Symplectic Numerical Schemes for Stochastic Systems Preserving Hamiltonian Functions

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Abstract. We present high-order symplectic schemes for stochastic Hamiltonian systems preserving Hamiltonian functions. The approach is based on the generating function method, and we show that for the stochastic Hamiltonian systems, the coefficients of the generating function are invariant under permutations. As a consequence, the high-order symplectic schemes have a simpler form than the explicit Taylor expansion schemes with the same order. Moreover, we demonstrate numerically that the symplectic schemes are effective for long time simulations.

Keywords: stochastic Hamiltonian systems, symplectic integration, mean-square convergence, high-order numerical schemes.

1 Introduction

We consider the autonomous stochastic differential equations (SDEs) in the sense of Stratonovich:

$$\begin{aligned} dP_i &= -\frac{\partial H^{(0)}(P,Q)}{\partial Q_i}dt - \sum_{r=1}^{m} \frac{\partial H^{(r)}(P,Q)}{\partial Q_i} \circ dw_t^r, \quad P(t_0) = p \\ dQ_i &= \frac{\partial H^{(0)}(P,Q)}{\partial P_i}dt + \sum_{r=1}^{m} \frac{\partial H^{(r)}(P,Q)}{\partial P_i} \circ dw_t^r, \quad Q(t_0) = q, \end{aligned} \tag{1}$$

where P, Q, p, q are n-dimensional vectors with the components P^i, Q^i, p^i, q^i, $i = 1, \ldots, n$, and $w_t^r, r = 1, \ldots, m$ are independent standard Wiener processes. The SDEs (1) are called the Stochastic Hamiltonian System (SHS) ([6]).

The stochastic flow $(p, q) \longrightarrow (P, Q)$ of the SHS (1) preserves the symplectic structure (Theorem 2.1 in [6]) as follows:

$$dP \wedge dQ = dp \wedge dq, \tag{2}$$

i.e. the sum over the oriented areas of its projections onto the two dimensional plane (p^i, q^i) is invariant. Here, we consider the differential 2-form

$$dp \wedge dq = dp^1 \wedge dq^1 + \cdots + dp^n \wedge dq^n, \tag{3}$$

I. Dimov, I. Faragó, and L. Vulkov (Eds.): NAA 2012, LNCS 8236, pp. 166–173, 2013.

and differentiation in (1) and (2) have different meanings: in (1) p, q are fixed parameters and differentiation is done with respect to time t, while in (2) differentiation is carried out with respect to the initial data p, q. We say that a method based on the one step approximation $\bar{P} = \bar{P}(t+h; t, p, q)$, $\bar{Q} = \bar{Q}(t+h; t, p, q)$ preserves symplectic structure if $d\bar{P} \wedge d\bar{Q} = dp \wedge dq$.

Milstein et al. [6] [7] introduced the symplectic numerical schemes for SHS, and they demonstrated the superiority of the symplectic methods for long time computation. Recently, Wang et al. [4],[8] proposed generating function methods to construct symplectic schemes for SHS. In the present study, we focus on SHS that preserve the Hamiltonian function (i.e. SHS for which $dH^{(r)} = 0$, $r = 0, \dots, m$). We propose higher order symplectic schemes that are computationally efficient for this special type of SHS .

2 The Generating Function Method and Symplectic Schemes

Similar with the deterministic case [3], we have the following result [4] relating the solutions of the Hamilton-Jacobi partial differential equation (HJ PDE) and the solutions of the SHS (1):

Theorem 1. *If $S^1_\omega(P, q)$ is a solution of the HJ PDE*

$$dS^1_\omega = H^{(0)}(P, q + \frac{\partial S^1_\omega}{\partial P})dt + \sum_{r=1}^{m} H^{(r)}(P, q + \frac{\partial S^1_\omega}{\partial P}) \circ dw^r_t, \quad S^1_\omega|_{t=t_0} = 0, \quad (4)$$

and if the matrix $(\frac{\partial^2 S_\omega}{\partial P_i \partial q_j})$ is invertible, then the map $(p, q) \to (P(t, \omega), Q(t, \omega))$ defined by

$$P = p - \frac{\partial S^1_\omega}{\partial q}(P, q), \quad Q = q + \frac{\partial S^1_\omega}{\partial P}(P, q), \quad (5)$$

is the flow of the SHS (1).

