers are $\tilde{N} = 2, 4$. For the method (5.3), $\tilde{N} = 2, 3$. The 'exact' solution of a truncated modified equation is taken as the numerical solution given by applying the midpoint scheme to this modified equation with a tiny step size $\delta = \frac{T}{10\times 2^{15}} = 2^{-14}$. Notice the fact that the preservation of the symplectic structure is equivalent to the preservation of the area of domains in two-dimensional case. The areas of domains remain unchanged




(a) Error for one trajectory (b) Energy error for one trajectory

FIG. 5. The explicit RK method (5.2).




(a) Error for one trajectory (b) Energy error for one trajectory

FIG. 6. The symplectic partitioned RK method (5.3).

under symplectic methods (5.1) and (5.3), as well as those given by the flows of associated truncated modified equations. However, the corresponding areas for the method (5.2) and its 4-truncated modified equation increase. In particular, we point out that the 2-truncated modified equation of the method (5.2) possesses the symplectic conservation law, since it coincides with the Wong–Zakai approximation of the original system and shares the same formula as the 2-truncated modified equation of the method (5.1). These numerical results confirm Theorem 3.11.

In Figures 4–6, we perform simulations for a trajectory with $a = 1$, $\sigma = 1$, $p = 1$, $q = 0$, $T = 50$, $N = 10 \times 2^8$ (i.e., $h = \frac{T}{N} = 0.0195$) by the three methods, successively. The errors $\|Y_n^h - Y_{t_n}\|$ and $\|Y_n^h - \tilde{y}_{t_n}^{\tilde{N}}\|$ are given in Figures 4(a)–6(a). The 'exact' solution of a truncated modified equation is simulated by applying the midpoint scheme to this modified equation with a tiny step size $\delta = \frac{T}{10\times 2^{15}}$. As expected, we see that the error decreases as $\tilde{N}$ becomes larger for a numerical method. Besides, the energy errors $|(Y_n^h)^\top Y_n^h - p^2 - q^2|$ and $|(\tilde{y}_{t_n}^{\tilde{N}})^\top \tilde{y}_{t_n}^{\tilde{N}} - p^2 - q^2|$ are presented in Figures 4(b)–6(b). Noting that the energy-preserving method (5.1) is also a symmetry method, we have that $f_\alpha(y) = 0$ for any $|\alpha| = 2k$, $k \in \mathbb{N}_+$. Therefore, what we observe is that the energy error is almost zero for the method (5.1) and its truncated modified equations. As to the other two methods, the energy is not preserved, but the energy error is generally controlled better by the symplectic method (5.3) than by the non-symplectic method (5.2).

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## Appendix

In this section, we prove Theorem 4.6. Before that, we recall Cauchy's estimate for analytic functions, and give four lemmas about estimates for the truncated increments, the numerical solution, the modified equation and the truncated modified equation, respectively.

Lemma A.1 (Cauchy's estimate) Suppose that $f$ is analytic on a neighbourhood of the closed ball $B_R(y^*)$ and $M_R = \max\{|f(y)| : y \in B_R(y^*)\} < \infty$, then

$$|f^{(n)}(y^*)| \leqslant \frac{n!\,M_R}{R^n}.$$

*Proof.* By Cauchy's integral formula,

$$|f^{(n)}(y^*)| = \left|\frac{n!}{2\pi i}\int_{|y-y^*|=R}\frac{f(y)}{(y-y^*)^{n+1}}\,\mathrm{d}y\right| \leqslant \frac{n!}{2\pi}\frac{M_R}{R^{n+1}}2\pi R = \frac{n!\,M_R}{R^n}.$$

□

Lemma A.2 (estimate for $\Delta_{n+1,l}$) Let $0 < \epsilon < \frac{1}{2}$ and $k \geqslant 1$. Then there exists a constant $C = C(\epsilon, k)$ such that

$$|\Delta_{n+1,l}| \leqslant h^{\frac{1}{2}-\epsilon} \quad \forall\, h < C. \tag{A.1}$$

