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SYMPLECTIC SCHEMES FOR STOCHASTIC HAMILTONIAN 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 prove that the coefficients of the generating function are invariant under permutations for this class of systems. As a consequence, the proposed high-order symplectic weak and strong schemes are computationally efficient because they require less stochastic multiple integrals than the Taylor expansion schemes with the same order.

Key words. Stochastic Hamiltonian systems, generating function, symplectic method, high-order schemes.

1. Introduction

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 $P_i, Q_i, p_i, q_i, i = 1,\dots,n$ and $w_t^r, r = 1,\dots,m$ are independent standard Wiener processes. The SDEs (1) are called the Stochastic Hamiltonian System (SHS) ([12], [11]).

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. However, by the chain rule of the Stratonovich stochastic integration, for any $i = 0,\dots,m$, we have

$$
\begin{aligned}
dH_i &= \sum_{k=1}^{n}\left(\frac{\partial H_i}{\partial P_k}dP_k + \frac{\partial H_i}{\partial Q_k}dQ_k\right) \\
&= \sum_{k=1}^{n}\left(-\frac{\partial H_i}{\partial P_k}\frac{\partial H_0}{\partial Q_k} + \frac{\partial H_i}{\partial Q_k}\frac{\partial H_0}{\partial P_k}\right)dt + \sum_{r=1}^{m}\sum_{k=1}^{n}\left(-\frac{\partial H_i}{\partial P_k}\frac{\partial H_r}{\partial Q_k} + \frac{\partial H_i}{\partial Q_k}\frac{\partial H_r}{\partial P_k}\right)\circ dw_t^r
\end{aligned} \tag{2}
$$

Thus, the Hamiltonian functions $H_i, i = 0,\dots,m$ are invariant for the flow of the system (1) (i.e. $dH_i = 0$), if and only if $\{H_i, H_j\} = 0$ for $i, j = 0,\dots,m$, where the Poisson bracket is defined as $\{H_i, H_j\} = \sum_{k=1}^{n}(\frac{\partial H_j}{\partial Q_k}\frac{\partial H_i}{\partial P_k} - \frac{\partial H_i}{\partial Q_k}\frac{\partial H_j}{\partial P_k})$. In this paper we propose symplectic schemes for SHS preserving the Hamiltonian functions. This type of SHS is a special case of integrable stochastic Hamiltonian dynamical systems which has been studied in [8]. An example of a SHS preserving Hamiltonian functions is the Kubo oscillator which is used, for instance, in [11] to illustrate the superior performance of symplectic schemes.

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We consider the differential 2-form

$$dp \wedge dq = dp_1 \wedge dq_1 + \cdots + dp_n \wedge dq_n. \tag{3}$$

The stochastic flow $(p, q) \longrightarrow (P, Q)$ of the SHS (1) preserves the symplectic structure (see Theorem 2.1 in [12]) as follows:

$$dP \wedge dQ = dp \wedge dq, \tag{4}$$

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. It should be noted that in (1) p, q are fixed parameters and the differentiation is done with respect to time t, while in (4) the 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

$$d\bar{P} \wedge d\bar{Q} = dp \wedge dq. \tag{5}$$

If for the approximation $\bar{X}_k = (\bar{P}, \bar{Q})$, $k = 0, 1, \ldots$, of the solution $X(t_k, \omega) = (P(t_k, \omega), Q(t_k, \omega))$, we have

$$\left[E|\bar{X}_k(\omega)) - X(t_k, \omega)|^2\right]^{1/2} \leq K h^j, \tag{6}$$

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 $\bar{X}_k$ approximates the solution $X(t_k)$ of (1) with mean square order of accuracy j ([7]). On the other hand, if

$$|E[F(\bar{X}_k(\omega))] - E[F(X(t_k, \omega)]| \leq K h^j, \tag{7}$$

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 $\bar{X}_k$ approximates the solution $X(t_k)$ of (1) in the weak sense with weak order of accuracy j ([7]).

