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WEAK SYMPLECTIC SCHEMES FOR STOCHASTIC HAMILTONIAN EQUATIONS*

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Abstract. We propose a systematic approach to construct symplectic schemes in the weak sense for stochastic Hamiltonian systems. This method is based on generating functions, so it is an extension of the techniques used for constructing high-order symplectic schemes for deterministic Hamiltonian systems. Although the developed symplectic schemes are implicit, they are comparable with the explicit weak Taylor schemes in terms of the number and the complexity of the multiple Itô stochastic integrals required. We study the convergence of the proposed symplectic weak order 2 schemes. The excellent long term performance of the symplectic schemes is verified numerically.

Key words. stochastic Hamiltonian systems, symplectic integration, numerical scheme in weak sense

AMS subject classifications. 65C30, 65P10, 60H10

1. Introduction.

Consider the stochastic differential equations in the sense of Stratonovich:

$$
\begin{aligned}
dP_i &= -\frac{\partial H_0}{\partial Q_i}(P,Q)dt - \sum_{r=1}^{d} \frac{\partial H_r}{\partial Q_i}(P,Q)\circ dw_t^r, \quad P(t_0)=p,\\
dQ_i &= \frac{\partial H_0}{\partial P_i}(P,Q)dt + \sum_{r=1}^{d} \frac{\partial H_r}{\partial P_i}(P,Q)\circ dw_t^r, \qquad Q(t_0)=q,
\end{aligned}
\tag{1.1}
$$

where $P=(P_1,\dots,P_n)^T$, $Q=(Q_1,\dots,Q_n)^T$, p, q are n-dimensional column vectors, and w_t^r, $r=1,\dots,d$, are independent standard Wiener processes for $t\in[t_0,t_0+T]$. We denote the solution of the stochastic Hamiltonian system (SHS) (1.1) by

$$X_{t_0,x}(t,\omega)=\left(P_{t_0,p}^T(t,\omega),Q_{t_0,q}^T(t,\omega)\right)^T,$$

where $t_0\le t\le t_0+T$, and ω is an elementary random event. It is known that if H_r, $r=0,\dots,d$, are sufficiently smooth, then $X_{t_0,x}(t,\omega)$ is a phase flow (diffeomorphism) for almost any ω [12]. To simplify the notation, we will remove any reference to the dependence on ω unless it is absolutely necessary to avoid confusion.

The equations (1.1) represent an autonomous SHS. A non-autonomous SHS is given by time-dependent Hamiltonian functions $H_r(t,P,Q)$, $r=0,\dots,d$. However, it can be rewritten as an autonomous SHS by introducing new variables e and f. Indeed, if we let $df_r = dt$ and $de_r=-\frac{\partial H_r(t,P,Q)}{\partial t}\circ dw_t^r$, where $dw_t^0 := dt$, with the initial condition $e_r(t_0)=-H_r(t_0,p,q)$ and $f_r(t_0)=t_0$, $r=0,\dots,d$, then the new Hamiltonian functions $\bar H_r(\bar P,\bar Q)=H_r(f_r,P,Q)$, $r=1,\dots,d$, and $\bar H_0(\bar P,\bar Q)=H_0(f_0,P,Q)+e_0+\dots+e_d$, define an autonomous SHS with $\bar P=(P^T,e_0,\dots,e_d)^T$ and $\bar Q=(Q^T,f_0,\dots,f_d)^T$. Hence, in this paper we will only investigate the autonomous case as given in (1.1)

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The stochastic flow $(p, q) \longrightarrow (P, Q)$ of the SHS (1.1) preserves the symplectic structure [16, Theorem 2.1] as follows:

$$dP \wedge dQ = dp \wedge dq, \tag{1.2}$$

i.e., the sum of the oriented areas of projections of a two-dimensional surface onto the coordinate planes (p_i, q_i), $i = 1, \ldots, n$, is invariant. Here, we consider the differential 2-form

$$dp \wedge dq = dp_1 \wedge dq_1 + \cdots + dp_n \wedge dq_n,$$

and differentiation in (1.1) and (1.2) have different meanings: in (1.1), p and q are fixed parameters and differentiation is done with respect to time t, while in (1.2) 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 the symplectic structure [16] if

$$d\bar{P} \wedge d\bar{Q} = dp \wedge dq.$$

If the approximation $\bar{X}_0 = x$, $\bar{X}_k = (\bar{P}(k), \bar{Q}(k))$, $k = 1, 2, \ldots,$ of the solution $X_{t_0,x}(t_k, \omega) = (P_{t_0,p}(t_k, \omega), Q_{t_0,q}(t_k, \omega))$, satisfies

$$|E[F(\bar{X}_k(\omega))] - E[F(X_{t_0,x}(t_k, \omega)]| \le K h^m, \tag{1.3}$$

for F from a sufficiently large class of functions, where $t_k = t_0 + kh \in [t_0, t_0 + T]$, h is the time step, and the constant K does not depend on k and h, then we say that $\bar{X}_k$ approximate the solution $X_{t_0,x}(t_k)$ of (1.1) in the weak sense with a weak order of accuracy m [17] .

Milstein et al. [15, 16] introduced symplectic numerical schemes for SHSs, and they demonstrated the mean-square convergence and the superiority of these symplectic methods for long-time computations. In [17] they also presented a weak first-order symplectic scheme for the system (1.1). Several symplectic schemes with weak orders 2 or 3 are proposed for special types of SHS (such as SHSs with additive noise or SHSs with separable Hamiltonians), but it is concluded that further investigation is needed to obtain higher-order symplectic schemes for the general SHS (1.1) with multiplicative noise; see Remark 4.2 in [17]. Our work presented here makes a contribution to the open problems proposed by Milstein et al. Our approach is a non-trivial extension of the methods based on generating functions from deterministic Hamiltonian systems [8, Chapter 4] to SHSs.

The generating function method in the stochastic case was introduced in [18], and it was applied to obtain symplectic schemes in [9, 10], but only the symplectic schemes with mean square orders up to $3/2$ were constructed because of the requirement of high complexity to determine the coefficients of the generating function. In [13] some low-stage stochastic symplectic Runge-Kutta methods with strong global order 1.0 are constructed. Low-rank Runge-Kutta methods that perform well in terms of the stationary distribution function and the evolution of the mean of the underlying Hamiltonian are reported in [6]. Stochastic variational integrators have been introduced in [5, 19], and it is interesting to note that the variational integrators can be used to construct some of the symplectic schemes proposed in [15, 16]. Weak second-order integrators preserving quadratic invariants were constructed in [1] based on modified equations.

In [7] we obtain general recursive formulas for the coefficients of the generating functions, and these results are used to develop symplectic schemes in the strong sense. In [2] we take advantage of the special properties of the stochastic Hamiltonian systems preserving

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the Hamiltonian functions to propose computationally efficient symplectic schemes. In this paper we propose a systematic approach to construct symplectic schemes in the weak sense.

Similar to the deterministic case, the interest on symplectic schemes for SHSs is motivated by the fact that unlike usual numerical schemes, symplectic integrators allow us to simulate Hamiltonian systems on very long time intervals with high accuracy. For example, in [3] we apply an expansion of the global error to explain theoretically the better performance of a weak first-order symplectic scheme proposed in [17], compared to the Euler method (which is also a weak order 1 method). Here we construct a weak second-order symplectic scheme for the general SHS (1.1), and we illustrate numerically that it gives more accurate results for long-time simulations than the Runge-Kutta weak second-order method; see [11, Chapter 15.1].

Preliminary results regarding the generating function method for SHS are reported in Section 2. Section 3 presents the construction of the symplectic schemes. In Section 4, we prove the convergence of the weak second-order schemes. The numerical simulations presented in Section 5 demonstrate the excellent long-term accuracy of the proposed schemes.

2. The generating functions. In this section, we present preliminary results regarding the generating function method for SHS [7, 18]. These results will be used in Section 3 to construct the weak symplectic schemes.

The generating functions associated with the SHS (1.1) were rigorously introduced in [4, Theorem 6.14] as the solutions of the associated Hamilton-Jacobi partial differential equations (HJ PDE); see also [12, Theorem 6.1.5]. Under appropriate conditions, we obtain the following results [7, Theorem 3.1]:

1. If $S^1_\omega(P,q,t)$ is a smooth solution of the HJ PDE written formally as

$$dS^1_\omega = H_0\left(P, q + \nabla_P S^1_\omega\right)dt + \sum_{r=1}^{d} H_r\left(P, q + \nabla_P S^1_\omega\right) \circ dw^r_t, \quad S^1_\omega|_{t=t_0} = 0, \tag{2.1}$$

and there exists a stopping time $\tau_1 > t_0$ a.s. such that the matrix $\partial(P^T q + S^1_\omega)/\partial P \partial q$ is a.s. invertible for $t_0 \le t < \tau_1$, then the map $(p,q) \to (P(t,\omega), Q(t,\omega))$, $t_0 \le t < \tau_1$, defined by

$$p_i = P_i + \frac{\partial S^1_\omega}{\partial q_i}(P,q), \quad Q_i = q_i + \frac{\partial S^1_\omega}{\partial P_i}(P,q), \quad i = 1,\ldots,n, \tag{2.2}$$

is the flow of the SHS (1.1).

2. If $S^2_\omega(Q,p,t)$ is a smooth solution of the HJ PDE written formally as

$$dS^2_\omega = H_0\left(p + \nabla_Q S^2_\omega, Q\right)dt + \sum_{r=1}^{d} H_r\left(p + \nabla_Q S^2_\omega, Q\right) \circ dw^r_t, \quad S^2_\omega|_{t=t_0} = 0, \tag{2.3}$$

and there exists a stopping time $\tau_2 > t_0$ a.s. such that the matrix $\partial(p^T Q + S^2_\omega)/\partial p \partial Q$ is a.s. invertible for $t_0 \le t < \tau_2$, then the map $(p,q) \to (P(t,\omega), Q(t,\omega))$, $t_0 \le t < \tau_2$, defined by

$$q_i = Q_i + \frac{\partial S^2_\omega}{\partial p_i}(p,Q), \quad P_i = p_i + \frac{\partial S^2_\omega}{\partial Q_i}(p,Q), \quad i = 1,\ldots,n, \tag{2.4}$$

is the flow of the SHS (1.1).