*Proof.* Consider the function $v_1(h) = k\ln h + h^{-2\epsilon}$. Since $\lim_{h\to 0} v_1(h) = +\infty$, we obtain that there exists a constant $C = C(\epsilon, k)$ such that

$$v_1(h) \geqslant 0 \quad \forall\, h < C.$$

Then we have

$$|\zeta_{n+1,l}| \leqslant A_h = \sqrt{k|\ln h|} \leqslant h^{-\epsilon} \quad \forall\, h < C,$$

which implies (A.1). □

LEMMA A.3 (estimate for $d_\alpha$) Denote $\kappa := \max_{i=1,\cdots,s}\left\{\sum_{j=1}^{s}|a_{ij}|\right\}$ and $\mu := \sum_{i=1}^{s}|b_i|$. Under assumptions as in Theorem 4.6, if

$$\max\{h, |\Delta_{1,1}|, \cdots, |\Delta_{1,d}|\} < \frac{R}{2\kappa M(d+1)\sqrt{s}}, \tag{A.2}$$

then it holds that

$$\|d_\alpha(y)\| \leqslant \mu(d+1)M\left[\frac{2\kappa M(d+1)\sqrt{s}}{R}\right]^{|\alpha|-1} \quad \forall\, y \in B_R(z),$$

where the coefficient $d_\alpha$ is defined by the expansion

$$Y_1^h(z) = z + \sum_{|\alpha|=1}^{\infty} d_\alpha(z)h^{\alpha_0}\Delta_{1,1}^{\alpha_1}\cdots\Delta_{1,d}^{\alpha_d}, \quad \alpha = (\alpha_0, \cdots, \alpha_d) \in \mathbb{N}^{d+1}.$$

*Proof.* For any $y \in B_{\frac{3}{2}R}(z)$ and $\|\Delta y\| \leqslant 1$, define $v(\theta) := V_l(y+\theta\Delta y)$, $|\theta| \leqslant \frac{R}{2}$. Then Cauchy's estimate shows

$$\|V_l'(y)\Delta y\| = \left\|v'(\theta)\big|_{\theta=0}\right\| \leqslant \frac{M}{\frac{R}{2}} = \frac{2M}{R},$$

which implies

$$\|V_l'(y)\| = \sup_{\|\Delta y\|\leqslant 1}\|V_l'(y)\Delta y\| \leqslant \frac{2M}{R} \quad \forall\, y \in B_{\frac{3}{2}R}(z). \tag{A.3}$$

For any $y \in B_R(z)$, define a map $F : \mathbb{C}^{m\times s} \to \mathbb{C}^{m\times s}$ by

$$F : g = (g_1, \cdots, g_s) \mapsto F(g) = (F(g)_1, \cdots, F(g)_s),$$
$$F(g)_i = y + \sum_{j=1}^{s} a_{ij}\left[V_0(g_j)h + \sum_{l=1}^{d} V_l(g_j)\Delta_{1,l}\right], \quad i = 1, \cdots, s.$$

We claim that $F$ is a contraction on the closed set $\mathbb{B} := \left\{(g_1, \cdots, g_s) : \|g_i - y\| \leqslant \frac{R}{2}, i = 1, \cdots, s\right\}$ with $y \in B_R(z)$. Indeed, for any $0 < \gamma < 1$ and

$$\max\{|h|, |\Delta_{1,1}|, \cdots, |\Delta_{1,d}|\} \leqslant \frac{\gamma R}{2\kappa M(d+1)\sqrt{s}} =: C_1(\gamma),$$

we have

$$\|F(g)_i - y\| \leqslant \sum_{j=1}^{s}|a_{ij}|M\left[h + \sum_{l=1}^{d}|\Delta_{1,l}|\right] < \frac{R}{2} \quad \forall\, g \in \mathbb{B}.$$

Besides, (A.3) yields

$$\|F(g)_i - F(\tilde{g})_i\| \leqslant \sum_{j=1}^{s} |a_{ij}| \frac{2M}{R} \left[ h + \sum_{l=1}^{d} |\Delta_{1,l}| \right] \|g - \tilde{g}\| \leqslant \frac{\gamma}{\sqrt{s}} \|g - \tilde{g}\| \quad \forall\, g, \tilde{g} \in \mathbb{B},$$

which leads to $\|F(g) - F(\tilde{g})\| \leqslant \gamma \|g - \tilde{g}\|$. Therefore, there exists a unique fixed point $g^* = (g_1^*, \cdots, g_s^*)$ for $F$ on the set $\mathbb{B}$. Denote

$$Y_1^h(y) := y + \sum_{i=1}^{s} b_i \left( V_0(g_i^*) h + \sum_{l=1}^{d} V_l(g_i^*) \Delta_{1,l} \right).$$