Milstein et al. [12] [11] have constructed a symplectic scheme with mean square order 0.5 for the general SHS (1), and several symplectic schemes with higher mean square order for special types of SHSs such as SHSs with additive noise or separable Hamiltonians. A symplectic scheme with weak order one is constructed in [10]. An approach to construct symplectic schemes for SHSs based on generating functions was proposed by Wang in [13]. More recently, Wang et al. have also proposed variational integrators [14] for SHSs, and have presented several applications of the generating functions method for SHSs in [5], [6].

In [1] and [4], we follow the approach based on generating functions and we propose a recurrence formula for finding the coefficients of the generating function for SHSs. We derive several higher order strong and weak schemes and we also illustrate by numerical simulations that symplectic schemes are more accurate for long term numerical calculations than the non-symplectic methods. In this study, we extend the results presented in [3] and we focus on SHS preserving the Hamiltonian functions.

In the next section, we introduce general results regarding the generating functions associated with the SHS (1). The main results are presented in Section 3 where we prove that the coefficients of the generating function are invariant under permutation for this type of systems. Hence, the construction of the strong and weak symplectic schemes of order two and three reported in Section 4 is simpler and more efficient than the non-symplectic explicit Taylor expansion schemes with the same order. In Section 5 we illustrate numerically the performance of the proposed strong and weak symplectic schemes.

2. Generating function method

The generating functions are stochastic processes connected with the SHS (1) by the following Hamilton-Jacobi partial differential equations (HJ PDE). Let $S_\omega^i(P,q,t)$, $i=1,\dots,3$ be the solutions of the partial differential equations

$$dS_\omega^1 = H_0(P, q+\nabla_P S_\omega^1)dt + \sum_{r=1}^m H_r(P, q+\nabla_P S_\omega^1)\circ dw_t^r, \quad S_\omega^1|_{t=t_0}=0, \tag{8}$$

$$dS_\omega^2 = H_0(p+\nabla_Q S_\omega^2, Q)dt + \sum_{r=1}^m H_r(p+\nabla_Q S_\omega^2, Q)\circ dw_t^r, \quad S_\omega^2|_{t=t_0}=0, \tag{9}$$

$$dS_\omega^3 = H_0(w+\frac{1}{2}J^{-1}\nabla S_\omega^3)dt + \sum_{r=1}^m H_r(w+\frac{1}{2}J^{-1}\nabla S_\omega^3)\circ dw_t^r, \quad S_\omega^3|_{t=t_0}=0, \tag{10}$$

where S_ω^1 depends on the coordinates (P,q), S_ω^2 depends on the coordinates (p,Q), and S_ω^3 depends on $w\in\mathbb{R}^{2n}$. Here J is the following matrix

$$J = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix}, \tag{11}$$

where I is the n dimensional unit matrix. Under appropriate conditions (see Theorem 3.1 in [4]) we have:

- The map $(p,q)\to(P(t,\omega),Q(t,\omega))$ defined by

$$P_i = p_i - \frac{\partial S_\omega^1}{\partial q_i}(P,q), \quad Q_i = q_i + \frac{\partial S_\omega^1}{\partial P_i}(P,q), \tag{12}$$

  $i=1,\dots,n$ is the flow of the SHS (1).
- The map $(p,q)\to(P(t,\omega),Q(t,\omega))$ defined by

$$P_i = p_i + \frac{\partial S_\omega^2}{\partial Q_i}(p,Q), \quad Q_i = q_i - \frac{\partial S_\omega^2}{\partial p_i}(p,Q), \tag{13}$$

  $i=1,\dots,n$, is the flow of the SHS (1).
- The map $(p,q)\to(P(t,\omega),Q(t,\omega))$ defined by

$$Y = y - J\nabla S_\omega^3((y+Y)/2), \tag{14}$$

  where $Y=(P^T,Q^T)^T$, $y=(p^T,q^T)^T$ is the flow of the SHS (1).