3. If $S^3_\omega(z)$, $z \in \mathbb{R}^{2n}$, is a smooth solution of the HJ PDE written formally as

$$dS^3_\omega = H_0(z + \frac{1}{2}J^{-1}\nabla S^3_\omega)dt + \sum_{r=1}^{d} H_r(z + \frac{1}{2}J^{-1}\nabla S^3_\omega) \circ dw^r_t, \quad S^3_\omega|_{t=t_0} = 0, \tag{2.5}$$

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where

$$J = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix},$$

with I the n-dimensional identity matrix, and there exists a stopping time $\tau_3 > t_0$ a.s. such that the matrix $\partial((P+p)^T(Q-q) - 2S^3_\omega(y+Y)/2)/\partial Y \partial y$, where $Y = (P^T, Q^T)^T$ and $y = (p^T, q^T)^T$, is a.s. invertible for $t_0 \le t < \tau_3$, then the map $y \to Y(t,\omega)$, $t_0 \le t < \tau_3$, defined by

$$Y = y - J\nabla S^3_\omega((y+Y)/2), \tag{2.6}$$

is the flow of the SHS (1.1).

The key idea to construct high-order symplectic schemes via generating functions [18] is to obtain approximations of the solutions of the HJ PDE (2.1), (2.3), or (2.5) and then to derive the symplectic numerical scheme through the relations (2.2), (2.4), or (2.6). As in [7] we assume that the generating function $S^i_\omega(P,q,t)$, $i = 1,2,3$, can be expressed locally by the following expansion:

$$S^i_\omega(P,q,t) = \sum_\alpha G^i_\alpha J_{\alpha;t_0,t}, \tag{2.7}$$

where $\alpha = (j_1, j_2, \ldots, j_l)$, $j_i \in \{0,\ldots,d\}$ is a multi-index of length $l(\alpha) = l$, and $J_{\alpha;t_0,t}$ is the multiple Stratonovich integral

$$J_{\alpha;t_0,t} = \int_{t_0}^t \int_{t_0}^{s_l} \ldots \int_{t_0}^{s_2} \circ dw^{j_1}_{s_1} \cdots \circ dw^{j_{l-1}}_{s_{l-1}} \circ dw^{j_l}_{s_l}. \tag{2.8}$$

For convenience, ds is denoted by dw^0_s, and we shall write $J_{\alpha;t_1,t_2}$ as J_α whenever the values of the time indices are obvious. In [7] we have derived a general formula for the coefficients G^i_α of the generating function S^i_ω, $i = 1,2,3$.

First, consider the case when the multi-index $\alpha = (j_1, j_2, \ldots, j_l)$ has no repeated elements (i.e., $j_m \ne j_n$ if $m \ne n$, $m,n = 1,\ldots,l$), and define the set $R(\alpha)$ to be the empty set, $R(\alpha) = \emptyset$, if $l = 1$, and $R(\alpha) = \{(j_m, j_n) | m < n, m,n = 1,\ldots,l\}$ if $l \ge 2$.

A general formula for the coefficients G^1_α of the generating function S^1_ω can be obtained by replacing the expansion (2.7) in (2.1) and is given by the following recurrence from [7]. If $\alpha = (j_1)$, $j_1 = 0,\ldots,d$, then $G^1_\alpha = H_{j_1}$. If $l(\alpha) = l > 1$, then

$$G^1_\alpha = \sum_{i=1}^{l(\alpha)-1} \frac{1}{i!} \sum_{k_1,\ldots,k_i=1}^{n} \frac{\partial^i H_{j_l}}{\partial q_{k_1}\ldots\partial q_{k_i}} \sum_{\substack{l(\alpha_1)+\cdots+l(\alpha_i)=l(\alpha)-1 \\ R(\alpha_1)\cup\cdots\cup R(\alpha_i)\subseteq R(\alpha-)}} \frac{\partial G^1_{\alpha_1}}{\partial P_{k_1}} \cdots \frac{\partial G^1_{\alpha_i}}{\partial P_{k_i}}, \tag{2.9}$$

where $\alpha- = (j_1, j_2, \ldots, j_{l-1})$ and the arguments are (P,q) everywhere. For example, for any $j = 0,\ldots,d$ and any $r = 1,\ldots,d$ we get:

$$G^1_{(j)} = H_j, \quad G^1_{(0,r)} = \sum_{k=1}^n \frac{\partial H_r}{\partial q_k}\frac{\partial H_0}{\partial P_k}, \quad G^1_{(r,0)} = \sum_{k=1}^n \frac{\partial H_0}{\partial q_k}\frac{\partial H_r}{\partial P_k},$$

where the arguments are (P,q) everywhere.

The coefficients of the generating function S^2_ω are obtained by replacing q by p and P by Q in the recurrence (2.9). A general formula for the coefficients G^3_α of the generating function S^3_ω is obtained using (2.5) and is given by the following recurrence [7]. If $\alpha = (j_1)$, $j_1 = 0, \ldots, d$, then $G^3_\alpha = H_{j_1}$. If $\alpha = (j_1, \ldots, j_{l-1}, j_l)$, $j_1, \ldots, j_l = 0, \ldots, d$ and $l > 1$, then

$$G^3_\alpha = \sum_{i=1}^{l(\alpha)-1} \frac{1}{i!} \sum_{k_1,\ldots,k_i=1}^{2n} \frac{\partial^i H_{j_l}}{\partial y_{k_1} \ldots \partial y_{k_i}} \cdot \sum_{\substack{l(\alpha_1)+\cdots+l(\alpha_i)=l(\alpha)-1 \\ R(\alpha_1)\cup\cdots\cup R(\alpha_i)\subseteq R(\alpha-)}} (\frac{1}{2} J^{-1}\nabla G^3_{\alpha_1})_{k_1} \ldots (\frac{1}{2} J^{-1}\nabla G^3_{\alpha_i})_{k_i}, \tag{2.10}$$

where $(J^{-1}\nabla G^3_{\alpha_i})_{k_i}$ is the k_i-th component of the column vector $J^{-1}\nabla G^3_{\alpha_i}$, $y = (p^T, q^T)^T$, $Y = (P^T, Q^T)^T$, and the arguments are $(Y+y)/2$ everywhere. For example, in the SHS (1.1) for S^3_ω we get

$$G^3_{(j)} = H_j, \quad G^3_{(r,0)} = \frac{1}{2}(\nabla H_0)^T J^{-1} \nabla H_r, \quad G^3_{(0,r)} = \frac{1}{2}(\nabla H_r)^T J^{-1} \nabla H_0, \tag{2.11}$$

for any $j = 0, \ldots, d$ and any $r = 1, \ldots, d$, where the arguments are $(Y + y)/2$ everywhere.

If the multi-index α contains any repeated components, then we first form a new multi-index α' without any duplicates by associating different subscripts to the repeating numbers (e.g., if $\alpha = (1, 0, 0, 1, 2, 1)$ then $\alpha' = (1_1, 0_1, 0_2, 1_2, 2, 1_3)$). Secondly, we apply (2.9) and (2.10) to find $G^1_{\alpha'}$ and $G^3_{\alpha'}$, respectively. Finally the formulas for G^1_α and G^3_α are derived by deleting the subscripts introduced for defining the multi-index α' from the formulas for $G^1_{\alpha'}$ and $G^3_{\alpha'}$ and by making any eventual simplifications.

For example, for $G^1_{(0,0,0)}$ we get

$$\begin{aligned} G^1_{(0,0,0)} &= G^1_{(0_1,0_2,0_3)} \\ &= \sum_{k_1=1}^{n} \frac{\partial H_{0_3}}{\partial q_{k_1}} \frac{\partial G^1_{(0_1,0_2)}}{\partial P_{k_1}} + \sum_{k_1,k_2=1}^{n} \frac{1}{2!} \frac{\partial^2 H_{0_3}}{\partial q_{k_1} \partial q_{k_2}} \left(\frac{\partial G^1_{(0_1)}}{\partial P_{k_1}} \frac{\partial G^1_{(0_2)}}{\partial P_{k_2}} + \frac{\partial G^1_{(0_2)}}{\partial P_{k_1}} \frac{\partial G^1_{(0_1)}}{\partial P_{k_2}} \right) \\ &= \sum_{k_1=1}^{n} \frac{\partial H_0}{\partial q_{k_1}} \frac{\partial G^1_{(0,0)}}{\partial P_{k_1}} + \sum_{k_1,k_2=1}^{n} \frac{\partial^2 H_0}{\partial q_{k_1} \partial q_{k_2}} \frac{\partial G^1_{(0)}}{\partial P_{k_1}} \frac{\partial G^1_{(0)}}{\partial P_{k_2}}. \end{aligned}$$

Using

$$G^1_{(0,0)} = G^1_{(0_1,0_2)} = \sum_{k=1}^{n} \frac{\partial H_{0_2}}{\partial q_k} \frac{\partial H_{0_1}}{\partial P_k} = \sum_{k=1}^{n} \frac{\partial H_0}{\partial q_k} \frac{\partial H_0}{\partial P_k},$$

we have

$$\begin{aligned} G^1_{(0,0,0)} = \sum_{k_1,k_2=1}^{n} \Bigg(& \frac{\partial^2 H_0}{\partial q_{k_1} \partial q_{k_2}} \frac{\partial H_0}{\partial P_{k_1}} \frac{\partial H_0}{\partial P_{k_2}} + \frac{\partial H_0}{\partial q_{k_1}} \frac{\partial H_0}{\partial P_{k_2}} \frac{\partial^2 H_0}{\partial q_{k_2} \partial P_{k_1}} \\ & + \frac{\partial H_0}{\partial q_{k_1}} \frac{\partial H_0}{\partial q_{k_2}} \frac{\partial^2 H_0}{\partial P_{k_1} \partial P_{k_2}} \Bigg), \end{aligned}$$

where again the arguments are (P, q) everywhere. Similarly, to find the coefficient $G^3_{(r,r)}$,

$r = 0, \dots, d$, of S^3_ω we use (2.10) and the first equation in (2.11), and thus we have

$$
\begin{aligned}
G^3_{(r,r)} &= G^3_{(r_1,r_2)} = \sum_{k=1}^{2n} \frac{\partial H_{r_2}}{\partial y_k}(\frac{1}{2}J^{-1}\nabla G^3_{r_1})_k = \sum_{k=1}^{2n} \frac{\partial H_r}{\partial y_k}(\frac{1}{2}J^{-1}\nabla G^3_r)_k \\
&= \frac{1}{2}\sum_{k=1}^{n}\left(-\frac{\partial H_r}{\partial y_k}\frac{\partial H_r}{\partial y_{k+n}} + \frac{\partial H_r}{\partial y_{k+n}}\frac{\partial H_r}{\partial y_k}\right) = 0,
\end{aligned}
\tag{2.12}
$$

where the arguments are $(Y+y)/2$ everywhere.