Together with the analyticity of $V$, $Y_1^h(y) - y$ is analytic for $|h|, |\Delta_{1,1}|, \cdots, |\Delta_{1,d}| \leqslant C_1(\gamma)$ and $y \in B_R(z)$. In this case, due to $g_i^* \in B_{\frac{3R}{2}}(z)$, the boundedness of $V$ implies

$$\|Y_1^h(y) - y\| \leqslant \mu(d+1) M C_1(\gamma).$$

Repeatedly applying Cauchy's estimate, we have

$$\begin{aligned} \|d_\alpha(y)\| &= \left\| \frac{1}{\alpha_0! \cdots \alpha_d!} \left[ \frac{d^{\alpha_d}}{d\Delta_{1,d}^{\alpha_d}} \cdots \left[ \frac{d^{\alpha_0}}{dh^{\alpha_0}} \left( Y_1^h(y) - y \right) \right] \Big|_{h=0} \cdots \right] \Big|_{\Delta_{1,d}=0} \right\| \\ &\leqslant \frac{\mu(d+1) M C_1(\gamma)}{C_1^{|\alpha|}(\gamma)} = \mu(d+1) M \left[ \frac{2\kappa M (d+1) \sqrt{s}}{\gamma R} \right]^{|\alpha|-1}. \end{aligned}$$

Letting $\gamma \to 1$, we obtain

$$\|d_\alpha(y)\| \leqslant \mu(d+1) M \left[ \frac{2\kappa M (d+1) \sqrt{s}}{R} \right]^{|\alpha|-1} \quad \forall\, y \in B_R(z).$$

□

REMARK A.4 Let $\epsilon = \frac{1}{4}$ and $k = 4$. Lemma A.2 shows that condition (A.2) holds if we simulate the random variable $\Delta_{1,l}$ in (4.3) by taking

$$h < \min \left\{ C(\epsilon, k), \frac{R}{2\kappa M (d+1) \sqrt{s}}, \left[ \frac{R}{2\kappa M (d+1) \sqrt{s}} \right]^4 \right\}. \tag{A.4}$$

LEMMA A.5 (estimate for $f_\alpha$) Denote $\eta := 2 \max\{\kappa, \mu/(2\ln 2 - 1)\}$. Under assumptions as in Theorem 4.6 and Lemmas A.2–A.3, then the coefficients of the associated stochastic modified equation (4.5) satisfy

$$\sum_{|\alpha|=J} \|f_\alpha(y)\| \leqslant (\ln 2) \eta M (d+1)^2 \sqrt{s} \left( \frac{\eta M (d+1)^2 \sqrt{s} J}{R} \right)^{J-1} \quad \forall\, y \in B_{\frac{1}{2}R}(z),\ J \in \mathbb{N}_+.$$

*Proof.* For $J = 1$, it follows from Lemma A.3 that for $y \in B_{\frac{1}{2}R}(z)$,

$$\sum_{|\alpha|=1} \|f_\alpha(y)\| \leqslant \mu M(d+1)^2 \leqslant (\ln 2)\eta M(d+1)^2\sqrt{s}.$$

Suppose $J \geqslant 2$. We consider $\alpha \in \mathbb{N}^{d+1}$ such that $1 \leqslant |\alpha| \leqslant J$. The definitions of $\{d_\alpha\}$ and $\{f_\alpha\}$ imply that $\{d_\alpha\}$ and $\{f_\alpha\}$ are composed by $V$ and its derivatives in general, which are analytic on a neighbourhood of $B_{2R}(z)$. For any analytic function $g$ on a neighbourhood of $B_{2R}(z)$, we define

$$\|g\|_m := \max\left\{\|g(y)\| : y \in B_{R-(m-1)\delta}(z),\ \delta = \frac{R}{2(J-1)}\right\} \quad \forall\, m \in \mathbb{N}_+.$$

It holds that $\|g\|_{m_1} \geqslant \|g\|_{m_2}$ if $m_1 \leqslant m_2$. Moreover, the function $v(\theta) := g(y + \theta f_\alpha(y))$ with $|\theta| \leqslant \frac{\delta}{\|f_\alpha\|_m}$ and $y \in B_{R-(m-1)\delta}(z)$ is analytic. It follows from Cauchy's estimate that

$$\begin{aligned}
\|D_\alpha g(y)\| &= \|g(y) f_\alpha(y)\| \\
&= \|v'(0)\| \\
&\leqslant \frac{\sup_{|\theta|\leqslant \delta/\|f_\alpha\|_m} \|v(\theta)\|}{\delta/\|f_\alpha\|_m} \\
&= \frac{1}{\delta}\|f_\alpha\|_m \|g\|_{m-1},
\end{aligned}$$