The key idea for deriving high order symplectic schemes via generating functions is to obtain an approximation of the solution of HJ PDE, and then to construct the symplectic numerical scheme through the relations (5). It is reasonable to assume that the generating function can be expressed by the following expansion locally [4]

$$S^1_\omega(P, q, t) = G_{(0)}(P, q)J_{(0)} + G_{(1)}(P, q)J_{(1)} + G_{(0,1)}(P, q)J_{(0,1)} + \cdots = \sum_{\alpha} G_\alpha J_\alpha, \quad (6)$$

where $\alpha = (j_1, j_2, \dots, j_l), j_i \in \{0, 1, \dots, m\}$, $i = 1, \dots, l$ is a multi-index of length $l(\alpha) = l$, and, with $dw^0_s := ds$, J_α is the multiple Stratonovich integral

$$J_\alpha = \int_0^t \int_0^{s_l} \dots \int_0^{s_2} \circ dw^{j_1}_{s_1} \cdots \circ dw^{j_{l-1}}_{s_{l-1}} \circ dw^{j_l}_{s_l}. \quad (7)$$

If the multi-index $\alpha = (j_1, j_2, \ldots, j_l)$ with $l > 1$, then $\alpha- = (j_1, j_2, \ldots, j_{l-1})$. For any two multi-indexes $\alpha = (j_1, j_2, \ldots, j_l)$ and $\alpha' = (j'_1, j'_2, \ldots, j'_{l'})$, we define the concatenation operation $'*'$ as $\alpha * \alpha' = (j_1, j_2, \ldots, j_l, j'_1, j'_2, \ldots, j'_{l'})$. The concatenation of a collection Λ of multi-indexes with the multi-index α gives the collection $\Lambda * \alpha = \{\alpha' * \alpha\}_{\alpha' \in \Lambda}$.

For any multi-index $\alpha = (j_1, j_2, \ldots, j_l)$ with no duplicated elements (i.e., $j_m \neq j_n$ if $m \neq n$, $1 \leq m, n \leq l$), we define the set $R(\alpha)$ to be the empty set $R(\alpha) = \Phi$ if $l = 1$ and $R(\alpha) = \{(j_m, j_n) | m < n, 1 \leq m, n \leq l\}$ if $l \geq 2$. $R(\alpha)$ defines a partial order on the set formed with the numbers included in the multi-index α, defined by $i \prec j$ if and only if $(i, j) \in R(\alpha)$. We suppose that there are no duplicated elements in or between the multi-indexes $\alpha = (j_1, j_2, \ldots, j_l)$ and $\alpha' = (j'_1, j'_2, \ldots, j'_{l'})$, and we define

$$\Lambda_{\alpha,\alpha'} = \{\beta \in \mathcal{M} | R(\alpha) \cup R(\alpha') \subseteq R(\beta) \text{ and } \beta \text{ has no duplicates}\} \tag{8}$$

where $\mathcal{M} = \{(\hat{j}_1, \hat{j}_2, \ldots, \hat{j}_{l+l'}) | \hat{j}_i \in \{j_1, j_2, \ldots, j_l, j'_1, j'_2, \ldots, j'_{l'}\}, i = 1, \ldots, l + l'\}$. Analogously if there are no duplicated elements in or between any of the multi-indexes $\alpha = (j_1^{(1)}, j_2^{(1)}, \ldots, j_{l_1}^{(1)})$, $\ldots$, $\alpha_n = (j_1^{(n)}, j_2^{(n)}, \ldots, j_{l_n}^{(n)})$, then we define

$$\Lambda_{\alpha_1,\ldots,\alpha_n} = \{\beta \in \mathcal{M} | \cup_{k=1}^{n} R(\alpha_k) \subseteq R(\beta) \text{ and } \beta \text{ has no duplicates}\}, \tag{9}$$