3. The weak symplectic schemes. In this section, we present a method to generate symplectic numerical schemes in the weak sense for the SHS (1.1).

From (2.34) and [11, Chapter 5], we have the following relationship between the Itô integrals

$$
I_\alpha[f(\cdot,\cdot)]_{t_0,t} = \int_{t_0}^{t}\int_{t_0}^{s_l}\cdots\int_{t_0}^{s_2} f(s_1,\cdot)dw^{j_1}_{s_1}\dots dw^{j_{l-1}}_{s_{l-1}}dw^{j_l}_{s_l}, \quad I_\alpha = I_\alpha[1]_{t_0,t},
$$

and the Stratonovich integrals J_α defined in (2.8): $I_\alpha = J_\alpha$ for $l(\alpha) = 1$ and

$$
J_\alpha = I_{(j_l)}\left[J_{\alpha-}\right] + \chi_{\{j_l = j_{l-1} \neq 0\}} I_{(0)}\left[\frac{1}{2}J_{(\alpha-)-}\right] \qquad \text{for } l(\alpha) \geq 2,
\tag{3.1}
$$

where $\alpha = (j_1, j_2, \dots, j_l)$, $j_i \in \{0, 1, \dots, d\}$, χ_A denotes the indicator function of the set A, and f is any appropriate process [11, Chapter 5].

Thus, in (3.1) we get $J_{(0)} = I_{(0)}$, $J_{(i)} = I_{(i)}$, $J_{(0,0)} = I_{(0,0)}$, $J_{(0,i)} = I_{(0,i)}$, $J_{(i,0)} = I_{(i,0)}$, $J_{(i,0,j)} = I_{(i,0,j)}$, $J_{(i,0,i)} = I_{(i,0,i)}$, $J_{(i,j)} = I_{(i,j)}$, $J_{(i,0,0)} = I_{(i,0,0)}$, $J_{(0,i,0)} = I_{(0,i,0)}$, $J_{(0,0,i)} = I_{(0,0,i)}$, $J_{(i,j,i)} = I_{(i,j,i)}$

$$
\begin{aligned}
J_{(i,i)} &= I_{(i,i)} + \frac{1}{2}I_{(0)}, & J_{(i,i,j)} &= I_{(i,i,j)} + \frac{1}{2}I_{(0,j)}\\
J_{(j,i,i)} &= I_{(j,i,i)} + \frac{1}{2}I_{(j,0)}, & J_{(i,i,0)} &= I_{(i,i,0)} + \frac{1}{2}I_{(0,0)},\\
J_{(0,i,i)} &= I_{(0,i,i)} + \frac{1}{2}I_{(0,0)}, & J_{(i,i,i)} &= I_{(i,i,i)} + \frac{1}{2}\left(I_{(0,i)} + I_{(i,0)}\right)\\
J_{(i,i,j,j)} &= I_{(i,i,j,j)} + \frac{1}{2}\left(I_{(0,j,j)} + I_{(i,i,0)}\right) + \frac{1}{4}I_{(0,0)}, \\
J_{(i,i,i,i)} &= I_{(i,i,i,i)} + \frac{1}{2}\left(I_{(0,i,i)} + I_{(i,0,i)} + I_{(i,i,0)}\right) + \frac{1}{4}I_{(0,0)},
\end{aligned}
\tag{3.2}
$$

for any $i \neq j$, $i, j = 1, \dots, d$.

To obtain a weak first-order scheme, in (2.7) we replace the Stratonovich integrals by Itô integrals according to (3.1), and we truncate the series to include only Itô integrals with multi-indices α with $l(\alpha) \leq 1$. Using $J_{(r)} = I_{(r)}$, $r = 0, \dots, d$, and the first equation in (3.2), we get the following approximations for the generating functions S^i_ω, $i = 1, 2, 3$:

$$
S^i_\omega \approx \left(G^i_{(0)} + \frac{1}{2}\sum_{k=1}^{d} G^i_{(k,k)}\right) I_{(0)} + \sum_{k=1}^{d} G^i_{(k)} I_{(k)},
$$

where the arguments are (P, q) if $i = 1$, (p, Q) if $i = 2$, or $(Y + y)/2$ if $i = 3$. If h is the time step, then $I_0 = h$ and for a scheme of weak order 1 we can replace the Gaussian

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increments $I_{(k)}$ by the two-point distributed mutually independent random variables $\sqrt{h}\varsigma_k$ with $P(\varsigma_k = \pm 1) = 1/2$, $k = 1, \ldots, d$; see [11, Chapter 14.1].

REMARK 3.1. The symplectic weak order 1 scheme with $\alpha = \beta = 1$ presented in [17] is obtained if we replace S^1_ω in (2.2) by the previous approximation. Since from (2.12) we know that $G^3_{(k,k)} = 0$, $k = 0, \ldots, d$, we can obtain the symplectic weak order 1 scheme in [17] with $\alpha = \beta = 1/2$ using the previous approximation of S^3_ω and (2.6).

3.1. The symplectic weak second-order schemes. Similarly, to obtain a weak second-order scheme, we replace the Stratonovich integrals J_α in (2.7) by Itô integrals using (3.1), and we truncate the series to include only Itô integrals corresponding to multi-indices α such that $l(\alpha) \leq 2$. Thus, from (3.2) we can easily verify the following approximations for the generating functions S^i_ω, $i = 1, 2, 3$:

$$\begin{aligned} S^i_\omega \approx & \left(G^i_{(0)} + \frac{1}{2}\sum_{k=1}^d G^i_{(k,k)} \right) I_{(0)} + \sum_{k=1}^d G^i_{(k)} I_{(k)} \\ & + \left(G^i_{(0,0)} + \frac{1}{2}\sum_{k=1}^d (G^i_{(k,k,0)} + G^i_{(0,k,k)}) + \frac{1}{4}\sum_{k,j=1}^d G^i_{(k,k,j,j)} \right) I_{(0,0)} \\ & + \sum_{k=1}^d \left(\left(G^i_{(0,k)} + \frac{1}{2}\sum_{j=1}^d G^i_{(j,j,k)} \right) I_{(0,k)} + \left(G^i_{(k,0)} + \frac{1}{2}\sum_{j=1}^d G^i_{(k,j,j)} \right) I_{(k,0)} \right) \\ & + \sum_{j,k=1}^d G^i_{(j,k)} I_{(j,k)}, \end{aligned} \tag{3.3}$$

where the arguments are (P, q), (p, Q), or $(Y + y)/2$ if $i = 1, 2, 3$, respectively. For a scheme of weak order 2, we can simulate the Itô stochastic integrals in (3.3) as described in [11, Chapter 14.2] and thus get the approximations

$$\begin{aligned} \bar{S}^i_\omega = & h \left(G^i_{(0)} + \frac{1}{2}\sum_{k=1}^d G^i_{(k,k)} \right) + \sum_{k=1}^d G^i_{(k)} \sqrt{h}\zeta_k \\ & + \frac{h^2}{2} \left(G^i_{(0,0)} + \frac{1}{2}\sum_{k=1}^d \left(G^i_{(k,k,0)} + G^i_{(0,k,k)} \right) + \frac{1}{4}\sum_{k,j=1}^d G^i_{(k,k,j,j)} \right) \\ & + \frac{h^{3/2}}{2}\sum_{k=1}^d \zeta_k \left(G^i_{(0,k)} + G^i_{(k,0)} + \frac{1}{2}\sum_{j=1}^d \left(G^i_{(k,j,j)} + G^i_{(j,j,k)} \right) \right) \\ & + \frac{h}{2}\sum_{j,k=1}^d G^i_{(j,k)} (\zeta_j\zeta_k + \zeta_{j,k}), \end{aligned} \tag{3.4}$$

where h is the time step and the arguments are (P, q), (p, Q), or $(Y + y)/2$ if $i = 1, 2, 3$, respectively. Here ζ_k, $\zeta_{j,k}$ for $j, k = 1, \ldots, d$ are mutually independent random variables with the following discrete distributions

$$P(\zeta_k = \pm\sqrt{3}) = \frac{1}{6}, \quad P(\zeta_k = 0) = \frac{2}{3}, \tag{3.5}$$

and $\zeta_{j_1,j_1} = -1$, $j_1 = 1, \ldots, d$,

$$P(\zeta_{j_1,j_2} = \pm 1) = \frac{1}{2}, j_2 = 1, \ldots, j_1 - 1, \quad \zeta_{j_1,j_2} = -\zeta_{j_2,j_1}, j_2 = j_1 + 1, \ldots, d. \tag{3.6}$$

Replacing S_ω^1 by $\bar{S}_\omega^1$ in (2.2), we get the scheme corresponding to the following one-step approximation:

$$
\begin{aligned}
\bar{P}_i = p_i &- h\left(\frac{\partial G^1_{(0)}}{\partial q_i} + \frac{1}{2}\sum_{k=1}^{d}\frac{\partial G^1_{(k,k)}}{\partial q_i}\right) - \sum_{k=1}^{d}\frac{\partial G^1_{(k)}}{\partial q_i}\sqrt{h}\zeta_k \\
&- \frac{h^2}{2}\left(\frac{\partial G^1_{(0,0)}}{\partial q_i} + \frac{1}{2}\sum_{k=1}^{d}\left(\frac{\partial G^1_{(k,k,0)}}{\partial q_i} + \frac{\partial G^1_{(0,k,k)}}{\partial q_i}\right) + \frac{1}{4}\sum_{k,j=1}^{d}\frac{\partial G^1_{(k,k,j,j)}}{\partial q_i}\right) \\
&- \frac{h^{3/2}}{2}\sum_{k=1}^{d}\zeta_k\left(\frac{\partial G^1_{(0,k)}}{\partial q_i} + \frac{\partial G^1_{(k,0)}}{\partial q_i} + \frac{1}{2}\sum_{j=1}^{d}\left(\frac{\partial G^1_{(k,j,j)}}{\partial q_i} + \frac{\partial G^1_{(j,j,k)}}{\partial q_i}\right)\right) \\
&- \frac{h}{2}\sum_{j,k=1}^{d}\frac{\partial G^1_{(j,k)}}{\partial q_i}(\zeta_j\zeta_k + \zeta_{j,k}),
\end{aligned}
\tag{3.7}
$$