The key idea to construct high-order symplectic schemes via generating functions is to obtain an approximation of the solution of the HJ PDE, and then to derive the symplectic numerical scheme through the relations (12) - (14).

As in [4], we assume that the generating function can be expressed by the following expansion locally:

$$S_\omega^i(P,q,t) = \sum_\alpha G_\alpha^i J_{\alpha;t_0,t}, \quad i=1,2,3, \tag{15}$$

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

$$J_{\alpha;t_0,t} = \int_{t_0}^t\int_{t_0}^{s_l}\cdots\int_{t_0}^{s_2}\circ dw_{s_1}^{j_1}\cdots\circ dw_{s_{l-1}}^{j_{l-1}}\circ dw_{s_l}^{j_l}. \tag{16}$$

For convenience, ds is denoted by dw_s^0, and we shall write J_α for $J_{\alpha;t_1,t_2}$ whenever the values of the time indexes are obvious.

We denote by $n(\alpha)$ the number of components of the multi-index α that are equal with 0 (e.g $n(\alpha) = 2$, if $\alpha = (0, 3, 0, 1)$). From equations (2.34) in Chapter 5 in [7], we have the following relationship between the Ito integrals

$$I_\alpha[f(\cdot,\cdot)]_{t_0,t} = \int_{t_0}^{t}\int_{t_0}^{s_l}\dots\int_{t_0}^{s_2} f(s_1,\cdot)dw_{s_1}^{j_1}\dots dw_{s_{l-1}}^{j_{l-1}}dw_{s_l}^{j_l}, \quad I_\alpha = I_\alpha[1]_{t_0,t}, \tag{17}$$

and the Stratonovich integrals J_α defined in equation (16): $I_\alpha = J_\alpha$ if $l(\alpha) = 1$ and

$$J_\alpha = I_{(j_l)}\left[J_{\alpha-}\right] + \chi_{\{j_l=j_{l-1}\neq 0\}} I_{(0)}\left[\frac{1}{2}J_{(\alpha-)-}\right], \quad l(\alpha) \geq 2, \tag{18}$$

where $\alpha = (j_1, j_2, \dots, j_l), j_i \in \{0, 1, \dots, m\}$, χ_A denotes the indicator function of the set A, and f is any appropriate process (see Chapter 5 in [7]) .

To introduce the formulas for the coefficients G^i_α, $i = 1, 2, 3$, we define some operations for the multi-indexes. If the multi-index $\alpha = (j_1, j_2, \dots, j_l)$ with $l > 1$ then $\alpha- = (j_1, j_2, \dots, j_{l-1})$, i.e. the last component is deleted. For any two multi-indexes $\alpha = (j_1, j_2, \dots, j_l)$ and $\alpha' = (j'_1, j'_2, \dots, j'_{l'})$, we define the concatenation operation $'*'$ as $\alpha * \alpha' = (j_1, j_2, \dots, j_l, j'_1, j'_2, \dots, j'_{l'})$. The concatenation of a collection Λ of multi-indexes with the multi-index α gives the collection formed by concatenating each element of the collection Λ with the multi-index α, i.e., $\Lambda * \alpha = \{\alpha' * \alpha | \alpha' \in \Lambda\}$. For example, if $\Lambda = \{(1, 1), (0, 1, 2), (1, 1)\}$ and $\alpha = (0)$ then $\Lambda * \alpha = \{(1, 1, 0), (0, 1, 2, 0), (1, 1, 0)\}$.