where $\mathcal{M} = \{(\hat{j}_1, \hat{j}_2, \ldots, \hat{j}_{\hat{l}}) | \hat{j}_i \in \{j_1^{(1)}, j_2^{(1)}, \ldots, j_{l_1}^{(1)}, \ldots j_1^{(n)}, j_2^{(n)}, \ldots, j_{l_n}^{(n)}\}, i = 1, \ldots, \hat{l}, \hat{l} = l_1 + \cdots + l_n\}$. For multi-indexes with duplicated elements, we extend the previous definitions by assigning a different subscript to each duplicated element, for example, $\Lambda_{(2,0),(0,1)} = \Lambda_{(2,0_1),(0_2,1)} = \{(2, 0_2, 1, 0_1), (0_2, 2, 1, 0_1), (0_2, 1, 2, 0_1), (0_2, 2, 0_1, 1), (2, 0_1, 0_2, 1), (2, 0_2, 0_1, 1)\} = \{(2, 0, 1, 0), (0, 2, 1, 0), (0, 1, 2, 0), (0, 2, 0, 1), (2, 0, 0, 1), (2, 0, 0, 1)\}$.

We can easily verify that $\Lambda_{\alpha,\alpha'} = \Lambda_{\alpha',\alpha}$, and the length of the multi indexes $\beta \in \Lambda_{\alpha,\alpha'}$, is $l(\beta) = l(\alpha) + l(\alpha')$.

It can be proved [2] that the multiplication of a finite sequence of multiple-indexes can be expressed by the following summation:

$$\prod_{i=1}^{n} J_{\alpha_i} = \sum_{\beta \in \Lambda_{\alpha_1,\ldots,\alpha_n}} J_\beta. \tag{10}$$

Inserting (6) into the HJ PDE (4), and using the previous equation, we get

$$\begin{aligned} S_\omega^1 &= \int_0^t H^{(0)}(P, q + \sum_\alpha \frac{\partial G_\alpha}{\partial P} J_\alpha) ds + \sum_{r=1}^{m} \int_0^t H^{(r)}(P, q + \sum_\alpha \frac{\partial G_\alpha}{\partial P} J_\alpha) \circ dw_s^r \\ &= \sum_{r=0}^{m} \sum_{i=0}^{\infty} \sum_{k_1,\ldots,k_i=1}^{n} \sum_{\alpha_1,\ldots,\alpha_i} \sum_{\beta \in \Lambda_{\alpha_1,\ldots\alpha_i}} \frac{1}{i!} \frac{\partial^i H^{(r)}}{\partial q_{k_1} \ldots \partial q_{k_i}} \frac{\partial G_{\alpha_1}}{\partial P_{k_1}} \cdots \frac{\partial G_{\alpha_i}}{\partial P_{k_i}} J_{\beta * (r)} \end{aligned} \tag{11}$$

where $(\sum_\alpha \frac{\partial G_{\alpha_i}}{\partial P})_{k_i}$ is the k_i-th component of the column vector $\sum_\alpha \frac{\partial G_{\alpha_i}}{\partial P}$. Equating the coefficients of J_α in (6) and (11), we obtain a recurrence formula for determining G_α.

If $\alpha = (r)$, $r = 0, \dots, m$ then $G_\alpha = H^{(r)}$. If $\alpha = (i_1, \dots, i_{l-1}, r)$, $l > 1$, $i_1, \dots, i_{l-1}, r = 0, \dots, m$ has no duplicates then

$$G_\alpha = \sum_{i=1}^{l(\alpha)-1} \frac{1}{i!} \sum_{k_1,\dots,k_i=1}^{n} \frac{\partial^i H^{(r)}}{\partial q_{k_1} \dots \partial q_{k_i}} \sum_{\substack{l(\alpha_1)+\dots+l(\alpha_i)=l(\alpha)-1 \\ \alpha- \in \Lambda_{\alpha_1,\dots,\alpha_i}}} \frac{\partial G_{\alpha_1}}{\partial P_{k_1}} \dots \frac{\partial G_{\alpha_i}}{\partial P_{k_i}}. \quad (12)$$

If the multi-index α contains any duplicates, then we apply formula (12) after we associate different subscripts to the repeating numbers.