which implies $\|D_\alpha g\|_m \leqslant \frac{1}{\delta}\|f_\alpha\|_m\|g\|_{m-1}$. Then given $k^{i,1}, \cdots, k^{i,i} \in \mathbb{N}^{d+1}$ such that $|k_{i,1}|, \cdots, |k_{i,i}| \geqslant 1$ and $|k^{i,1}| + \cdots + |k^{i,i}| = |\alpha|$, $i = 1, \cdots, |\alpha|$, we get

$$\begin{aligned}
\|D_{k^{i,1}} \cdots D_{k^{i,i-1}} f_{k^{i,i}}\|_{|\alpha|} &\leqslant \frac{1}{\delta}\|f_{k^{i,1}}\|_{|\alpha|}\|D_{k^{i,2}} \cdots D_{k^{i,i-1}} f_{k^{i,i}}\|_{|\alpha|-1} \\
&\leqslant \frac{1}{\delta^2}\|f_{k^{i,1}}\|_{|\alpha|}\|f_{k^{i,2}}\|_{|\alpha|-1}\|D_{k^{i,3}} \cdots D_{k^{i,i-1}} f_{k^{i,i}}\|_{|\alpha|-2} \\
&\leqslant \cdots \\
&\leqslant \frac{1}{\delta^{i-1}}\|f_{k^{i,1}}\|_{|\alpha|}\|f_{k^{i,2}}\|_{|\alpha|-1} \cdots \|f_{k^{i,i}}\|_{|\alpha|-(i-1)} \\
&\leqslant \frac{1}{\delta^{i-1}}\|f_{k^{i,1}}\|_{|k^{i,1}|} \cdots \|f_{k^{i,i}}\|_{|k^{i,i}|}.
\end{aligned}$$

Combining with (3.7), we have

$$\|f_\alpha\|_{|\alpha|} \leqslant \|d_\alpha\|_{|\alpha|} + \sum_{i=2}^{|\alpha|} \frac{1}{i!} \sum_{(k^{i,1},\cdots,k^{i,i})\in O_i^\alpha} \frac{1}{\delta^{i-1}}\|f_{k^{i,1}}\|_{|k^{i,1}|} \cdots \|f_{k^{i,i}}\|_{|k^{i,i}|}.$$

By the notation $F_{\tilde{\alpha}} := \sum_{|\alpha|=\tilde{\alpha}} \|f_\alpha\|_{|\alpha|}$ and $G_{\tilde{\alpha}} := \sum_{|\alpha|=\tilde{\alpha}} \|d_\alpha\|_{|\alpha|}$, the above inequality yields

$$F_{\tilde{\alpha}} \leqslant G_{\tilde{\alpha}} + \sum_{i=2}^{\tilde{\alpha}} \frac{1}{i!} \sum_{\tilde{k}^{i,1}+\cdots+\tilde{k}^{i,i}=\tilde{\alpha}} \frac{1}{\delta^{i-1}} F_{\tilde{k}^{i,1}} \cdots F_{\tilde{k}^{i,i}}. \tag{A.6}$$

Lemma A.3 produces

$$\|d_\alpha\|_{|\alpha|} \leqslant \mu(d+1)M\left[\frac{2\kappa M(d+1)\sqrt{s}}{R}\right]^{\tilde{\alpha}-1}, \quad |\alpha| = \tilde{\alpha}.$$

Together with $\#\{\alpha = (\alpha_0, \cdots, \alpha_d) : |\alpha| = \tilde{\alpha}\} = \frac{(\tilde{\alpha}+(d+1)-1)!}{((d+1)-1)!\tilde{\alpha}!} = \frac{(d+\tilde{\alpha})!}{d!\tilde{\alpha}!}$, we have

$$\begin{aligned} G_{\tilde{\alpha}} &\leqslant \frac{(d+\tilde{\alpha})!}{d!\,\tilde{\alpha}!}\mu(d+1)M\left[\frac{2\kappa M(d+1)\sqrt{s}}{R}\right]^{\tilde{\alpha}-1} \\ &\leqslant (d+1)^{\tilde{\alpha}}\mu(d+1)M\sqrt{s}\left[\frac{2\kappa M(d+1)\sqrt{s}}{R}\right]^{\tilde{\alpha}-1} \\ &= \mu M(d+1)^2\sqrt{s}\left[\frac{2\kappa M(d+1)^2\sqrt{s}}{R}\right]^{\tilde{\alpha}-1}. \end{aligned} \tag{A.7}$$