In [4] we define recursively the collection $\Lambda_{\alpha_1,\dots,\alpha_k}$ depending on the multi-indexes α_1, …, α_k. If $\alpha_1 = (j_1, j_2, \dots, j_l)$ and $\alpha_2 = (j'_1, j'_2, \dots, j'_{l'})$, then $\Lambda_{\alpha_1,\alpha_2}$ is the collection of multi-indexes depending on α_1 and α_2 and given by the following recurrence relation:

$$\Lambda_{\alpha_1,\alpha_2} = \begin{cases} \{(j_1, j'_1), (j'_1, j_1)\}, & \text{if } \quad l = 1 \text{ and } l' = 1 \\ \{\Lambda_{(j_1),\alpha_2-} * (j'_{l'}), \alpha_2 * (j_l)\}, & \text{if } \quad l = 1 \text{ and } l' \neq 1 \\ \{\Lambda_{\alpha_1-,(j'_1)} * (j_l), \alpha_1 * (j'_l)\}, & \text{if } \quad l \neq 1 \text{ and } l' = 1 \\ \{\Lambda_{\alpha_1-,\alpha_2} * (j_l), \Lambda_{\alpha_1,\alpha_2-} * (j'_{l'})\}, & \text{if } \quad l \neq 1 \text{ and } l' \neq 1 \end{cases} \tag{19}$$

For any $k > 2$, we define $\Lambda_{\alpha_1,\dots,\alpha_k} = \{\Lambda_{\beta,\alpha_k} | \beta \in \Lambda_{\alpha_1,\dots,\alpha_{k-1}}\}$. For example, $\Lambda_{(1),(0),(0)} = \{\Lambda_{\beta,(0)} | \beta \in \Lambda_{(1),(0)}\} = \{\Lambda_{(0,1),(0)}, \Lambda_{(1,0),(0)}\} = \{(0, 0, 1), (0, 0, 1), (0, 1, 0), (1, 0, 0), (0, 1, 0), (1, 0, 0)\}$.

In addition to the previous recurrence relation, we can also compute explicitly the collection $\Lambda_{\alpha_1,\dots,\alpha_k}$ (see Lemma 4.4 in [4]). First, for any multi-index $\alpha = (j_1, j_2, \dots, j_l)$ with no duplicated elements, (i.e., $j_m \neq j_n$ if $m \neq n$, $m, n = 1, \dots, l$) we define the set $R(\alpha)$ to be the empty set $R(\alpha) = \emptyset$ if $l = 1$ and $R(\alpha) = \{(j_m, j_n) | m < n, m, n = 1, \dots, l\}$ if $l \geq 2$. $R(\alpha)$ defines a partial order on the set $\{0, \dots, m\}$, defined by $i \prec j$ if and only if $(i, j) \in R(\alpha)$. If there are no duplicated elements in or between any of the multi-indexes $\alpha_1 = (j_1^{(1)}, j_2^{(1)}, \dots, j_{l_1}^{(1)})$, …, $\alpha_k = (j_1^{(k)}, j_2^{(k)}, \dots, j_{l_k}^{(k)})$, then

$$\Lambda_{\alpha_1,\dots,\alpha_k} = \{\beta \in \mathcal{M} | \cup_{i=1}^k R(\alpha_i) \subseteq R(\beta) \text{ and there are no duplicated elements in } \beta\}, \tag{20}$$

where $\mathcal{M} = \{(\hat{j}_1, \hat{j}_2, \dots, \hat{j}_{\hat{l}}) | \hat{j}_i \in \{j_1^{(1)}, j_2^{(1)}, \dots, j_{l_1}^{(1)}, \dots j_1^{(k)}, j_2^{(k)}, \dots, j_{l_k}^{(k)}\}, i = 1, \dots, \hat{l}$, $\hat{l} = l_1 + \dots + l_k\}$. For multi-indexes with duplicated elements, we need to assign a different subscript to each duplicated element. For example, $\Lambda_{(2,0),(0,1)} = \Lambda_{(2,0_1),(0_2,1)} = \{(2, 0_2, 1, 0_1), (0_2, 2, 1, 0_1), (2, 0_1, 0_2, 1), (0_2, 2, 0_1, 1), (0_2, 1, 2, 0_1), (2, 0_2, 0_1, 1)\} = \{(2, 0, 1, 0), (0, 2, 1, 0), (2, 0, 0, 1), (0, 2, 0, 1), (0, 1, 2, 0), (2, 0, 0, 1)\}$.