In [2], we prove that the symplectic schemes based on truncations of S^1_ω for multi-indexes $\alpha \in \mathcal{A}_k = \{\alpha : l(\alpha) + n(\alpha) \leq 2k\}$ have mean square order k, for $k = 1, 1.5, 2$. Here $n(\alpha)$ is the number of components equal with 0 in the multi-index α. For example, using the following truncation of S^1_ω based on $\mathcal{A}_1$, we can get a scheme with mean square order 1:

$$S^1_\omega \approx G_{(0)} J_{(0)} + \sum_{r=1}^{m} \left(G_{(r)} J_{(r)} + G_{(r,r)} J_{(r,r)} \right) + \sum_{i,j=1, i \neq j}^{m} G_{(i,j)} J_{(i,j)}. \quad (13)$$

3 Symplectic Schemes for SHS Preserving the Hamiltonian Functions

Unlike the deterministic cases, in general the SHS (1) no longer preserves the Hamiltonian functions $H_i, i = 0, \dots, n$ with respect to time.

Proposition 1. *The Hamiltonian functions $H^{(i)}, i = 0, \dots, m$ are invariant for the flow of the system (1), if and only if $\{H^{(i)}, H^{(j)}\} = 0$ for $i, j = 0, \dots, m$, where the Poisson bracket is defined as $\{H^{(i)}, H^{(j)}\} = \sum_{k=1}^{n} (\frac{\partial H^{(j)}}{\partial Q_k} \frac{\partial H^{(i)}}{\partial P_k} - \frac{\partial H^{(i)}}{\partial Q_k} \frac{\partial H^{(j)}}{\partial P_k})$.*

Proof. By the chain rule of the Stratonovich stochastic integration, the Hamiltonian functions $H^{(i)}, i = 0, \dots, m$ are invariant for the system (1), if and only if for every $i = 0, \dots, m$

$$\begin{aligned} dH^{(i)} &= \sum_{k=1}^{n} (\frac{\partial H^{(i)}}{\partial P_k} dP_k + \frac{\partial H^{(i)}}{\partial Q_k} dQ_k) = \sum_{k=1}^{n} (-\frac{\partial H^{(i)}}{\partial P_k} \frac{\partial H^{(0)}}{\partial Q_k} \\ &+ \frac{\partial H^{(i)}}{\partial Q_k} \frac{\partial H^{(0)}}{\partial P_k}) dt + \sum_{r=1}^{m} \sum_{k=1}^{n} (-\frac{\partial H^{(i)}}{\partial P_k} \frac{\partial H^{(r)}}{\partial Q_k} + \frac{\partial H^{(i)}}{\partial Q_k} \frac{\partial H^{(r)}}{\partial P_k}) \circ dw^r_t = 0. \end{aligned} \quad (14)$$

For any permutation on $\{1, \dots, l\}$, $l \geq 1$ (i.e. for any bijective function $\pi : \{1, \dots, l\} \to \{1, \dots, l\}$), and for any multi-index $\alpha = (i_1, \dots, i_l)$ with $l(\alpha) = l$, let denote by $\pi(\alpha)$ the multi-index defined as $\pi(\alpha) := (i_{\pi(1)}, \dots, i_{\pi(l)})$. For systems preserving the Hamiltonian functions, the coefficients G_α of S^1_ω are invariant under the permutations on α, when $l(\alpha) = 2$ because for any $r_1, r_2 = 0, \dots, m$, we have

$$G_{(r_1,r_2)} = \sum_{k=1}^{n} \frac{\partial H^{(r_2)}}{\partial q_k} \frac{\partial H^{(r_1)}}{\partial P_k} = \sum_{k=1}^{n} \frac{\partial H^{(r_1)}}{\partial q_k} \frac{\partial H^{(r_2)}}{\partial P_k} = G_{(r_2,r_1)}. \tag{15}$$

A simple calculation verifies that G_α are invariant under the permutations on α when $l(\alpha) = 3$. By induction we can prove that this invariance also holds in the general case ([1]).