For all $\tilde{\alpha} \in \mathbb{N}_+$, we let

$$\beta_{\tilde{\alpha}} := \frac{\mu M(d+1)^2\sqrt{s}}{\delta}\left(\frac{2\kappa M(d+1)^2\sqrt{s}}{R}\right)^{\tilde{\alpha}-1} + \sum_{i=2}^{\tilde{\alpha}} \frac{1}{i!} \sum_{\tilde{k}^{i,1}+\cdots+\tilde{k}^{i,i}=\tilde{\alpha}} \beta_{\tilde{k}^{i,1}} \cdots \beta_{\tilde{k}^{i,i}}. \tag{A.8}$$

Based on (A.5), we have that $F_{\tilde{\alpha}} \leqslant \delta\beta_{\tilde{\alpha}}$ holds for $\tilde{\alpha} = 1$. Moreover, assume by induction that $F_{\tilde{\alpha}} \leqslant \delta\beta_{\tilde{\alpha}}$ holds for $\alpha = 1, \cdots, n$. Then according to (A.6)–(A.8), we know that for $\tilde{\alpha} = n+1$,

$$F_{\tilde{\alpha}} \leqslant \mu M(d+1)^2\sqrt{s}\left[\frac{2\kappa M(d+1)^2\sqrt{s}}{R}\right]^{\tilde{\alpha}-1} + \sum_{i=2}^{\tilde{\alpha}} \frac{1}{i!} \sum_{\tilde{k}^{i,1}+\cdots+\tilde{k}^{i,i}=\tilde{\alpha}} \frac{1}{\delta^{i-1}}\left(\delta\beta_{\tilde{k}^{i,1}}\right)\cdots\left(\delta\beta_{\tilde{k}^{i,i}}\right) = \delta\beta_{\tilde{\alpha}}.$$

Therefore, we have that $F_{\tilde{\alpha}} \leqslant \delta\beta_{\tilde{\alpha}}$ for $\tilde{\alpha} = 1, \cdots, J$. In order to estimate $F_J$, it suffices to estimate $\beta_J$. Let $c_1 := \frac{\mu M(d+1)^2\sqrt{s}}{\delta}$, $c_2 := \frac{2\kappa M(d+1)^2\sqrt{s}}{R}$. For $|\xi| \leqslant 1/c_2$, multiplying (A.8) by $\xi^{\tilde{\alpha}}$ and summarizing for $\tilde{\alpha}$ leads to

$$\begin{aligned} \sum_{\tilde{\alpha}=1}^{\infty} \beta_{\tilde{\alpha}}\xi^{\tilde{\alpha}} &= \sum_{\tilde{\alpha}=1}^{\infty} c_1 c_2^{\tilde{\alpha}-1}\xi^{\tilde{\alpha}} + \sum_{\tilde{\alpha}=1}^{\infty}\sum_{i=2}^{\tilde{\alpha}} \frac{1}{i!} \sum_{\tilde{k}^{i,1}+\cdots+\tilde{k}^{i,i}=\tilde{\alpha}} \beta_{\tilde{k}^{i,1}}\cdots\beta_{\tilde{k}^{i,i}}\xi^{\tilde{\alpha}} \\ &= c_1\xi\sum_{\tilde{\alpha}=1}^{\infty}(c_2\xi)^{\tilde{\alpha}-1} + \sum_{i=2}^{\infty}\frac{1}{i!}\sum_{\tilde{\alpha}=i}^{\infty}\sum_{\tilde{k}^{i,1}+\cdots+\tilde{k}^{i,i}=\tilde{\alpha}} \beta_{\tilde{k}^{i,1}}\cdots\beta_{\tilde{k}^{i,i}}\xi^{\tilde{\alpha}}, \end{aligned}$$

which produces

$$b(\xi) = \frac{c_1 \xi}{1 - c_2 \xi} + e^{b(\xi)} - 1 - b(\xi)$$

with

$$b(\xi) := \sum_{\tilde{\alpha}=1}^{\infty} \beta_{\tilde{\alpha}} \xi^{\tilde{\alpha}}. \tag{A.9}$$

Consider the function

$$q(b, \xi) = \frac{c_1 \xi}{1 - c_2 \xi} + e^b - 1 - 2b = 0.$$

If $\frac{\partial q(b,\xi)}{\partial b} = e^b - 2 \neq 0$ (i.e., $b \neq \ln 2$), the implicit function theorem shows that there exists a map $b : \xi \mapsto b(\xi)$ and the series in (A.9) is convergent. Since $c_1, c_2 > 0$, we know that the range of the increasing function $\xi \mapsto \frac{c_1 \xi}{1 - c_2 \xi}$ for $|\xi| \in \big[0,\ (2\ln 2 - 1)/(c_1 + c_2(2\ln 2 - 1))\big)$ is

$$\big( - 2\ln 2 + 1 + (2c_2(2\ln 2 - 1)^2)/(c_1 + 2c_2(2\ln 2 - 1)),\ 2\ln 2 - 1\big).$$

