

A Lie algebraic approach for a class of highly oscillatory stochastic Hamiltonian systems^{*}

RUAN Jialin, WANG Lijin[†]

(School of Mathematical Sciences, University of Chinese Academy of Sciences, Beijing 100049, China)

(Received 26 September 2017; Revised 4 January 2018)

Ruan J L, Wang L J. A Lie algebraic approach for a class of highly oscillatory stochastic Hamiltonian systems[J]. Journal of University of Chinese Academy of Sciences, 2019,36(1):5-10.

Abstract In this work, we propose a Lie algebraic approach for numerically solving a class of highly oscillatory stochastic Hamiltonian systems (SHSs). For a concrete highly oscillatory SHS, we construct two numerical schemes based on the Lie algebraic approach, and prove their near preservation of the symplecticity. We also show by numerical tests their root mean-square convergence orders, as well as their effectiveness and merits in solving the highly oscillatory SHS.

Keywords numerical solutions of stochastic differential equations; stochastic Hamiltonian systems; highly oscillatory SDEs; operator splitting methods; Lie algebraic approach

CLC number: O241.8 **Document code:** A **doi:**10.7523/j.issn.2095-6134.2019.01.002

一类高振荡随机哈密顿系统的李代数方法

阮家麟, 王丽瑾

(中国科学院大学数学科学学院, 北京 100049)

摘 要 为一类高振荡随机哈密顿系统提出一种李代数数值方法。对一个具体的高振荡随机哈密顿系统, 给出两个基于李代数方法的数值格式, 并证明它们近似保辛结构。通过数值实验展示这两种格式的根均方收敛阶, 以及它们在数值求解该高振荡随机哈密顿系统中的有效性和优越性。

关键词 随机微分方程数值解; 随机哈密顿系统; 高振荡随机微分方程; 算子分裂方法; 李代数方法

Stochastic differential equations (SDEs) play an important role in the description of phenomena in many subjects^[1-2], such as biology, mechanics, chemistry, and microelectronics. The Hamiltonian system is one of the most important dynamical systems. All the real physical processes where the dissipation can be neglected can be formulated as Hamiltonian systems^[3]. Stochastic Hamiltonian

^{*} Supported by the National Nature Science Foundation of China (11471310, 11071251)
[†] Corresponding author, E-mail: ljwang@ucas.ac.cn

systems (SHSs) are the Hamiltonian systems with stochastic disturbances.

A $2n$ -dimensional SHS can be written as the SDE of Stratonovich sense^[4-5] with initial values $P(0) = p$, $Q(0) = q$,

$$\begin{aligned} dP &= f(t, P, Q)dt + \sum_{r=1}^m \sigma_r(t, P, Q) \circ dW_r(t), \\ dQ &= g(t, P, Q)dt + \sum_{r=1}^m \gamma_r(t, P, Q) \circ dW_r(t), \end{aligned} \quad (1)$$

where f , g , σ_r , and γ_r , $r = 1, \dots, m$, are n -dimensional column vectors, and $W_r(t)$, $r = 1, \dots, m$, are independent standard Wiener processes. There are functions $H(t, P, Q)$, $H_r(t, P, Q)$, $r = 1, \dots, m$, such that

$$\begin{aligned} f^i &= -\partial H / \partial q^i, g^i = \partial H / \partial p^i, \\ \sigma_r^i &= -\partial H_r / \partial q^i, \gamma_r^i = \partial H_r / \partial p^i (i = 1, \dots, n). \end{aligned} \quad (2)$$

Similar to deterministic Hamiltonian systems, the phase flow of SHS (1) preserves the symplectic structure characterized by

$$\left(\frac{\partial Y(t)}{\partial y_0} \right)^T J \left(\frac{\partial Y(t)}{\partial y_0} \right) = J, \forall t \geq 0, \text{ a.s.},$$

where $Y(t) = (P(t)^T Q(t)^T)^T$, $y_0 = (p^T q^T)^T$, $J = \begin{pmatrix} 0 & I_n \\ -I_n & 0 \end{pmatrix}$.