Proposition 2. *For SHS preserving the Hamiltonian functions, the coefficients G_α are invariants to permutations, i.e $G_\alpha = G_{\pi(\alpha)}$.*

The invariance under permutations of G_α makes higher order symplectic schemes computationally attractive for systems preserving the Hamiltonian functions. For example, for the system (1) with $m = 1$, since $J_{(0,1)} + J_{(1,0)} = J_{(1)}J_{(0)}$ and $J_{(0,1,1)} + J_{(1,0,1)} + J_{(1,1,0)} = J_{(1,1)}J_{(0)}$ (see (10)), we get the following generating function based on the set $\mathcal{A}_2$

$$\begin{aligned} S^1_\omega \approx\; & G_{(0)}h + G_{(1)}\sqrt{h}\xi_h + \frac{G_{(0,0)}}{2}h^2 + \frac{G_{(1,1)}}{2}h\xi_h^2 + G_{(1,0)}\xi_h h^{\frac{3}{2}} \\ & + \frac{G_{(1,1,1)}}{6}h^{\frac{3}{2}}\xi_h^3 + \frac{G_{(1,1,0)}}{2}\xi_h^2 h^2 + \frac{G_{(1,1,1,1)}}{24}h^2\xi_h^4. \end{aligned} \tag{16}$$

Here, we proceed as reported in [7] to construct an implicit scheme based on S^1_ω and ensuring it is well-defined. If the time step $h < 1$, then when simulating the stochastic integrals J_1, J_{11}, J_{110}, J_{111} and J_{1111}, we replace the random variable $\xi \sim N(0, 1)$ with the bounded random variable ξ_h:

$$\xi_h = \begin{cases} -A_h(2) & \text{if } \xi < -A_h(2) \\ \xi & \text{if } |\xi| \le A_h(2) \\ A_h(2) & \text{if } \xi > A_h(2), \end{cases} \tag{17}$$

where $A_h(2) = 2\sqrt{2|\ln h|}$. Using (5) and (16) we construct the following symplectic scheme:

$$\begin{aligned} P_i(k+1) = P_i(k) - \Bigg(& \frac{\partial G_{(0)}}{\partial Q_i}h + \frac{\partial G_{(1)}}{\partial Q_i}\sqrt{h}\xi_h + \frac{\partial G_{(0,0)}}{\partial Q_i}\frac{h^2}{2} + \frac{\partial G_{(1,1)}}{\partial Q_i}\frac{h\xi_h^2}{2} \\ & + 2\frac{\partial G_{(1,0)}}{\partial Q_i}\xi_h h^{\frac{3}{2}} + \frac{\partial G_{(1,1,1)}}{\partial Q_i}\frac{h^{\frac{3}{2}}\xi_h^3}{6} + \frac{\partial G_{(1,1,0)}}{\partial Q_i}\frac{3\xi_h^2 h^2}{2} + \frac{\partial G_{(1,1,1,1)}}{\partial Q_i}\frac{h^2\xi_h^4}{24}\Bigg) \\ Q_i(k+1) = Q_i(k) + \Bigg(& \frac{\partial G_{(0)}}{\partial P_i}h + \frac{\partial G_{(1)}}{\partial P_i}\sqrt{h}\xi_h + \frac{\partial G_{(0,0)}}{\partial P_i}\frac{h^2}{2} + \frac{\partial G_{(1,1)}}{\partial P_i}\frac{h\xi_h^2}{2} \\ & + 2\frac{\partial G_{(1,0)}}{\partial P_i}\xi_h h^{\frac{3}{2}} + \frac{\partial G_{(1,1,1)}}{\partial P_i}\frac{h^{\frac{3}{2}}\xi_h^3}{6} + \frac{\partial G_{(1,1,0)}}{\partial P_i}\frac{3\xi_h^2 h^2}{2} + \frac{\partial G_{(1,1,1,1)}}{\partial P_i}\frac{h^2\xi_h^4}{24}\Bigg), \end{aligned} \tag{18}$$

where everywhere the arguments are $(P(k+1), Q(k))$. From [7] we know that $E(\xi - \xi_h)^2 \le h^4$ and $0 \le E(\xi^2 - \xi_h^2) \le 7h^{7/2}$, so proceeding as in [2] we can prove that (18) is a mean square second-order scheme.