Meanwhile, the range of the increasing function $b \mapsto -e^b + 1 + 2b$ for $|b| \in [0, \ln 2)$ is

$$(-2\ln 2 + 1/2, 2\ln 2 - 1),$$

which includes the range of the function. Then we have that for any $\xi$ satisfying $|\xi| \in \big[0,\ (2\ln 2 - 1)/(c_1 + c_2(2\ln 2 - 1))\big)$, there exists $b(\xi) \in (-\ln 2, \ln 2)$ such that $q(b, \xi) = 0$, which implies

$$|b(\xi)| \leqslant \ln 2 \quad \forall\, |\xi| < (2\ln 2 - 1)/(c_1 + c_2(2\ln 2 - 1)).$$

Since $b(\xi)$ equals to a convergent polynomials series (A.9) of $\xi$, $b(\xi)$ is analytic with respect to $\xi$. By Cauchy's estimate, we derive

$$|\beta_{\tilde{\alpha}}| \leqslant \frac{\ln 2}{((2\ln 2 - 1)/(c_1 + c_2(2\ln 2 - 1)))^{\tilde{\alpha}}}, \quad \tilde{\alpha} \in \mathbb{N}_+,$$

and then

$$F_J \leqslant \delta\beta_J \leqslant \frac{R}{2(J-1)} \frac{\ln 2}{((2\ln 2 - 1)/(c_1 + c_2(2\ln 2 - 1)))^J} \leqslant \frac{(\ln 2)R}{2(J-1)} \left( \frac{\eta M (d+1)^2 \sqrt{s} J}{R} \right)^J.$$

Therefore,

$$\sum_{|\alpha|=J} \|f_\alpha(y)\| \leqslant (\ln 2)\eta M (d+1)^2 \sqrt{s} \left( \frac{\eta M (d+1)^2 \sqrt{s} J}{R} \right)^{J-1} \qquad \forall\, y \in B_{\frac{1}{2}R}(z).$$

□

In order to estimate the exact solution of the $\tilde{N}$-truncated modified equation (4.6), we consider the infinite expansion for its solution with respect to the initial value $z$:

$$\tilde{y}_{t_1}^{\tilde{N}} = z + \sum_{|\alpha|=1}^{\infty} f_\alpha^{\tilde{N}}(z) h^{\alpha_0} \Delta_{1,1}^{\alpha_1} \cdots \Delta_{1,d}^{\alpha_d}.$$

LEMMA A.6 (estimate for $f_\alpha^{\tilde{N}}$) Let $0 < \epsilon < \frac{1}{2}$. Under assumptions as in Theorem 4.6 and Lemmas A.2–A.5, then there exist constants $C = C(\epsilon, R, M)$ and $\tau = \tau(\epsilon, R, M)$ such that for any $h \in (0, \tau)$, if the truncation number $\tilde{N}$ satisfies

$$1 \leqslant \tilde{N} \leqslant \frac{R}{\eta M(d+1)^2 \sqrt{s} h^{\frac{1}{2}-\epsilon}}, \tag{A.10}$$

then we have

$$\|f_\alpha^{\tilde{N}}(z)\| \leqslant \frac{(\ln 2)\eta M(d+1)^2\sqrt{s}C}{\left[\frac{R}{2(\ln 2)\eta M(d+1)^2\sqrt{s}C}\right]^{(\frac{1}{1/2-\epsilon})|\alpha|-1}}.$$

*Proof.* For simplicity, we let $\epsilon = \frac{1}{4}$, as the proof is similar for $\epsilon \in \left(0, \frac{1}{2}\right)$.

According to Lemma A.5, as long as $\{\tilde{y}_t^{\tilde{N}} : t \leqslant t_1 = h\} \subset B_{\frac{R}{2}}(z)$, we have the estimate

$$\begin{aligned}
\|\tilde{y}_t^{\tilde{N}} - z\| &\leqslant \sum_{J=1}^{\tilde{N}} h^{\frac{1}{4}J} (\ln 2)\eta M(d+1)^2\sqrt{s} \left(\frac{\eta M(d+1)^2\sqrt{s}J}{R}\right)^{J-1} \\
&\leqslant h^{\frac{1}{4}} (\ln 2)\eta M(d+1)^2\sqrt{s} \left(1 + \sum_{J=2}^{\tilde{N}} \left(\frac{\eta M(d+1)^2\sqrt{s}Jh^{\frac{1}{4}}}{R}\right)^{J-1}\right) \quad \forall\, t \leqslant h.
\end{aligned}$$