The exact solutions to SDEs are in general very difficult to obtain. Therefore numerical methods become important tools for simulating solutions to SDEs. In recent decades, there arose many studies regarding different aspects of numerical methods of SDEs^[6-8]. The study of numerical solutions for highly oscillatory problems is an important branch, to which many works were devoted, such as Refs. [9-12]. Standard numerical methods are usually not suitable for treating such problems because they require very small time step sizes and thus make the computations prohibitively expensive.

In this work we focus on the stochastic highly oscillatory problem with initial values $P(0) = p$, $Q(0) = q$,

$$\begin{aligned} dP &= (\epsilon^{-1} - f(P, Q))Qdt - \sigma Q \circ dW(t), \\ dQ &= (-\epsilon^{-1} + f(P, Q))Pdt + \sigma P \circ dW(t), \end{aligned} \quad (3)$$

where $\epsilon > 0$ is a small number, and f is a scalar function. It is called the highly oscillatory nonlinear Kubo oscillator with multiplicative noise^[10]. According to the integrability lemma^[13], it is not difficult to obtain that the oscillator (3) is a stochastic Hamiltonian system under the conditions

$$Pf_p^T = f_p P^T, Qf_q^T = f_q Q^T, Qf_p^T = Pf_q^T. \quad (4)$$

Our motivation is to employ the Lie algebraic approach to solve this class of highly oscillatory SHSs (3) with conditions (4), and we establish two numerical schemes for a concrete highly oscillatory SHS based on the Lie algebraic approach. Further, we analyze the symplecticity of the two schemes and prove that they nearly preserve the symplectic structure. Next we investigate their root mean-square convergence orders, efficiency, and superiority via numerical experiments.

1 The Lie algebraic approach

Let $(\Omega, \mathcal{F}, \{\mathcal{F}_t\}_{t \geq 0}, P)$ be a complete probability space with filtration $\{\mathcal{F}_t\}_{t \geq 0}$. Consider the SDE of Stratonovich sense under the probability space $(\Omega, \mathcal{F}, \{\mathcal{F}_t\}_{t \geq 0}, P)$, with initial value $S(0) = s_0$,

$$dS(t) = b(S(t))dt + \sum_{j=1}^r g_j(S(t)) \circ dW^j(t), \quad (5)$$

where b, g_j , $j = 1, \dots, r$, are d -dimensional \mathbb{C}^∞ functions and $W(t) = (W^1(t), \dots, W^r(t))$ is a m -dimensional standard Wiener process. Define the \mathbb{C}^∞ vector fields

$$X_0 = \sum_{i=1}^d b^i \partial_i, X_j = \sum_{i=1}^d g_j^i \partial_i (j = 1, \dots, r), \quad (6)$$

where $\partial_i = \partial / \partial S^i$. There is a representation theorem in Ref. [14] for the solution of SDE (5), which is the base of the Lie algebraic approach. To state the theorem, we first introduce some notations.

Given a multi-index $J = (j_1, \dots, j_m)$ and $[X, Y] = XY - YX$, X^J is defined as

$$X^J = [[\dots [X_{j_1}, X_{j_2}], \dots], X_{j_m}].$$

The divided index \hat{J} is a division of the multi-index J in the form

$$\hat{J} = (J_1, \dots, J_{k_1})(J_{k_1+1}, \dots, J_{k_2}) \cdots (J_{k_{l-1}+1}, \dots, J_{k_l}). \quad (7)$$

\hat{J} is called a single divided index when each $J_k (k = 1, \dots, k_l)$ contains a single element, and \hat{J} is a double divided index if each $J_k (k = 1, \dots, k_l)$ has either one element or two duplicated elements.