Based on (5) and the truncation (13) we can build the symplectic mean square first-order scheme:

$$
\begin{aligned}
P_i(k+1) &= P_i(k) - \left(\frac{\partial G_{(0)}}{\partial Q_i} h + \frac{\partial G_{(1)}}{\partial Q_i} \sqrt{h}\zeta_h + \frac{\partial G_{(1,1)}}{\partial Q_i} \frac{h\zeta_h^2}{2} \right) \\
Q_i(k+1) &= Q_i(k) + \left(\frac{\partial G_{(0)}}{\partial P_i} h + \frac{\partial G_{(1)}}{\partial P_i} \sqrt{h}\zeta_h + \frac{\partial G_{(1,1)}}{\partial P_i} \frac{h\zeta_h^2}{2} \right),
\end{aligned}
\tag{19}
$$

where everywhere the arguments are $(P(k+1), Q(k))$ and ζ_h is defined as in (17), but with $A_h(2)$ replaced by $A_h(1) = 2\sqrt{|\ln h|}$.

4 Numerical Simulations and Conclusions

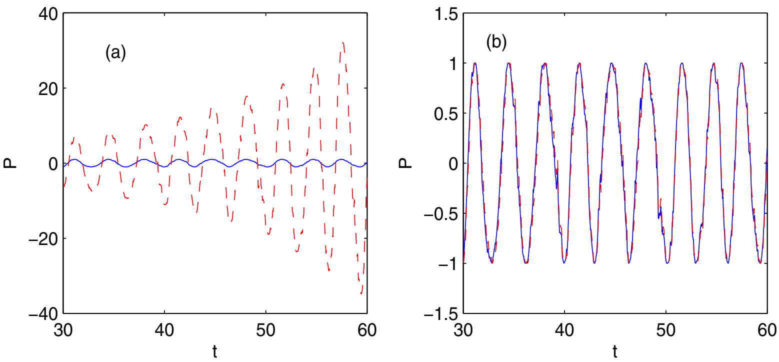

Fig. 1. Sample path for (20): (-) exact solution , (- -) numerical solution from (a) the explicit Milstein scheme and (b) the mean square second-order symplectic scheme

The mathematical model for the Kubo oscillator is given by

$$
\begin{aligned}
dP &= -aQdt - \sigma Q \circ dw_t^1, \quad P(0) = p_0, \\
dQ &= aPdt + \sigma P \circ dw_t^2, \quad Q(0) = q_0,
\end{aligned}
\tag{20}
$$

where a and σ are constants. This example has been studied in [7] to demonstrate the performance of the stochastic symplectic scheme for long time computation. The linear system with constant coefficients (20) can be solved analytically (see chapter 4 in [5]) , so we can easily simulate trajectories of the exact solution. The Hamiltonian functions are $H^{(0)}(P(t), Q(t)) = a\frac{P(t)^2+Q(t)^2}{2}$ and $H^{(1)}(P(t), Q(t)) = \sigma\frac{P(t)^2+Q(t)^2}{2}$, and it is easy to verify that they are preserved under the phase flow of the systems. As a consequence, the phase trajectory of (20) lies on the circle with the center at the origin and the radius $\sqrt{p_0^2 + q_0^2}$.

Replacing in (12), we obtain the following coefficients $G_\alpha(P,q)$ of $S^1_\omega(P,q)$:

$$G_{(0)} = \frac{a}{2}(P^2+q^2), \quad G_{(1)} = \frac{\sigma}{2}(P^2+q^2), \quad G_{(0,0)} = a^2Pq, \quad G_{(1,1)} = \sigma^2 Pq,$$
$$G_{(1,0)} = G_{(0,1)} = a\sigma Pq, \quad G_{(0,0,0)} = a^3(P^2+q^2), \quad G_{(1,1,1)} = \sigma^3(P^2+q^2),$$
$$G_{(1,1,0)} = G_{(1,0,1)} = G_{(0,1,1)} = a\sigma^2(P^2+q^2), \quad G_{(1,1,1,1)} = 5\sigma^4 Pq. \tag{21}$$