Since $1 \leqslant \tilde{N} \leqslant \frac{R}{\eta M(d+1)^2\sqrt{s}h^{\frac{1}{4}}}$, we know

$$1 + \sum_{J=2}^{\tilde{N}} \left(\frac{\eta M(d+1)^2\sqrt{s}Jh^{\frac{1}{4}}}{R}\right)^{J-1} \leqslant 1 + \sum_{J=2}^{\tilde{N}} \left(\frac{J}{\tilde{N}}\right)^{J-1} \leqslant C_0.$$

Then a sufficient condition for $\{\tilde{y}_t^{\tilde{N}} : t \leqslant h\} \subset B_{\frac{R}{2}}(z)$ is

$$h \leqslant \left(\frac{R}{2(\ln 2)\eta M(d+1)^2\sqrt{s}C_0}\right)^4. \tag{A.11}$$

In this case, it has

$$\|\tilde{y}_t^{\tilde{N}} - z\| \leqslant h^{\frac{1}{4}} (\ln 2)\eta M(d+1)^2\sqrt{s}C_0 \quad \forall\, t \leqslant h.$$

Moreover, since the coefficients $\{f_\alpha\}$ of (4.6) are generally composed by $V$ and its derivatives, $\{f_\alpha\}$ are also analytic. Then $\{\tilde{y}_t^{\tilde{N}} : t \leqslant h\} \subset B_{\frac{R}{2}}(z)$ produces that $\tilde{y}_h^{\tilde{N}} - z$ is analytic for $h$ satisfying (A.11).

Combining the conditions (A.4) and (A.11) on $h$ together, we obtain that there exists a sufficiently large $C_1$ such that

$$\left[\frac{R}{2(\ln 2)\eta M(d+1)^2\sqrt{s}C_1}\right]^4$$
$$< \min\left\{C(\epsilon,k), \frac{R}{2\kappa M(d+1)\sqrt{s}}, \left[\frac{R}{2\kappa M(d+1)\sqrt{s}}\right]^4, \left[\frac{R}{2(\ln 2)\eta M(d+1)^2\sqrt{s}C_0}\right]^4\right\}.$$

Defining $C_2 := \left[\frac{R}{2(\ln 2)\eta M(d+1)^2\sqrt{s}C_1}\right]^4$, we use Cauchy's estimate to get

$$\|f_\alpha^{\tilde{N}}(z)\| = \frac{1}{\alpha_0!\cdots\alpha_d!}\left[\frac{d^{\alpha_d}}{d\Delta_{1,d}^{\alpha_d}}\cdots\left[\frac{d^{\alpha_0}}{dh^{\alpha_0}}\left(\tilde{y}_h^{\tilde{N}} - z\right)\right]\Big|_{h=0}\cdots\right]\Bigg|_{\Delta_{1,d}=0}$$
$$\leqslant \frac{C_2^{\frac{1}{4}}(\ln 2)\eta M(d+1)^2\sqrt{s}C_0}{C_2^{|\alpha|}}$$
$$\leqslant \frac{(\ln 2)\eta M(d+1)^2\sqrt{s}C_1}{\left[\frac{R}{2(\ln 2)\eta M(d+1)^2\sqrt{s}C_1}\right]^{4|\alpha|-1}}.$$

□

Now we can proceed to the proof of Theorem 4.6.

*Proof of Theorem* 4.6. We know that $d_\alpha = f_\alpha^{\tilde{N}}$ with $1 \leqslant |\alpha| \leqslant \tilde{N}$, then it remains to estimate the terms for $|\alpha| \geqslant \tilde{N}+1$. For simplicity, we let $\epsilon = \frac{1}{4}$, since the proof is similar for $0 < \epsilon < \frac{1}{2}$.

For the numerical solution given by (4.4), Lemma A.3 yields that the sum of remainder terms is bounded by

$$\sum_{|\alpha|=\tilde{N}+1}^{\infty} \|d_\alpha(z)\| h^{\alpha_0}|\Delta_{1,1}^{\alpha_1}|\cdots|\Delta_{1,d}^{\alpha_d}|$$
$$\leqslant \sum_{J=\tilde{N}+1}^{\infty} \mu M(d+1)^2\sqrt{s}\left[\frac{2\kappa M(d+1)^2\sqrt{s}}{R}\right]^{J-1} h^{\frac{J}{4}}$$
$$\leqslant \left\{\sum_{J=0}^{\infty} h^{\frac{J}{4}}\left[\frac{2\kappa M(d+1)^2\sqrt{s}}{R}\right]^{J-1}\right\}\mu M(d+1)^2\sqrt{s}\left[\frac{2\kappa M(d+1)^2\sqrt{s}}{R}\right]^{\tilde{N}+1} h^{\frac{\tilde{N}+1}{4}}$$
$$\leqslant C\tilde{C}^{\tilde{N}} h^{\frac{\tilde{N}+1}{4}}.$$