For a single divided index \hat{J} , the multiple Stratonovich integral $W^{\hat{J}}(t)$ is defined as

$$W^{\hat{J}}(t) := \int \cdots \int \circ dW^{j_1}(t_1) \cdots \circ dW^{j_m}(t_m), \quad (8)$$

where $W^0(t) = t$. For a double divided index \hat{J} ,

$$W^{\hat{J}}(t) := \int \cdots \int \circ dW^{j_1}(t_1) \cdots \circ dW^{j_{k_l}}(t_{k_l}), \quad (9)$$

where

$$W^{J_k}(t) = \begin{cases} W^{i_k}(t), & \text{if } J_k = \{i_k\}, \\ t, & \text{if } J_k = \{i_k, i_k\} \text{ and } i_k \neq 0, \\ 0, & \text{if } J_k = \{0, 0\}. \end{cases}$$

Lemma 1.1 Suppose that the Lie algebra $L = L(X_0, X_1, \dots, X_r)$ generated by X_0, X_1, \dots, X_r is nilpotent of step p . Then the solution $S(t)$ of (5) with $S(0) = s$ is represented as $S(t) = \exp(Y_t)(s)$, where $Y_t(\omega)$ is the vector field given by

$$Y_t = \sum_{i=0}^r W^i(t) X_i + \sum_{2 \leq |J| \leq p} \left\{ \sum_J^* c_J W^{\hat{J}}(t) \right\} X^J \quad (10)$$

almost surely for each t .

In (10), $|J|$ denotes the length of the multi-index J , and $\sum_{\hat{J}}^*$ is the sum taken over all single and double divided indices \hat{J} of J . Besides, the coefficients c_J are given by

$$c_{\hat{J}} = \frac{1}{m} \sum_{s=0}^{l-1} \sum_{*} \binom{l-1}{s} (-1)^{u_1 + \dots + u_{k_l} - s - 1} \times \frac{(u_1 + \dots + u_{k_l} - s)^{-1}}{n_1^{(1)}! \cdots n_1^{(u_1)}! \cdots n_{k_l}^{(1)}! \cdots n_{k_l}^{(u_{k_l})}!}, \quad (11)$$

where $n_k^{(v)} (k = 1, \dots, k_l, v = 1, \dots, u_k)$ denotes the v -th element of J_k , and u_k is the number of elements of J_k .

Given a time discretization $\{t_n\}$ of the interval $[0, T]$ with an equidistant step size h , i.e., $t_n = nh$, $n = 0, 1, \dots, N$. The Lie algebraic approach to construction of numerical methods follows the procedure^[2] as follows.

• Based on the representation of the solution of

the SDE (5), write the time discretization scheme $S_{n+1} = \exp(Y_{n,h})(S_n)$;

• After obtaining a truncated vector field $\hat{Y}_{n,h}$ by discarding the higher order terms, construct the truncated scheme $\hat{S}_{n+1} = \exp(\hat{Y}_{n,h})(\hat{S}_n)$;

• Split $\hat{Y}_{n,h}$ into $\hat{Y}_{n,h} = A_{n,h} + B_{n,h}$ where $\exp(A_{n,h})$ and $\exp(B_{n,h})$ can both be explicitly calculated. Then, use $\exp(A_{n,h}) \exp(B_{n,h})$ to approximate $\exp(\hat{Y}_{n,h})$ to get the numerical approximation $\tilde{S}_{n+1} = \exp(A_{n,h}) \exp(B_{n,h})(\tilde{S}_n)$, with $\tilde{S}_0 = s_0$.

2 The Lie algebraic methods for highly oscillatory SHSs

According to Refs. [2, 14], we write the coefficients $c_{\hat{J}}$ in (11) for $|J| = 2, 3$ explicitly. Furthermore, for convenience of calculations, we replace the multiple Stratonovich integrals in Y_t in (10) by their equivalent multiple Itô integrals. For SDE (5) with one single noise, we have

$$\begin{aligned} Y_t = & I_{(0)}(t) X_0 + I_{(1)}(t) X_1 + \\ & \frac{1}{2} (I_{(0,1)}(t) - I_{(1,0)}(t)) [X_0, X_1] + \\ & \frac{C_1}{18} [[X_0, X_1], X_0] + \frac{C_2}{18} [[X_0, X_1], X_1] + \\ & \frac{1}{36} \{ I_{(0,0)} + \{ I_{(0)}(t) \}^2 \} [[X_0, X_1], X_1] + \\ & \sum_{4 \leq |J|} H^J(t) X^J, \end{aligned} \quad (12)$$