$$
\begin{aligned}
\bar{Q}_i = q_i &+ h\left(\frac{\partial G^1_{(0)}}{\partial \bar{P}_i} + \frac{1}{2}\sum_{k=1}^{d}\frac{\partial G^1_{(k,k)}}{\partial \bar{P}_i}\right) + \sum_{k=1}^{d}\frac{\partial G^1_{(k)}}{\partial \bar{P}_i}\sqrt{h}\zeta_k \\
&+ \frac{h^2}{2}\left(\frac{\partial G^1_{(0,0)}}{\partial \bar{P}_i} + \frac{1}{2}\sum_{k=1}^{d}\left(\frac{\partial G^1_{(k,k,0)}}{\partial \bar{P}_i} + \frac{\partial G^1_{(0,k,k)}}{\partial \bar{P}_i}\right) + \frac{1}{4}\sum_{k,j=1}^{d}\frac{\partial G^1_{(k,k,j,j)}}{\partial \bar{P}_i}\right) \\
&+ \frac{h^{3/2}}{2}\sum_{k=1}^{d}\zeta_k\left(\frac{\partial G^1_{(0,k)}}{\partial \bar{P}_i} + \frac{\partial G^1_{(k,0)}}{\partial \bar{P}_i} + \frac{1}{2}\sum_{j=1}^{d}\left(\frac{\partial G^1_{(k,j,j)}}{\partial \bar{P}_i} + \frac{\partial G^1_{(j,j,k)}}{\partial \bar{P}_i}\right)\right) \\
&+ \frac{h}{2}\sum_{j,k=1}^{d}\frac{\partial G^1_{(j,k)}}{\partial \bar{P}_i}(\zeta_j\zeta_k + \zeta_{j,k}),
\end{aligned}
\tag{3.8}
$$

where $i = 1, \ldots, n$, the arguments are $(\bar{P}, q)$, and the random variables ζ_k, $\zeta_{j,k}$ for $j, k = 1, \ldots, d$ are mutually independent and are independently generated at each time step according to the distributions given in (3.5)–(3.6).

The one-step approximation (3.7)–(3.8) corresponds to an implicit scheme. In Section 4 we will prove that it is well-defined and of weak order 2, but first we show the following result.

LEMMA 3.2. *For the SHS (1.1), the scheme corresponding to the one-step approximation (3.7)–(3.8) is symplectic.*

Proof. The scheme is symplectic if it preserves the symplectic structure, i.e., if we have $\bar{P} \wedge \bar{Q} = dp \wedge dq$ [16]. This can be proved by adapting the proof of Theorem 3.1 in [15]. Notice that we have

$$
\bar{P}_i = p_i - \frac{\partial \bar{S}^1_\omega}{\partial q_i}(\bar{P}, q), \quad \bar{Q}_i = q_i + \frac{\partial \bar{S}^1_\omega}{\partial \bar{P}_i}(\bar{P}, q),
\tag{3.9}
$$

where $\bar{S}^1_\omega$ is given in (3.4). Using the second equation in (3.9), we get

$$
\begin{aligned}
\bar{P} \wedge \bar{Q} &= \sum_{i=1}^{n} d\bar{P}_i \wedge d\bar{Q}_i = \sum_{i=1}^{n} d\bar{P}_i \wedge \left(dq_i + \sum_{j=1}^{n}\frac{\partial^2 \bar{S}^1_\omega}{\partial \bar{P}_i \partial \bar{P}_j}d\bar{P}_j + \sum_{j=1}^{n}\frac{\partial^2 \bar{S}^1_\omega}{\partial \bar{P}_i \partial q_j}dq_j\right) \\
&= \sum_{i=1}^{n} d\bar{P}_i \wedge dq_i + \sum_{i=1}^{n}\sum_{j=1}^{n}\frac{\partial^2 \bar{S}^1_\omega}{\partial \bar{P}_i \partial q_j}d\bar{P}_i \wedge dq_j.
\end{aligned}
\tag{3.10}
$$

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Here, we use $d\bar{P}_i \wedge d\bar{P}_j = -d\bar{P}_j \wedge d\bar{P}_i$, $i, j = 1, \ldots, n$. From the first equation in (3.9), we have

$$d\bar{P}_i = dp_i - \sum_{j=1}^{n} \frac{\partial^2 \bar{S}^1_\omega}{\partial q_i \partial \bar{P}_j} d\bar{P}_j - \sum_{j=1}^{n} \frac{\partial^2 \bar{S}^1_\omega}{\partial q_i \partial q_j} dq_j,$$

so replacing $\sum_{j=1}^{n} \frac{\partial^2 \bar{S}^1_\omega}{\partial q_i \partial \bar{P}_j} d\bar{P}_j$ in (3.10) and using again $dq_j \wedge dq_i = -dq_i \wedge dq_j$, we get

$$\bar{P} \wedge \bar{Q} = \sum_{i=1}^{n} dp_i \wedge dq_i = dp \wedge dq. \qquad \square$$

Analogously, using the approximation $\bar{S}^2_\omega$ of S^2_ω in (2.4) or replacing S^3_ω by $\bar{S}^3_\omega$ in (2.6), we can obtain two more schemes of weak order 2 for the SHS (1.1). Notice that the proof of Lemma 3.2 can be adapted in an obvious way to show that these schemes are symplectic.

We can extend the method used to construct symplectic weak first- and second-order schemes for the derivation of symplectic schemes of weak order m in a similar way, by replacing the Stratonovich integrals in (2.7) by Itô integrals using (3.1) and keeping the Itô integrals I_α with $l(\alpha) \leq m$. However, for $m > 2$ the schemes become too complex and require extensive simulations. The error due to these Monte-Carlo simulations could overcome the advantage of using a weak higher-order scheme.

4. Convergence study. In this section, we study the convergence of the symplectic weak second-order numerical schemes proposed in the previous section for the SHS (1.1). We will illustrate the idea of the proof for the scheme of weak order 2 corresponding to the one-step approximation (3.7)–(3.8). This scheme is based on the approximation (3.4) of $\bar{S}^1_\omega$, but the same approach can be followed for the symplectic schemes obtained using the approximation $\bar{S}^2_\omega$ of S^2_ω in (2.4), or replacing S^3_ω by $\bar{S}^3_\omega$ in (2.6).

For any functions F defined on $\mathbb{R}^{2n}$ and any multi-index $\alpha = (\alpha_1, \ldots, \alpha_{2n})$, with $\alpha_i = 0, 1, \ldots$, $i = 1, \ldots, 2n$, with length $|\alpha| = \alpha_1 + \cdots, +\alpha_{2n}$, let $\partial_\alpha F$ denote the partial derivative of order $|\alpha|$:

$$\frac{\partial^{|\alpha|} F}{\partial^{\alpha_1} x_1 \cdots \partial^{\alpha_{2n}} x_{2n}}.$$

As in [17], we define the class $\mathcal{F}$ to consist of the functions F on $\mathbb{R}^{2n}$ for which there exist constants $K > 0$ and $\chi > 0$ such that

$$|F(x)| \leq K(1 + \|x\|)^\chi,$$

for any $x \in \mathbb{R}^{2n}$, where $\|\cdot\|$ is the Euclidean norm. We assume that the function F in (1.3) together with its partial derivatives up to order 6 belong to the class $\mathcal{F}$. We also suppose that the functions H_r, $r = 0, \ldots, d$, are smooth enough such that their partial derivatives of order 1 up to order 7 are bounded. Consequently, $\partial_\alpha H_r \in \mathcal{F}$ with $\chi = 1$, for any multi-index α with $|\alpha| = 1, \ldots, 7$, and $r = 0, \ldots, d$, and we have the following global Lipschitz condition: there exists a constant $L > 0$ such that for any $(P^T, Q^T)^T, (p^T, q^T)^T \in \mathbb{R}^{2n}$, $|\alpha| = 1, \ldots, 6$, and $r = 0, \ldots, d$, we have

$$|\partial_\alpha H_r(P, Q) - \partial_\alpha H_r(p, q)| \leq L(\|P - p\| + \|Q - q\|). \tag{4.1}$$

For the one-step approximation (3.7)–(3.8) and any $i = 1, \ldots, 2n$, we use the notation $\bar{\Delta}_i = \bar{X}_i - x_i$, $i = 1, \ldots, 2n$, where $\bar{X} = (\bar{P}^T, \bar{Q}^T)^T$, $x = (p^T, q^T)^T$.

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LEMMA 4.1. *There exist constants $K_e > 0$ and $h_0 > 0$, such that for any $h < h_0$, $x = (p^T, q^T)^T \in \mathbb{R}^{2n}$, the system formed by (3.7) for $i = 1, \dots, n$ has a unique solution $\bar{P} = (\bar{P}_1, \dots, \bar{P}_n)^T$ which satisfies*

$$|\bar{\Delta}_i| \le K_e(1 + \|x\|)\sqrt{h}, \quad i = 1, \dots, n. \tag{4.2}$$

Proof. The lemma can easily be proven similarly as Lemma 2.4 in [15] using the contraction principle, the global Lipschitz condition (4.1), the boundedness of the partial derivatives of H_r, $r = 0, \dots, d$, of orders 1 to 7, and the fact that at each time step the random variables $\zeta_r, \zeta_{r,k}$ satisfy $|\zeta_r| \le \sqrt{3}$, $|\zeta_{r,k}| \le 1$, $r, k = 1, \dots, d$. The solution can be found by the method of simple iteration with $x = (p^T, q^T)^T$ as the initial approximation. □

REMARK 4.2. Substituting the solution $\bar{P} = (\bar{P}_1, \dots, \bar{P}_n)^T$ in the explicit system of equations (3.8) with $i = 1, \dots, n$ and using again the global Lipschitz condition (4.1) and the boundedness assumptions, we show that there exist constants $K > 0$ and $h_0 > 0$ such that for any $h \le h_0$, $x = (p^T, q^T)^T \in \mathbb{R}^{2n}$, the system (3.7)–(3.8) has a unique solution $\bar{X} = (\bar{P}^T, \bar{Q}^T)^T \in \mathbb{R}^{2n}$ which satisfies the inequality

$$\|\bar{X} - x\| \le K(1 + \|x\|)\sqrt{h}.$$

Thus the scheme corresponding to the one-step approximation (3.7)–(3.8) is well-defined.