The last inequality holds if $h^{\frac{1}{4}}\left[\frac{2\kappa M(d+1)^2\sqrt{s}}{R}\right] < 1$, i.e., $h < \left[\frac{R}{2\kappa M(d+1)^2\sqrt{s}}\right]^4$.

For the exact solution of the $\tilde{N}$-truncated modified equation (4.6), Lemma A.6 leads to that the sum of remainder terms is bounded by

$$\begin{aligned}
&\sum_{|\alpha|=\tilde{N}+1}^{\infty} \|f_{\alpha}^{\tilde{N}}(z)\| h^{\alpha_0} |\Delta_{1,1}^{\alpha_1}| \cdots |\Delta_{1,d}^{\alpha_d}| \\
&\leqslant \sum_{J=\tilde{N}+1}^{\infty} (d+1)^J \frac{(\ln 2)\eta M (d+1)^2 C_1 \sqrt{s}}{\left[\frac{R}{2(\ln 2)\eta M(d+1)^2 C_1 \sqrt{s}}\right]^{4J-1}} h^{\frac{J}{4}} \\
&\leqslant \left\{ \sum_{J=0}^{\infty} \frac{h^{\frac{J}{4}} (d+1)^J}{\left[\frac{R}{2(\ln 2)\eta M(d+1)^2 C_1 \sqrt{s}}\right]^{4J-1}} \right\} \frac{(\ln 2)\eta M (d+1)^2 C_1 \sqrt{s} (d+1)^{\tilde{N}+1}}{\left[\frac{R}{2(\ln 2)\eta M(d+1)^2 C_1 \sqrt{s}}\right]^{4(\tilde{N}+1)}} h^{\frac{\tilde{N}+1}{4}} \\
&\leqslant C \tilde{C}^{\tilde{N}} h^{\frac{\tilde{N}+1}{4}}.
\end{aligned}$$

The last inequality holds if $\frac{(d+1)h^{\frac{1}{4}}}{\left[\frac{R}{2(\ln 2)\eta M(d+1)^2 C_1 \sqrt{s}}\right]^{4}} < 1$, i.e., $h < \left(\frac{1}{d+1}\right)^4 \left[\frac{R}{2(\ln 2)\eta M(d+1)^2 C_1 \sqrt{s}}\right]^{16}$.

Define $h_0 := \frac{R}{\eta M(d+1)^2 \sqrt{s}}$. Then the condition (A.10) reads $\tilde{N} \leqslant h_0 h^{-\frac{1}{4}}$. We choose $\tilde{N}$ for the largest integer under this condition and then

$$C \tilde{C}^{\tilde{N}} h^{\frac{\tilde{N}+1}{4}} = C \tilde{C}^3 h \tilde{C}^{\tilde{N}-3} h^{\frac{1}{4}(\tilde{N}-3)} = C \tilde{C}^3 h \left(\tilde{C} h^{\frac{1}{4}}\right)^{\tilde{N}-3}.$$

Due to $h_0 h^{-\frac{1}{4}} < \tilde{N}+1$, we have

$$\left(\tilde{C} h^{\frac{1}{4}}\right)^{\tilde{N}-3} \leqslant e^{-(\tilde{N}-3)} \leqslant e^4 e^{-(\tilde{N}+1)} \leqslant e^4 e^{-h_0/h^{\frac{1}{4}}} \quad \forall\, h \leqslant (\tilde{C} e)^{-4}.$$

Therefore, if the time step size $h \in (0, \tau)$ with

$$\tau = \min\left\{ \left[\frac{R}{2(\ln 2)\eta M (d+1)^2 \sqrt{s} C_1}\right]^4, \left[\frac{R}{2\kappa M (d+1)^2 \sqrt{s}}\right]^4, \left(\frac{1}{d+1}\right)^4 \left[\frac{R}{2(\ln 2)\eta M (d+1)^2 C_1 \sqrt{s}}\right]^{16}, (\tilde{C} e)^{-4} \right\},$$

then the local error is

$$\|\tilde{y}_{t_1}^{\tilde{N}} - Y_1^h\| \leqslant C h e^{-h_0/h^{\frac{1}{4}}}.$$

□