where $H^J(t)$ is a version of $\sum_{\hat{J}}^* c_{\hat{J}} W^{\hat{J}}(t)$, $C_1 = 2I_{(0,1,0)} - 2I_{(1,0,0)} + I_{(0)}I_{(1,0)} - I_{(0)}I_{(0,1)}$ and $C_2 = 2I_{(0,1,1)} - 2I_{(1,0,1)} + I_{(1)}I_{(1,0)} - I_{(1)}I_{(0,1)}$.

Now let us consider the highly oscillatory SDE (3). Let $f(P, Q) = P^2 + Q^2$ and the dimension of the system $d = 2$, i.e.,

$$\begin{aligned} dP = & (\epsilon^{-1} - (P^2 + Q^2)) Q dt - \sigma Q \circ dW(t), \\ dQ = & (-\epsilon^{-1} + (P^2 + Q^2)) P dt + \sigma P \circ dW(t). \end{aligned} \quad (13)$$

According to the conditions (4), it is clear that (13) is an SHS, with Hamiltonian functions

$$H(P, Q) = \frac{-\epsilon^{-1}}{2} (P^2 + Q^2) + \frac{1}{4} (P^2 + Q^2)^2,$$

$$H_1(\mathbf{P}, \mathbf{Q}) = \frac{\sigma}{2}(\mathbf{P}^2 + \mathbf{Q}^2).$$

Therefore, (13) is a highly oscillatory SHS.

Performing the change of variable $s = t/\epsilon$ in (13), we get the equivalent system of (13)

$$\begin{aligned} d\mathbf{P} &= (1 - \epsilon(\mathbf{P}^2 + \mathbf{Q}^2))\mathbf{Q}ds - \sqrt{\epsilon}\sigma\mathbf{Q} \circ dW(s), \\ d\mathbf{Q} &= (-1 + \epsilon(\mathbf{P}^2 + \mathbf{Q}^2))\mathbf{P}ds + \sqrt{\epsilon}\sigma\mathbf{P} \circ dW(s). \end{aligned} \quad (14)$$

It is not difficult to see that (14) is also an SHS. Now we apply the Lie algebraic approach to system (14), for which

$$\begin{aligned} X_0 &= (1 - \epsilon(\mathbf{P}^2 + \mathbf{Q}^2))\mathbf{Q}\partial\mathbf{P} + \\ &\quad (-1 + \epsilon(\mathbf{P}^2 + \mathbf{Q}^2))\mathbf{P}\partial\mathbf{Q}, \end{aligned}$$

$$X_1 = -\sqrt{\epsilon}\sigma\mathbf{Q}\partial\mathbf{P} + \sqrt{\epsilon}\sigma\mathbf{P}\partial\mathbf{Q}.$$

We take the truncation $\hat{Y}_{n,h} = hX_0 + \Delta W_n X_1$, and let

$$\begin{aligned} A_{n,h} &= ((1 - \epsilon(\mathbf{P}^2 + \mathbf{Q}^2))\mathbf{Q}h - \sqrt{\epsilon}\sigma\mathbf{Q}\Delta W_n)\partial\mathbf{P}, \\ B_{n,h} &= ((-1 + \epsilon(\mathbf{P}^2 + \mathbf{Q}^2))\mathbf{P}h + \\ &\quad \sqrt{\epsilon}\sigma\mathbf{P}\Delta W_n)\partial\mathbf{Q}. \end{aligned}$$

For simplicity, we denote $F(p, q) = (1 - \epsilon(p^2 + q^2))h - \sqrt{\epsilon}\sigma\Delta W_n$. If we choose the operator splitting $\hat{Y}_{n,h} = A_{n,h} + B_{n,h}$, we get the scheme

$$\begin{aligned} P_{n+1} &= P_n + F(P_n, Q_{n+1}) \frac{\exp(-2\epsilon P_n Q_{n+1}h) - 1}{-2\epsilon P_n h}, \\ Q_{n+1} &= Q_n - F(P_n, Q_n) \frac{\exp(2\epsilon P_n Q_n h) - 1}{2\epsilon Q_n h}. \end{aligned} \quad (15)$$