Here, we consider the mean square first-order scheme (19), and the mean square

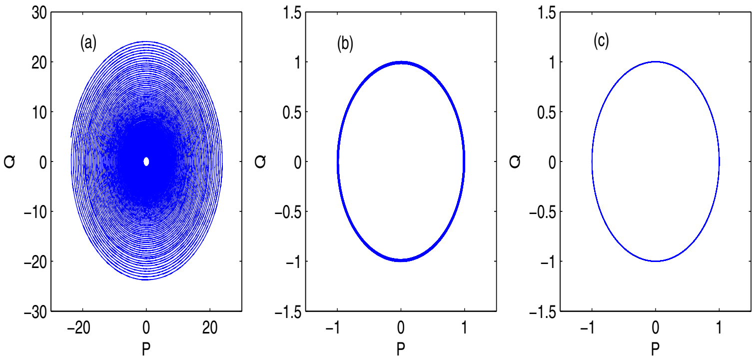

Fig. 2. A sample phase trajectory: (a) the Milstein scheme; (b) S^1_ω first-order scheme; (c) S^1_ω second-order scheme

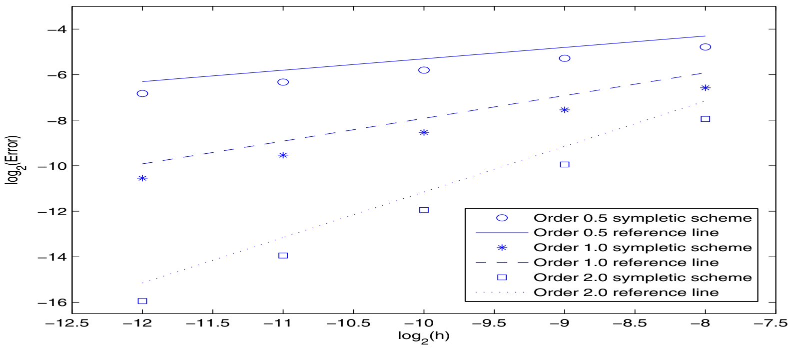

Fig. 3. Convergence rate of different order S^1_ω symplectic schemes

second-order scheme given in (18). Fig. 1 displays sample paths computed using the scheme (18) and the explicit mean square order one Milstein scheme ([5]) for $a = 2$, $\sigma = 0.3$, $p_0 = 1$ and $q_0 = 0$. Comparing with the exact solution we notice that the explicit scheme gives a divergent solution (see Fig. 1 a), while the symplectic scheme (18) produce accurate results (see Fig. 1 b).

Moreover, to validate the performance of symplectic schemes for long term simulations, in Fig. 2, we display sample phase trajectories of (20) computed using the explicit order one Milstein scheme given in [5] and the mean square order one and two symplectic schemes proposed in this paper. The time interval is $0 \leq T \leq 200$ and the time step $h = 2^{-8}$. It is clear that the phase trajectory of the Milstein non-symplectic scheme deviates from the circle $P(t)^2 + Q(t)^2 = 1$, while the proposed symplectic schemes produce accurate numerical solutions.

In [7], a mean square order 0.5 symplectic scheme is presented. Fig. 3 confirms the expected convergence rate for the symplectic schemes with the mean square orders 0.5, 1, 2, where the error is the maximum error of (P, Q) at $T = 100$.

4.1 Conclusions

We construct high-order symplectic schemes based on the generating functions for stochastic Hamiltonian systems preserving Hamiltonian functions. Since the coefficients of the generating function are invariant under permutations, the high-order implicit symplectic schemes have simpler forms and require less multiple stochastic integrals than the explicit Taylor expansion schemes. Based on the numerical simulations presented in this study, we conclude that the symplectic schemes are very effective for long term computations.

Acknowledgement. The authors are grateful for the support provided by the Natural Sciences and Engineering Research Council of Canada.

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