Notice that

$$\Lambda_{\alpha_1,\ldots,\alpha_k} = \Lambda_{\alpha_{\tau(1)},\ldots,\alpha_{\tau(k)}}, \tag{21}$$

for any permutation τ on the set $\{1,\ldots,k\}$ (i.e. for any bijective function $\tau : \{1,\ldots,k\} \to \{1,\ldots,k\}$).

Replacing the expansion (15) into the HJPDE (8)-(10) and using

$$\prod_{i=1}^{n} J_{\alpha_i} = \sum_{\beta \in \Lambda_{\alpha_1,\ldots,\alpha_n}} J_\beta, \tag{22}$$

we obtain recursive formulas for the coefficients G^i_α, $i = 1, 2, 3$ (see Proposition 4.1 in [4]).

For the coefficients of S^1_ω, if $\alpha = (r)$, $r = 0,\ldots,m$ then $G^1_\alpha = H_r$. If $\alpha = (i_1,\ldots,i_{l-1},r)$, $l > 1$, $i_1,\ldots,i_{l-1},r = 0,\ldots,m$ has no duplicates then

$$\begin{aligned} G^1_\alpha &= \sum_{i=1}^{l(\alpha)-1} \frac{1}{i!} \sum_{k_1,\ldots,k_i=1}^{n} \frac{\partial^i H_r}{\partial q_{k_1}\ldots\partial q_{k_i}} \sum_{\substack{l(\alpha_1)+\cdots+l(\alpha_i)=l(\alpha)-1 \\ R(\alpha_1)\cup\cdots\cup R(\alpha_i)\subseteq R(\alpha-)}} \frac{\partial G^1_{\alpha_1}}{\partial P_{k_1}} \cdots \frac{\partial G^1_{\alpha_i}}{\partial P_{k_i}} \\ &= \sum_{i=1}^{l(\alpha)-1} \frac{1}{i!} \sum_{k_1,\ldots,k_i=1}^{n} \frac{\partial^i H_r}{\partial q_{k_1}\ldots\partial q_{k_i}} \sum_{\substack{l(\alpha_1)+\cdots+l(\alpha_i)=l(\alpha)-1 \\ \alpha-\in\Lambda_{\alpha_1,\ldots,\alpha_i}}} \frac{\partial G^1_{\alpha_1}}{\partial P_{k_1}} \cdots \frac{\partial G^1_{\alpha_i}}{\partial P_{k_i}}. \end{aligned} \tag{23}$$

If the multi-index α contains any duplicates, then we apply formula (23) after associating different subscripts to the repeating numbers. The coefficients of the generating function S^2_ω are obtained by replacing q by p and P by Q in the recurrence (23) .

Proceeding as for S^1_ω, we obtain a general recurrence for finding the coefficients G_α of S^3_ω. Hence If $\alpha = (r)$, $r = 0,\ldots,m$ then $G^3_\alpha = H_r$. If $\alpha = (i_1,\ldots,i_{l-1},r)$, $l > 1$, $i_1,\ldots,i_{l-1},r = 0,\ldots,m$ has no duplicates then