If we choose the operator splitting $\hat{Y}_{n,h} = \frac{B_{n,h}}{2} + A_{n,h} + \frac{B_{n,h}}{2}$, we obtain the scheme

$$\begin{aligned} P_{n+1} &= P_n + F(P_n, \tilde{Q}_n) \frac{\exp(-2\epsilon P_n \tilde{Q}_n h) - 1}{-2\epsilon P_n h}, \\ Q_{n+1} &= \tilde{Q}_n - \frac{1}{2}F(P_{n+1}, \tilde{Q}_n) \frac{\exp(2\epsilon P_{n+1} \tilde{Q}_n h) - 1}{2\epsilon \tilde{Q}_n h}, \end{aligned} \quad (16)$$

where $\tilde{Q}_n = Q_n - \frac{1}{2}F(P_n, Q_n) \frac{\exp(2\epsilon P_n Q_n h) - 1}{2\epsilon Q_n h}$.

Theorem 2.1 The Lie algebraic schemes (15) and (16) for the highly oscillatory SHS (14) nearly preserve the symplectic structure with error of root mean-square order $3/2$, i.e.,

$$\left(\frac{\partial(P_{n+1}, Q_{n+1})}{\partial(P_n, Q_n)} \right)^T \mathbf{J} \left(\frac{\partial(P_{n+1}, Q_{n+1})}{\partial(P_n, Q_n)} \right) = (1 + R_s) \mathbf{J} \quad (17)$$

with $(E(R_s))^2)^{\frac{1}{2}} = O(h^{\frac{3}{2}})$.

Proof (17) holds if and only if

$$\frac{\partial P_{n+1}}{\partial P_n} \frac{\partial Q_{n+1}}{\partial Q_n} - \frac{\partial Q_{n+1}}{\partial P_n} \frac{\partial P_{n+1}}{\partial Q_n} = 1 + R_s \quad (18)$$

with $(E(R_s))^2)^{\frac{1}{2}} = O(h^{\frac{3}{2}})$.

For convenience, the left parts of (18) for the Lie algebraic schemes (15) and (16) are denoted by \bar{I}_1 and \bar{I}_2 , respectively. Then, according to (15) and (16), we have

$$\bar{I}_1 = 1 + \epsilon^{\frac{3}{2}}\sigma(3q_n^2 + p_n^2)h\Delta W_n + O(h^2),$$

$$\bar{I}_2 = 1 + \epsilon^{\frac{3}{2}}\sigma(2q_n^2 + \frac{5}{2}p_n^2)h\Delta W_n + O(h^2).$$

Due to $(E(\Delta W))^2)^{\frac{1}{2}} = h^{\frac{1}{2}}$, it is not difficult to get the conclusion. \square

3 Numerical experiments

In this section, we illustrate the performance of the Lie algebraic schemes via numerical tests. Throughout the section, the reference solution is computed by high-order schemes with a sufficiently small step size.

In Fig.1(a) we show the sample trajectories of the numerical solutions (15) (blue), (16) (yellow), and a trigonometric integrator in Ref. [11] (green) for the highly oscillatory SHS (13), with the initial values $p = 0$, $q = 1$ and the parameters $\epsilon = 0.01$, $\sigma = 0.3$, on $t \in [0, 1]$. The step size is $h = 2^{-5}$. The blue and yellow lines coincide visually with the red line which is the sample trajectory of the reference solution. Hereby we construct the two schemes (15) and (16) by involving the time-rescaling change of variable in our Lie algebraic methods, on the equivalent but time-rescaled system (14) of (13), and we apply the trigonometric method directly to (13) to draw the green line, with the same time step size $h = 2^{-5}$.