To prove the convergence with weak order 2, we use the general result stated in [17, Theorem 4.1]; see also [14, Theorem 9.1]. The idea of the proof is to compare the scheme corresponding to the one-step approximation (3.7)–(3.8) with the Taylor scheme of weak order 2; cf. [11, Chapter 14.2]. To simplify notation, let us denote for $i = 1, \dots n$,

$$\begin{aligned}
f_i(P,Q) &= -\frac{\partial H_0}{\partial Q_i}(P,Q) \\
&\quad + \frac{1}{2}\sum_{r=1}^{d}\sum_{j=1}^{n}\left(\frac{\partial H_r}{\partial Q_j}(P,Q)\frac{\partial^2 H_r}{\partial P_j \partial Q_i}(P,Q) - \frac{\partial H_r}{\partial P_j}(P,Q)\frac{\partial^2 H_r}{\partial Q_j \partial Q_i}(P,Q)\right), \\
g_i(P,Q) &= \frac{\partial H_0}{\partial P_i}(P,Q) \\
&\quad + \frac{1}{2}\sum_{r=1}^{d}\sum_{j=1}^{n}\left(-\frac{\partial H_r}{\partial Q_j}(P,Q)\frac{\partial^2 H_r}{\partial P_j \partial P_i}(P,Q) + \frac{\partial H_r}{\partial P_j}(P,Q)\frac{\partial^2 H_r}{\partial P_i \partial Q_j}(P,Q)\right), \\
\sigma_{ir}(P,Q) &= -\frac{\partial H_r}{\partial Q_i}(P,Q), \qquad \gamma_{ir}(P,Q) = \frac{\partial H_r}{\partial P_i}(P,Q), \quad r = 1, \dots, d.
\end{aligned}$$

Using Itô stochastic integration, we rewrite the SHS (1.1) as

$$dP_i = f_i(P,Q)dt + \sum_{r=1}^{d}\sigma_{ir}(P,Q)dw_t^r, \qquad P(t_0) = p, \tag{4.3}$$

$$dQ_i = g_i(P,Q)dt + \sum_{r=1}^{d}\gamma_{ir}(P,Q)dw_t^r, \qquad Q(t_0) = q, \tag{4.4}$$

The Taylor scheme with weak order 2 (cf. [11, Chapter 14.2]) for the Itô system (4.3)–(4.4)

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corresponds to the following one-step approximation:

$$\begin{aligned}\tilde{P}_i &= p_i + hf_i + h^{1/2}\sum_{r=1}^{d}\zeta_r\sigma_{ir} + \frac{h^2}{2}L_0(f_i) + \frac{h^{3/2}}{2}\sum_{r=1}^{d}\zeta_r\left(L_0(\sigma_{ir}) + L_r(f_i)\right)\\ &\quad + \frac{h}{2}\sum_{r,k=1}^{d}L_r(\sigma_{ik})(\zeta_r\zeta_k + \zeta_{r,k}),\end{aligned} \tag{4.5}$$

$$\begin{aligned}\tilde{Q}_i &= q_i + hg_i + h^{1/2}\sum_{r=1}^{d}\zeta_r\gamma_{ir} + \frac{h^2}{2}L_0(g_i) + \frac{h^{3/2}}{2}\sum_{r=1}^{d}\zeta_r\left(L_0(\gamma_{ir}) + L_r(g_i)\right)\\ &\quad + \frac{h}{2}\sum_{r,k=1}^{d}L_r(\gamma_{ik})(\zeta_r\zeta_k + \zeta_{r,k}),\end{aligned} \tag{4.6}$$

where the arguments are (p, q) everywhere, and the operators L_0 and L_r, $r = 1, \ldots, d$, are given by

$$\begin{aligned}L_0 &= \sum_{j=1}^{n}\left(f_j\frac{\partial}{\partial P_j} + g_j\frac{\partial}{\partial Q_j}\right)\\ &\quad + \frac{1}{2}\sum_{r=1}^{d}\sum_{i=1}^{n}\sum_{j=1}^{n}\left(\sigma_{ir}\sigma_{jr}\frac{\partial^2}{\partial P_iP_j} + \gamma_{ir}\gamma_{jr}\frac{\partial^2}{\partial Q_iQ_j} + 2\sigma_{ir}\gamma_{jr}\frac{\partial^2}{\partial P_iQ_j}\right),\\ L_r &= \sum_{i=1}^{n}\left(\sigma_{ir}\frac{\partial}{\partial P_i} + \gamma_{ir}\frac{\partial}{\partial Q_i}\right).\end{aligned}$$

The mutually independent random variables ζ_k and $\zeta_{r,k}$, $r, k = 1, \ldots, d$, are generated independently at each time step according to the discrete distributions given in (3.5) and (3.6).

For $i = 1, \ldots, 2n$, let $\tilde{\Delta}_i = \tilde{X}_i - x_i$, where $\tilde{X} = (\tilde{P}^T, \tilde{Q}^T)^T$, $x = (p^T, q^T)^T$, and $\Delta_i = X_i(t+h) - x_i$, where $X(t+h) = (P_{t,p}^T(t+h), Q_{t,q}^T(t+h))^T$ is the solution of the system (1.1) and $X(t) = x$. Then from [14, Chapter 8] we know that

$$\left|E\left(\prod_{j=1}^{s}\Delta_{i_j} - \prod_{j=1}^{s}\tilde{\Delta}_{i_j}\right)\right| \leq F_0(x)h^3, \quad s = 1, \ldots, 5, \tag{4.7}$$

where $i_j = 1, \ldots, 2n$, and $F_0 \in \mathcal{F}$.

We define ρ by

$$\rho_j = \tilde{X}^j - \bar{X}^j = \tilde{\Delta}^j - \bar{\Delta}^j, \quad j = 1, \ldots, 2n.$$

LEMMA 4.3. *There exists $K_l \in \mathcal{F}$, $l = 1, ..., 4$ such that for any $i, j, k = 1, \ldots, 2n$, we have*

$$|\rho_j| \leq K_1(x)h^{3/2}, \tag{4.8}$$

$$|E(\rho_j\bar{\Delta}_i\bar{\Delta}_k)| \leq K_2(x)h^3, \tag{4.9}$$

$$|E(\rho_j\bar{\Delta}_i)| \leq K_3(x)h^3, \tag{4.10}$$

$$|E(\rho_j)| = \left|E\left(\tilde{\Delta}_j - \bar{\Delta}_j\right)\right| \leq K_4(x)h^3. \tag{4.11}$$

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Proof. Expanding the terms on the right-hand side of (3.7)–(3.8) around $x = (p^T, q^T)^T$, we get

$$\begin{aligned}
\bar{P}_i - p_i = &-\sum_{k=1}^{d} \frac{\partial G^1_{(k)}}{\partial q_i}(x)\sqrt{h}\zeta_k - \sum_{k=1}^{d} \sqrt{h}\zeta_k \sum_{j=1}^{n} \bar{\Delta}_j \frac{\partial^2 G^1_{(k)}}{\partial q_i \partial \bar{P}_j}(p + \theta_{i,k}(\bar{P} - p), q) \\
&- h\left(\frac{\partial G^1_{(0)}}{\partial q_i}(\bar{P}, q) + \frac{1}{2}\sum_{k=1}^{d} \frac{\partial G^1_{(k,k)}}{\partial q_i}(\bar{P}, q)\right) - \frac{h^2}{2}\left(\frac{\partial G^1_{(0,0)}}{\partial q_i}(\bar{P}, q)\right. \\
&+ \frac{1}{2}\sum_{k=1}^{d}\left(\frac{\partial G^1_{(k,k,0)}}{\partial q_i}(\bar{P}, q) + \frac{\partial G^1_{(0,k,k)}}{\partial q_i}(\bar{P}, q)\right) + \left.\frac{1}{4}\sum_{k,j=1}^{d} \frac{\partial G^1_{(k,k,j,j)}}{\partial q_i}(\bar{P}, q)\right) \\
&- \frac{h^{3/2}}{2}\sum_{k=1}^{d} \zeta_k\left(\frac{\partial G^1_{(0,k)}}{\partial q_i}(\bar{P}, q) + \frac{\partial G^1_{(k,0)}}{\partial q_i}(\bar{P}, q) + \frac{1}{2}\sum_{j=1}^{d}\left(\frac{\partial G^1_{(k,j,j)}}{\partial q_i}(\bar{P}, q)\right.\right. \\
&+ \left.\left.\frac{\partial G^1_{(j,j,k)}}{\partial q_i}(\bar{P}, q)\right)\right) - \frac{h}{2}\sum_{j,k=1}^{d} \frac{\partial G^1_{(j,k)}}{\partial q_i}(\bar{P}, q)(\zeta_j\zeta_k + \zeta_{j,k}),
\end{aligned}$$

$$\begin{aligned}
\bar{Q}_i - q_i = &\sum_{k=1}^{d} \frac{\partial G^1_{(k)}}{\partial p_i}(x)\sqrt{h}\zeta_k + \sum_{k=1}^{d} \sqrt{h}\zeta_k \sum_{j=1}^{n} \bar{\Delta}_j \frac{\partial^2 G^1_{(k)}}{\partial \bar{P}_i \partial \bar{P}_j}(p + \theta_{i+n,k}(\bar{P} - p), q)) \\
&+ h\left(\frac{\partial G^1_{(0)}}{\partial \bar{P}_i}(\bar{P}, q) + \frac{1}{2}\sum_{k=1}^{d} \frac{\partial G^1_{(k,k)}}{\partial \bar{P}_i}(\bar{P}, q)\right) + \frac{h^2}{2}\left(\frac{\partial G^1_{(0,0)}}{\partial \bar{P}_i}(\bar{P}, q)\right. \\
&+ \frac{1}{2}\sum_{k=1}^{d}\left(\frac{\partial G^1_{(k,k,0)}}{\partial \bar{P}_i}(\bar{P}, q) + \frac{\partial G^1_{(0,k,k)}}{\partial \bar{P}_i}(\bar{P}, q)\right) + \left.\frac{1}{4}\sum_{k,j=1}^{d} \frac{\partial G^1_{(k,k,j,j)}}{\partial \bar{P}_i}(\bar{P}, q)\right) \\
&+ \frac{h^{3/2}}{2}\sum_{k=1}^{d} \zeta_k\left(\frac{\partial G^1_{(0,k)}}{\partial \bar{P}_i}(\bar{P}, q) + \frac{\partial G^1_{(k,0)}}{\partial \bar{P}_i}(\bar{P}, q) + \frac{1}{2}\sum_{j=1}^{d}\left(\frac{\partial G^1_{(k,j,j)}}{\partial \bar{P}_i}(\bar{P}, q)\right.\right. \\
&+ \left.\left.\frac{\partial G^1_{(j,j,k)}}{\partial \bar{P}_i}(\bar{P}, q)\right)\right) + \frac{h}{2}\sum_{j,k=1}^{d} \frac{\partial G^1_{(j,k)}}{\partial \bar{P}_i}(\bar{P}, q)(\zeta_j\zeta_k + \zeta_{j,k}),
\end{aligned}$$

where $0 < \theta_{i,k} < 1$, $i = 1, \ldots, 2n$, $k = 1, \ldots, d$.