In Fig.1(b) is the sample trajectory of the Lie algebraic scheme (15) under a higher frequency parameter $\epsilon = 0.001$, which is also visually in good

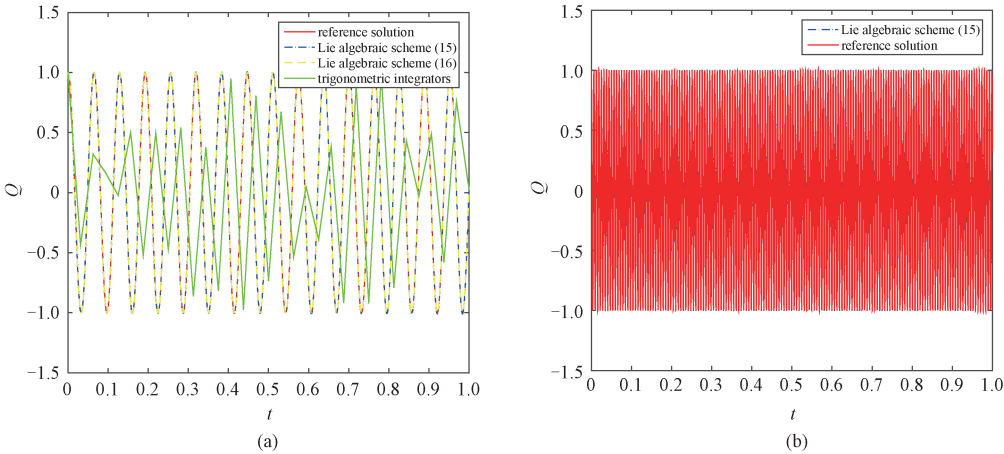


Fig.1 The sample trajectories

coincidence with the reference solution. The initial values are $p = 0$, $q = 1$. We take $\sigma = 0.3$ and the step size $h = 2^{-5}$.

In Fig.2(a) and Fig.2(b) we show the preservation of the invariant quantity $P(t)^2 + Q(t)^2 = p^2 + q^2$ of system (13)^[10] by the two Lie algebraic schemes.

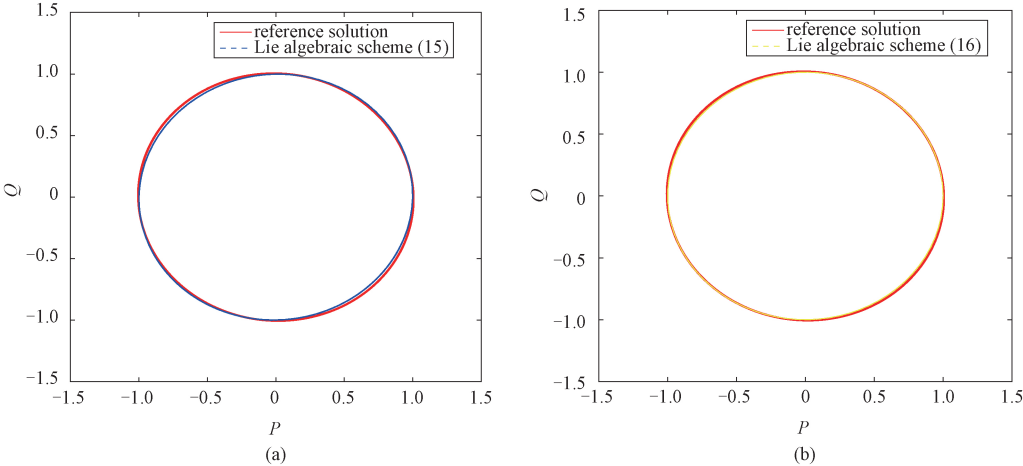


Fig.2 The phase trajectories

In Fig.2, the initial values $p = 0$, $q = 1$ and the parameters $\epsilon = 0.01$, $\sigma = 0.3$. The step size is $h = 2^{-5}$.

schemes (15) and (16) are both 1. Here we compute the error at $T = 1$ and take $p = 0$, $q = 1$, $\epsilon = 0.01$, $\sigma = 0.3$. Five hundred trajectories are sampled for approximating the expectation.