Using (4.2) and the fact that $|\zeta_r| \leq \sqrt{3}$, $|\zeta_{r,k}| \leq 1$, $r, k = 1, \ldots, d$, and the partial derivatives of H_r, $r = 0, \ldots, d$ of order 1 up to order 7 are bounded, we show that there exists a positive constant K_0 such that for any $i = 1, \ldots, 2n$,

$$\bar{\Delta}_i = \bar{\Delta}_{i,1}(x) + R_{i,1}(\bar{P}, q), \quad |R_{i,1}(\bar{P}, q)| \leq K_0(1 + \|x\|)h, \tag{4.12}$$

where, for $i = 1, \ldots, n$, we have

$$\bar{\Delta}_{i,1}(x) = -\sum_{k=1}^{d} \frac{\partial G^1_{(k)}}{\partial q_i}(x)\sqrt{h}\zeta_k, \quad \bar{\Delta}_{i+n,1}(x) = \sum_{k=1}^{d} \frac{\partial G^1_{(k)}}{\partial p_i}(x)\sqrt{h}\zeta_k. \tag{4.13}$$

Increasing the order of the deterministic Taylor expansions around $x = (p^T, q^T)^T$ in equations (3.7)–(3.8) and using additionally (4.12), we show that there exists $F_2 \in \mathcal{F}$ such that for any $i=1,\dots,2n$, we have $\bar\Delta_i=\bar\Delta_{i,2}(x)+R_{i,2}(\bar P,q)$, with $|R_{i,2}(\bar P,q)|\le F_2(x)h^{\frac32}$. Here, for $i=1,\dots,n$, we have

$$\begin{aligned}\bar\Delta_{i,2}&=-h^{1/2}\sum_{k=1}^{d}\zeta_k\left(\frac{\partial G^1_{(k)}}{\partial q_i}+\sum_{j=1}^{n}\bar\Delta_{j,1}\frac{\partial^2 G_{(k)}}{\partial q_i\partial p_j}\right)-h\left(\frac{\partial G^1_{(0)}}{\partial q_i}+\frac12\sum_{k=1}^{d}\frac{\partial G^1_{(k,k)}}{\partial q_i}\right)\\&\quad-\frac h2\sum_{j,k=1}^{d}\frac{\partial G^1_{(j,k)}}{\partial q_i}(\zeta_j\zeta_k+\zeta_{j,k}),\\ \bar\Delta_{i+n,2}&=h^{1/2}\sum_{k=1}^{d}\zeta_k\left(\frac{\partial G^1_{(k)}}{\partial p_i}+\sum_{j=1}^{n}\bar\Delta_{j,1}\frac{\partial^2 G_{(k)}}{\partial p_i\partial p_j}\right)+h\left(\frac{\partial G^1_{(0)}}{\partial p_i}+\frac12\sum_{k=1}^{d}\frac{\partial G^1_{(k,k)}}{\partial p_i}\right)\\&\quad+\frac h2\sum_{j,k=1}^{d}\frac{\partial G^1_{(j,k)}}{\partial p_i}(\zeta_j\zeta_k+\zeta_{j,k}).\end{aligned}$$

The arguments are $x=(p^T,q^T)^T$ everywhere.

Replacing the formulas for the coefficients G^1_α according to (2.9) and using (3.6) and (4.13), after simple but tedious calculations, we have the following result for $i=1,\dots,n$,

$$\begin{aligned}\bar\Delta_{i,2}&=hf_i+h^{1/2}\sum_{r=1}^{d}\zeta_r\sigma_{ir}+\frac h2\sum_{r,k=1}^{d}L_r(\sigma_{ik})(\zeta_r\zeta_k+\zeta_{r,k}),\\ \bar\Delta_{i+n,2}&=hg_i+h^{1/2}\sum_{r=1}^{d}\zeta_r\gamma_{ir}+\frac h2\sum_{r,k=1}^{d}L_r(\gamma_{ik})(\zeta_r\zeta_k+\zeta_{r,k}).\end{aligned}$$

Comparing with (4.5)–(4.6) we get the inequality (4.8).

Similarly, by successively increasing the order of the Taylor expansions in (3.7)–(3.8), we have

$$\bar\Delta_i=\bar\Delta_{i,j}(x)+R_{i,j}(\bar P,q),\quad |R_{i,j}(\bar P,q)|\le F_j(x)h^{\frac{j+1}{2}},\quad i=1,\dots,2n,$$

where $F_j\in\mathcal F$, $j=3,4,5$. For $j=3,4,5$ the calculations required to obtain the exact formulas for $\bar\Delta_{i,j}$, $i=1,\dots,2n$, are obvious but lengthy, and they were done using MAPLE software. Since ζ_k, $\zeta_{r,m}$, are mutually independent, and we have $E(\zeta_k^l)=0$ for any odd power l, $E(\zeta_{r,m}^l)=0$, $k,r,m=1,\dots,d$, $r\neq m$, from the formulas for $\bar\Delta_{i,3}$, $\bar\Delta_{i,4}$ and $\bar\Delta_{i,5}$, $i=1,\dots,2n$, we obtain the inequalities (4.9), (4.10), and (4.11), respectively. ◻

THEOREM 4.4. *The implicit method corresponding to the one-step approximation (3.7)–(3.8) for the system (1.1) is symplectic and of weak order 2.*

Proof. From Lemmas 3.2 and 4.1, it is clear that the scheme is well-defined and symplectic. To prove the convergence with weak order 2, we verify conditions (2) and (4) in [17, Theorem 4.1] (or [14, Theorem 9.1]).

Firstly we prove that there exists $K_5\in\mathcal F$ such that

$$\left|E\left(\prod_{j=1}^{s}\tilde\Delta_{i_j}-\prod_{j=1}^{s}\bar\Delta_{i_j}\right)\right|\le K_5(x)h^3,\quad s=1,\dots,5. \tag{4.14}$$

For $s=1$, from (4.11), there exists $K_4\in\mathcal F$ such that for any $i=1,\dots,2n$, we have

$$|E(\tilde\Delta_i-\bar\Delta_i)|=|E(\rho_i)|\le K_4(x)h^3.$$

For $s = 2, \dots, 5$, we can write

$$\left| E\left(\prod_{j=1}^{s} \tilde{\Delta}_{i_j} - \prod_{j=1}^{s} \bar{\Delta}_{i_j}\right)\right| = \left| E\left(\prod_{j=1}^{s} (\bar{\Delta}_{i_j} + \rho_{i_j}) - \prod_{j=1}^{s} \bar{\Delta}_{i_j}\right)\right|, \quad i_j = 1, \dots, 2n. \tag{4.15}$$

Hence for $s = 2$ and any $i_1, i_2 = 1, \dots, 2n$ we have

$$\left| E\left(\prod_{j=1}^{2} \tilde{\Delta}_{i_j} - \prod_{j=1}^{2} \bar{\Delta}_{i_j}\right)\right| \le |E(\bar{\Delta}_{i_1}\rho_{i_2})| + |E(\bar{\Delta}_{i_2}\rho_{i_1})| + E|\rho_{i_1}\rho_{i_2}|,$$

so (4.8) and (4.10) imply (4.14).

For $s = 3, 4, 5$, from (4.15) the difference $\prod_{j=1}^{s} \tilde{\Delta}_{i_j} - \prod_{j=1}^{s} \bar{\Delta}_{i_j}$ consists of the terms including either a product $\rho_{i_j}\bar{\Delta}_{i_k}\bar{\Delta}_{i_m}$, or a product $\rho_{i_j} \cdots \rho_{i_k}$ with at least two factors, or a product $\rho_{i_j}(\bar{\Delta}_{i_k} \cdots \bar{\Delta}_{i_m})$ with at least four factors. For the first type and from (4.9), there exists $K_2 \in \mathcal{F}$ such that

$$|E(\rho_{i_j}\bar{\Delta}_{i_k}\bar{\Delta}_{i_m})| \le K_2(x)h^3. \tag{4.16}$$

For the second type and from (4.8), there exists $K_{4,1} \in \mathcal{F}$ such that

$$|E(\rho_{i_j} \cdots \rho_{i_k})| \le E|\rho_{i_j} \cdots \rho_{i_k}| \le K_{4,1}(x)h^3. \tag{4.17}$$

For the third type and applying the Cauchy–Schwarz inequality using (4.2) and (4.8), there exists $K_{4,2} \in \mathcal{F}$ such that

$$|E(\rho_{i_j}(\bar{\Delta}_{i_k} \cdots \bar{\Delta}_{i_m})| \le \sqrt{E(\rho_{i_j}^2)E(\bar{\Delta}_{i_k}^2 \cdots \bar{\Delta}_{i_m}^2)} \le K_{4,2}(x)h^3. \tag{4.18}$$

The inequalities (4.16)–(4.18) imply that (4.14) is true also for $s = 3, 4, 5$. Using (4.14) and (4.7) we can easily show that there exists $k \in \mathcal{F}$ such that

$$\left| E\left(\prod_{j=1}^{s} \Delta_{i_j} - \prod_{j=1}^{s} \bar{\Delta}_{i_j}\right)\right| \le k(x)h^3, \quad s = 1, \dots, 5, \quad i_j = 1, \dots, 2n,$$

and condition (2) in [17, Theorem 4.1] is satisfied.

To conclude the proof, we have to show that for a sufficiently large number m, the moments $E(\|\bar{X}(k)\|^{2m})$ exist and are uniformly bounded with respect to N and $k = 0, \dots, N$, where $h = T/N$ (see condition (4) in [14, Theorem 9.1]). Since at each time step k we have $E(\zeta_r) = 0$, $r = 1, \dots, d$, from (4.12) and (4.13), for any $i = 1, \dots, 2n$, we have

$$|E(\bar{\Delta}_i)| = |E(R_{i,1}(\bar{P}, q))| \le K_0(1 + \|x\|)h.$$

This inequality and (4.2) ensure the existence and uniform boundedness of the moments $E(\|\bar{X}(k)\|^{2m})$; see [14, Lemma 9.1]. □

Analogously, we can prove a similar result for the midpoint scheme constructed by replacing S_ω^3 by $\bar{S}_\omega^3$ in (2.6).

5. Numerical tests. To validate the performance of the proposed symplectic schemes, we present numerical simulations in this section. First, we consider a non-linear SHS with additive noise. Then we investigate two systems with multiplicative noise: a linear case for the Kubo oscillator and a non-linear model for synchrotron oscillations. Since we work with schemes in the weak sense, we only need to simulate uniformly distributed random numbers for the Monte Carlo simulations. In all computations, we use 100 000 samples to calculate the expectations (unless we specify otherwise).

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5.1. A non-linear model with additive noise. We consider the SHS with additive noise given by the following equations:

$$\begin{aligned} dP &= (Q - Q^3)dt + \epsilon dw_t, \\ dQ &= Pdt, \end{aligned} \tag{5.1}$$

where ϵ is a constant. Notice that the Itô and the Stratonovich formulations are the same for this model with additive noise, and we have the separable Hamiltonian functions

$$H_0(P,Q) = \frac{Q^4}{4} - \frac{Q^2}{2} + \frac{P^2}{2} = U(Q) + V(P), \quad H_1(P,Q) = -\epsilon Q.$$

This is also referred to as the Double Well problem, and it is used in [6] to illustrate the accuracy of some low-rank Runge-Kutta methods to estimate the expectation of the Hamiltonian H_0. Notice that we have [6]

$$E(H_0(P_{0,p}(T), Q_{0,q}(T))) = H_0(p,q) + \frac{\epsilon^2}{2}T. \tag{5.2}$$

Here, we estimate $E(H_0(T))$ using the weak second-order schemes based on S^1_ω and S^3_ω. From the general formula (2.9), the coefficients G^1_α of S^1_ω are given by:

$$\begin{aligned} &G^1_{(0)} = \frac{q^4}{4} - \frac{q^2}{2} + \frac{P^2}{2}, \qquad G^1_{(1)} = -\epsilon q, \qquad G^1_{(0,0)} = P(q^3 - q), \\ &G^1_{(0,1)} = -\epsilon P, \qquad G^1_{(0,1,1)} = \epsilon^2, \end{aligned}$$

where the arguments are (P,q) everywhere. Similarly, by (2.10), we get the following coefficients G^3_α of S^3_ω:

$$G^3_{(0)}(p,q) = \frac{q^4}{4} - \frac{q^2}{2} + \frac{p^2}{2}, \quad G^3_{(1)}(p,q) = -\epsilon q, \quad G^3_{(1,0)}(p,q) = -G^3_{(0,1)}(p,q) = \frac{\epsilon p}{2},$$
$$G^3_{(1,1,0)}(p,q) = G^3_{(0,1,1)}(p,q) = \frac{\epsilon^2}{4}.$$

All other G^i_α, $i = 1,3$ included in the weak second-order symplectic schemes are zero, and the weak first- and second-order symplectic schemes based on S^1_ω are explicit for the SHS (5.1).

To compare with the results reported in [6], we consider the same values of the parameters, namely the noise term $\epsilon = 0.5$, the initial values are $p = q = \sqrt{2}$, and the number of simulations is $M = 50000$. In Figure 5.1 we plot the values of $E(H_0(P_{0,p}(t), Q_{0,q}(t)))$ for $t \in [0,60]$ obtained using the weak second-order symplectic schemes based on S^i_ω with $i = 1,3$. These approximations are in excellent agreement with the exact values given in (5.2) and are visually similar with the ones displayed in Figure 2 in [6]. To illustrate the accuracy of the symplectic methods, we have also included the values obtained using the Runge-Kutta method of weak order 2; see [11, Chapter 15.1]. In [6] the time step is $h = 0.1$, but since the Runge-Kutta method of weak order 2 is not convergent for $h = 0.1$, for all the simulations presented in Figure 5.1, we consider $h = 0.05$. We notice that, in addition to requiring a smaller time step for convergence, the non-symplectic method is less accurate for long-term simulations than the symplectic methods.

We also carry out a Monte Carlo simulation for the weak second-order symplectic scheme based on S^1_ω (given by the one-step approximation (3.7)–(3.8)), and we estimate 95% confidence intervals for $E(H_0(P_{0,p}(T), Q_{0,q}(T)))$ as

$$\bar{H}_{0p,q}(T) \pm 1.96\frac{s_{p,q}(T)}{\sqrt{M}}, \tag{5.3}$$

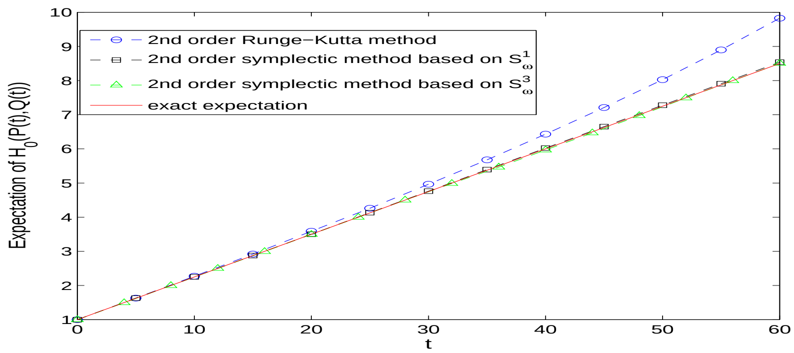

FIG. 5.1. *Expected value of* H_0.

where M is the number of independent realizations in the Monte Carlo simulations, $\bar{H}_{0p,q}(T)$ is the sample average, and $s_{p,q}(T)$ is the sample standard deviation; see also [17, Formula 7.7]. In addition to the weak scheme error, we also have the Monte Carlo error, but the margin of error in the confidence intervals (5.3) reflects the Monte Carlo error only. The results in Table 5.1 are in good agreement with the exact value obtained from (5.2), namely $E(H_0(P_{0,\sqrt{2}}(40), Q_{0,\sqrt{2}}(40))) = 6$.

TABLE 5.1
Estimation of $E(H_0(P_{0,\sqrt{2}}(40), Q_{0,\sqrt{2}}(40)))$ *by the weak second-order symplectic scheme based on the one-step approximation* (3.7)–(3.8).

h	M	$\bar{H}_{0\sqrt{2},\sqrt{2}}(40)$	95% confidence interval
0.1	$5\cdot 10^5$	6.1431	6.122 to 6.164
0.05	$5\cdot 10^5$	6.0256	6.005 to 6.046
0.01	$5\cdot 10^5$	6.0036	5.983 to 6.023
0.01	$4\cdot 10^6$	5.9990	5.991 to 6.006

5.2. Kubo oscillator. In [15] the Kubo oscillator based on the following SDEs in the sense of Stratonovich is used to demonstrate the advantage of using a stochastic symplectic scheme for long-time computations:

$$
\begin{aligned}
dP &= -aQdt - \sigma Q \circ dw_t, \qquad P(0) = p_0,\\
dQ &= aPdt + \sigma P \circ dw_t, \qquad Q(0) = q_0,
\end{aligned}
\tag{5.4}
$$

where a and σ are constants.

Here, we consider four stochastic symplectic schemes in the weak sense, namely the weak first- and second-order schemes based on S^1_ω and S^3_ω. The coefficients G^1_α of S^1_ω for the system (5.4) are given by (see the general formula (2.9)):

$$
\begin{aligned}
&G^1_{(0)} = \frac{a}{2}(P^2+q^2), \quad G^1_{(1)} = \frac{\sigma}{2}(P^2+q^2), \quad G^1_{(0,0)} = a^2 Pq, \quad G^1_{(1,1)} = \sigma^2 Pq,\\
&G^1_{(1,0)} = G^1_{(0,1)} = a\sigma Pq, \quad G^1_{(0,0,0)} = a^3(P^2+q^2), \quad G^1_{(1,1,1)} = \sigma^3(P^2+q^2),\\
&G^1_{(1,1,0)} = G^1_{(1,0,1)} = G^1_{(0,1,1)} = a\sigma^2(P^2+q^2), \quad G^1_{(1,1,1,1)} = 5\sigma^4 Pq,
\end{aligned}
$$

where the arguments are (P, q) everywhere. The symplectic schemes of various weak orders are obtained by truncating the generating function S^1_ω appropriately.

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For S^3_ω in the general formula (2.10), we get $G^3_\alpha = 0$ when $|\alpha| = 2$ and $G^3_{(1,1,1,1)} = 0$. Therefore,

$$\begin{aligned} G^3_{(0)}(p,q) &= \frac{a}{2}(p^2+q^2), & G^3_{(1)}(p,q) &= \frac{\sigma}{2}(p^2+q^2),\\ G^3_{(0,0,0)}(p,q) &= \frac{a^3}{4}(p^2+q^2), & G^3_{(1,1,1)}(p,q) &= \frac{\sigma^3}{4}(p^2+q^2),\\ G^3_{(1,1,0)}(p,q) &= G^3_{(1,0,1)}(p,q) = G^3_{(0,1,1)}(p,q) = \frac{a\sigma^2}{4}(p^2+q^2). \end{aligned}$$

It is well-known [15] that the Hamiltonian functions $H_0(P(t),Q(t)) = a(P(t)^2+Q(t)^2)/2$ and $H_1(P(t),Q(t)) = \sigma(P(t)^2+Q(t)^2)/2$ are preserved under the phase flow of the system. Therefore, the expected value of $P(t)^2+Q(t)^2$ is also invariant with respect to time and we have

$$\begin{aligned} E(P_{0,p}(T)) &= e^{-\frac{\sigma^2 T}{2}}(\cos(aT)p - \sin(aT)q),\\ E(Q_{0,q}(T)) &= e^{-\frac{\sigma^2 T}{2}}(\sin(aT)p + \cos(aT)q). \end{aligned} \tag{5.5}$$

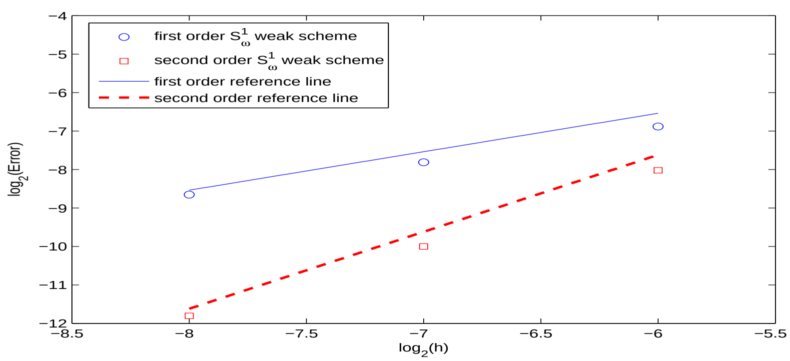

FIG. 5.2. *Convergence rate of different order S^1_ω symplectic weak scheme.*

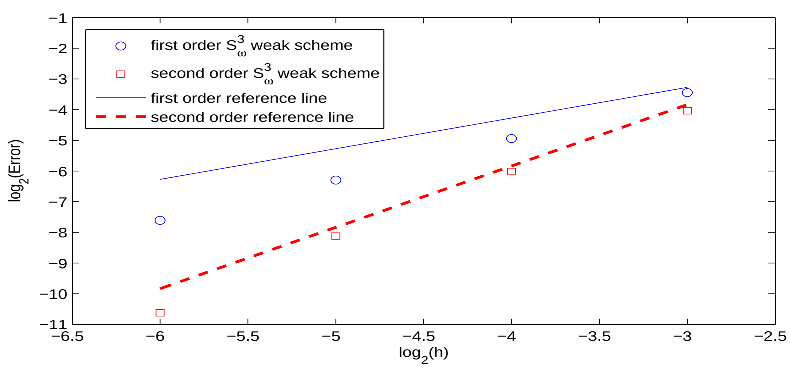

FIG. 5.3. *Convergence rate of different order S^3_ω symplectic weak scheme.*

The convergence rates of various symplectic weak schemes are investigated numerically by comparing the estimations of the expected values of the solutions to the exact values (5.5).