As shown in Fig. 3(a) and Fig. 3(b), the root mean-square convergence orders of the Lie algebraic

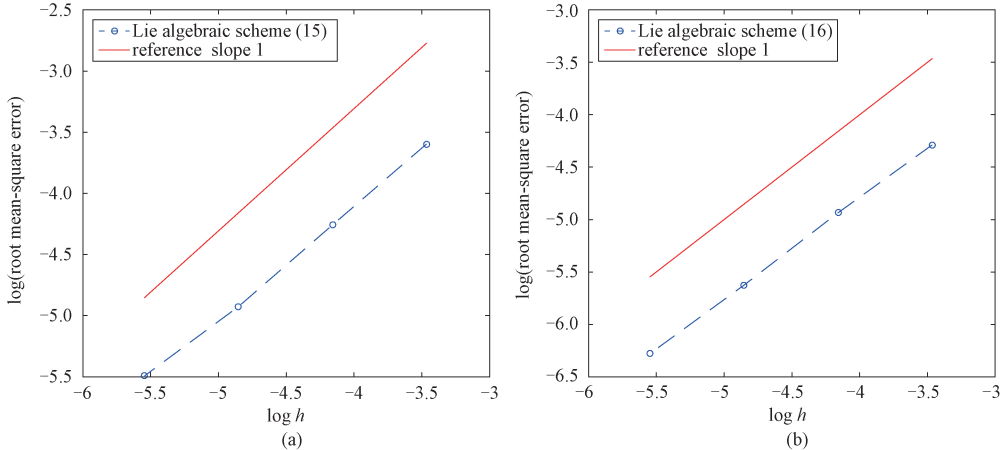


Fig.3 The convergence orders

References

- [1] Higham D J. An algorithmic introduction to numerical simulation of stochastic differential equations [J]. SIAM review, 2001, 43(3): 525-546.
- [2] Misawa T. A Lie algebraic approach to numerical integration of stochastic differential equations [J]. SIAM Journal on Scientific Computing, 2001, 23(3): 866-890.
- [3] Feng K, Qin M. Symplectic geometric algorithms for hamiltonian systems [M]. Berlin: Springer, 2010.
- [4] Milstein G N, Repin Y M, Tretyakov M V. Symplectic integration of Hamiltonian systems with additive noise [J]. SIAM Journal on Numerical Analysis, 2002, 39(6): 2 066-2 088.
- [5] Milstein G N, Repin Y M, Tretyakov M V. Numerical methods for stochastic systems preserving symplectic structure [J]. SIAM Journal on Numerical Analysis, 2002, 40(4): 1 583-1 604.
- [6] Kloeden P E, Platen E. Numerical solution of stochastic differential equations [M]. Springer-Verlag, 1992.
- [7] Milstein G N. Numerical integration of stochastic differential equations [M]. Springer Science & Business Media, 1994.
- [8] Milstein G N, Tretyakov M V. Stochastic numerics for mathematical physics [M]. Springer Science & Business Media, 2013.
- [9] Chartier P, Makazaga J, Murua A, et al. Multi-revolution composition methods for highly oscillatory differential equations [J]. Numerische Mathematik, 2014, 128(1): 167-192.
- [10] Vilmart G. Weak second order multirevolution composition methods for highly oscillatory stochastic differential equations with additive or multiplicative noise [J]. Siam Journal on Scientific Computing, 2015, 36(4): A1 770-A1 796.
- [11] Cohen D. On the numerical discretisation of stochastic oscillators [J]. Mathematics & Computers in Simulation, 2012, 82(8): 1 478-1 495.
- [12] Cohen D. Convergence analysis of trigonometric methods for stiff second-order stochastic differential equations [J]. Numerische Mathematik, 2012, 121(1): 1-29.
- [13] Hairer E, Lubich C, Wanner G. Geometric numerical integration: structure-preserving algorithms for ordinary differential equations [J]. Series in Computational Mathematics, 2006, 25(1): 805-882.
- [14] Kunita H. On the representation of solutions of stochastic differential equations [M]. Séminaire de Probabilités XIV 1978/79. Springer Berlin Heidelberg, 1980: 282-304.