The results presented in Figure 5.2 and Figure 5.3 confirm the expected convergence rates of the proposed symplectic schemes. The error is defined as the difference between the estimation of the expected value of the numerical solution and the exact value (5.5) at $T = 10$. The values of the parameters are $a = 2$, $\sigma = 0.2$, the initial values are $p = 1$, $q = 0$, and the time step is $h = 2^{-5}$.

A study of the computing time required for the symplectic schemes compared to Taylor non-symplectic schemes of the same weak order is presented in [2]. For this system preserving the Hamiltonian functions, the symplectic schemes of weak order 2 require less computing time than the Itô-Taylor scheme of weak order 2 corresponding to the one-step approximation (4.5)–(4.6).

5.3. Synchrotron oscillations. The mathematical model for the oscillations of the particles in storage rings [15] is given by:

$$\begin{aligned} dP &= -\beta^2 \sin Q dt - \sigma_1 \cos Q \circ dw_t^1 - \sigma_2 \sin Q \circ dw_t^2, \\ dQ &= P dt. \end{aligned} \tag{5.6}$$

Notice that $H_0(P,Q) = -\beta^2 \cos Q + P^2/2 = U(Q) + V(P)$, $H_1(Q) = \sigma_1 \sin Q$, and $H_2(Q) = -\sigma_2 \cos Q$. Thus (5.6) is a SHS with separable Hamiltonians and the explicit symplectic schemes in [17, Section 4.2] can be applied.

From the general formula (2.9), we obtain the following formulas for the coefficients G^1_α of S^1_ω,

$$\begin{aligned} G^1_{(0)} &= \frac{P^2}{2} - \beta^2 \cos q, & G^1_{(1)} &= \sigma_1 \sin q, & G^1_{(2)} &= -\sigma_2 \cos q, \\ G^1_{(0,0)} &= \beta^2 P \sin q, & G^1_{(0,1)} &= \sigma_1 P \cos q, & G^1_{(0,2)} &= \sigma_2 P \sin q, \\ G^1_{(0,1,1)} &= \sigma_1^2 \cos^2 q, & G^1_{(0,2,2)} &= \sigma_2^2 \sin^2 q, \end{aligned}$$

where the arguments are (P, q) everywhere. All other G^1_α included in the weak second-order symplectic scheme based on the one-step approximation (3.7)–(3.8) are zero, and the weak first- and second-order symplectic schemes based on S^1_ω are explicit for the SHS (5.6).

The mean energy of the system (5.6) is defined as $E(e(p,q))$, where [17]

$$e(p,q) = p^2/2 - \beta^2 \cos(q).$$

If $\sigma_1 = \sigma_2$, we have [17]

$$E(e(P_{0,p}(T), Q_{0,q}(T))) = e(p,q) + \frac{\sigma^2}{2} T. \tag{5.7}$$

To investigate the accuracy of the proposed symplectic schemes in the weak sense, we carry out a Monte Carlo simulation and estimate the 95% confidence intervals for

$$E(e(P_{0,p}(T), Q_{0,q}(T)))$$

as

$$\bar{e}_{0,p,q}(T) \pm 1.96 \frac{s_{0,p,q}(T)}{\sqrt{M}},$$

where M is the number of independent realizations in the Monte Carlo simulations, $\bar{e}_{0,p,q}(T)$ is the sample average, and $s_{0,p,q}(T)$ is the sample standard deviation.

TABLE 5.2
Estimation of $E(e(P_{0,1}(200), Q_{0,0}(200)))$ *by the weak second-order symplectic scheme based on the one-step approximation* (3.7)–(3.8).

h	M	$\bar{e}_{0,1,0}(200)$	95% confidence interval
0.05	10^5	-6.609	-6.665 to -6.552
0.025	10^5	-6.544	-6.601 to -6.488
0.01	10^5	-6.497	-6.553 to -6.44
0.01	$4 \cdot 10^6$	-6.502	-6.511 to -6.493

The experiments presented in Table 5.2 demonstrate that the weak second-order symplectic scheme based on the one-step approximation (3.7)–(3.8) has a similar accuracy compared to the explicit symplectic schemes (7.3) and (7.5) proposed by Milstein and Tretyakov; see [17, Table 1]. The values of the parameters used in the simulations are $\sigma_1 = \sigma_2 = 0.3$, $\beta = 4$, the initial values are $p = 1$, $q = 0$, and $T = 200$. The sample averages $\bar{e}_{0,1,0}(200)$ displayed in Table 5.2 corresponding to various time steps h and number of realizations M are good estimations of the exact solution $E(e(P_{0,1}(200), Q_{0,0}(200))) = -6.5$ obtained from (5.7). This confirms the excellent performance for a long-term simulation of the weak second-order symplectic scheme based on the one-step approximation (3.7)–(3.8).

6. Conclusions. In this paper, we present an approach based on the generating function method to construct symplectic schemes in the weak sense. The derived weak order 1 schemes are the same as the ones proposed by Milstein and Tretyakov in [17]. However, it should be noted that a different approach is presented in [17], and no detail is provided how the approach can be extended to construct symplectic scheme of weak orders $m > 1$ for general SHSs. To our knowledge, this may be the first paper to present the weak second-order symplectic schemes which can be applied to general SHSs.

For the symplectic weak order 2 schemes, we present a convergence study and we validate their accuracy by numerical simulations for three different stochastic Hamiltonian systems. It is known that there are effective explicit methods of weak order 2 for general stochastic differential equations [11, Chapters 14, 15], but these methods are not symplectic. Compared to the methods based on Taylor expansion, the proposed symplectic weak second-order methods are implicit, but they are comparable in terms of the number and the complexity of the multiple Itô stochastic integrals or the derivatives of the Hamiltonian functions required. Moreover, since we can use bounded discrete random variables to simulate the multiple Itô stochastic integrals for the weak schemes, the derived weak schemes are well defined and they are also computationally efficient.

REFERENCES

[1] A. ABDULLE, D. COHEN, G. VILMART, AND K. C. ZYGALAKIS, *High weak order methods for stochastic differential equations based on modified equations*, SIAM J. Sci. Comput., 34 (2012), pp. A1800–A1823.
[2] C. ANTON, Y. WONG, AND J. DENG, *Symplectic schemes for stochastic Hamiltonian systems preserving Hamiltonian functions*, Int. J. Numer. Anal. Model., 11 (2014), pp. 427–451.
[3] ———, *On global error of symplectic schemes for stochastic Hamiltonian systems*, Int. J. Numer. Anal. Model. Ser. B, 4 (2013), pp. 80–93.
[4] J.-M. BISMUT, *Méchanique Aléatoire*, Springer, Berlin, 1981.
[5] N. BOU-RABEE AND H. OWHADI, *Stochastic variational integrators*, IMA J. Numer. Anal., 29 (2009), pp. 421–443.
[6] K. BURRAGE AND P. M. BURRAGE, *Low rank Runge-Kutta methods, symplecticity and stochastic Hamiltonian problems with additive noise*, J. Comput. Appl. Math., 236 (2012), pp. 3920–3930.

[7] J. DENG, C. ANTON, AND Y. WONG, *High-order symplectic schemes for stochastic Hamiltonian systems*, Commun. Comput. Phys., 16 (2014), pp. 169–200.

[8] E. HAIRER, C. LUBICH, AND G. WANNER, *Geometric Numerical Integration*, Springer, Heidelberg, 2006.

[9] J. HONG, L. WANG, AND R. SCHERER, *Simulation of stochastic Hamiltonian systems via generating functions*, in Proceedings of the 4th IEEE Intern. Conf. on Computer Science and Information Technology, ICCSIT 2011, IEEE Conference Proceedings, Los Alamitos, 2011, pp. 523–528.

[10] ———, *Symplectic numerical methods for a linear stochastic oscillator with two additive noises*, in Proceedings of the World Congress on Engineering vol. 1, S. I. Ao, L. Gelman, D. W. L. Hukins, A. Hunter, and A. M. Korsunsky, eds., Newswood Limited, London, 2011, pp. 19–23.

[11] P. KLOEDEN AND E. PLATEN, *Numerical Solutions of Stochastic Differential Equations*, Springer, Berlin, 1992.

[12] H. KUNITA, *Stochastic Flows and Stochastic Differential Equations*, Cambridge University Press, Cambridge, 1990.

[13] Q. MA, D. DING, AND X. DING, *Symplectic conditions and stochastic generating functions of stochastic Runge-Kutta methods for stochastic Hamiltonian systems with multiplicative noise*, Appl. Math. Comput., 219 (2012), pp. 635–643.

[14] G. N. MILSTEIN, *Numerical Integration of Stochastic Differential Equations*, Kluwer Dordrecht, 1995.

[15] G. N. MILSTEIN, Y. M. REPIN, AND M. V. TRETYAKOV, *Numerical methods for stochastic systems preserving symplectic structure*, SIAM J. Numer. Anal., 40 (2002), pp. 1583–1604.

[16] ———, *Symplectic integration of Hamiltonian systems with additive noise*, SIAM J. Numer. Anal., 39 (2002), pp. 2066–2088.

[17] G. N. MILSTEIN AND M. V. TRETYAKOV, *Quasi-symplectic methods for Langevin-type equations*, IMA J. Numer. Anal., 23 (2003), pp. 593–626.

[18] L. WANG, *Variational Integrators and Generating Functions for Stochastic Hamiltonian Systems*, PhD. Thesis, IANM, University of Karlsruhe, KIT Scientific Publishing, University of Karlsruhe, Germany, 2007.

[19] L. WANG, J. HONG, R. SCHERER, AND F. BAI, *Dynamics and variational integrators of stochastic Hamiltonian systems*, Int. J. Numer. Anal. Model., 6 (2009), pp. 586–602.