$$\begin{aligned} G^3_\alpha &= \sum_{i=1}^{l(\alpha)-1} \frac{1}{i!} \sum_{k_1,\ldots,k_i=1}^{2n} \frac{\partial^i H_r}{\partial y_{k_1}\ldots\partial y_{k_i}} \sum_{\substack{l(\alpha_1)+\cdots+l(\alpha_i)=l(\alpha)-1 \\ R(\alpha_1)\cup\cdots\cup R(\alpha_i)\subseteq R(\alpha-)}} (\frac{1}{2}J^{-1}\nabla G^3_{\alpha_1})_{k_1} \\ &\quad \ldots (\frac{1}{2}J^{-1}\nabla G^3_{\alpha_i})_{k_i} \\ &= \sum_{i=1}^{l(\alpha)-1} \frac{1}{2^i i!} \sum_{k_1,\ldots,k_i=1}^{2n} \frac{\partial^i H_r}{\partial y_{k_1}\ldots\partial y_{k_i}} \sum_{\substack{l(\alpha_1)+\cdots+l(\alpha_i)=l(\alpha)-1 \\ \alpha-\in\Lambda_{\alpha_1,\ldots,\alpha_i}}} (J^{-1}\nabla G^3_{\alpha_1})_{k_1} \\ &\quad \ldots (J^{-1}\nabla G^3_{\alpha_i})_{k_i}, \end{aligned} \tag{24}$$

where $y = (p^T, q^T)^T$ and $(J^{-1}\nabla G^3_{\alpha_i})_{k_i}$ is the k_i-th component of the column vector $J^{-1}\nabla G^3_{\alpha_i}$. If the multi-index α contains any duplicates, then we apply formula (24) after associating different subscripts with the repeating numbers.

3. Properties of G_α

We now prove an invariance property of the coefficients G^i_α of the generating functions S^i_ω, $i = 1, 2, 3$. For any permutation on $\{1,\ldots,l\}$, $l \geq 1$ and for any multi-index $\alpha = (i_1,\ldots,i_l)$ with $l(\alpha) = l$, let denote by $\pi(\alpha)$ the multi-index defined as $\pi(\alpha) := (i_{\pi(1)},\ldots,i_{\pi(l)})$.

Based on formula (23), we have the following result.

Theorem 3.1. *For SHS preserving the Hamiltonian functions, the coefficients G^1_α of the generating function S^1_ω are invariants under permutations, i.e. $G^1_\alpha = G^1_{\pi(\alpha)}$, for any permutation π on $\{1,\dots,l\}$, where $l = l(\alpha)$.*

Proof. The proof is based on induction on the length of the multi-index α. For systems preserving the Hamiltonian functions the coefficients G^1_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

$$G^1_{(r_1,r_2)} = \sum_{k=1}^{n} \frac{\partial H_{r_2}}{\partial q_k}\frac{\partial H_{r_1}}{\partial P_k} = \sum_{k=1}^{n} \frac{\partial H_{r_1}}{\partial q_k}\frac{\partial H_{r_2}}{\partial P_k} = G^1_{(r_2,r_1)}. \tag{25}$$

We assume that $G^1_\alpha = G^1_{\pi(\alpha)}$ for any multi-index α with $l(\alpha) < l$ and any permutation π on $\{1,\dots,l(\alpha)\}$. Let consider any multi-index α with $l(\alpha) = l$. We suppose that the components of the multi-index α are distinct, otherwise we rename the repeating ones with distinct subscripts. To prove that $G^1_\alpha = G^1_{\pi(\alpha)}$, we analyze several cases depending on the permutation π on $\{1,\dots,l\}$.

Case 1 Let first consider any permutation π such that $\pi(l) = l$. Then we can write $\alpha = (i_1,\dots,i_{l-1},r)$ and $\pi(\alpha) = (i_{\pi(1)},\dots,i_{\pi(l-1)},r)$, with $r = i_l \in \{0,\dots,m\}$. From (23) and $G^1_\beta = G^1_{\pi(\beta)}$ for any multi-index β with $l(\beta) < l$, we get

$$\begin{aligned} G^1_\alpha &= \sum_{i=1}^{l-1}\frac{1}{i!}\sum_{k_1,\dots,k_i=1}^{n}\frac{\partial^i H_r}{\partial q_{k_1}\dots\partial q_{k_i}}\sum_{\substack{l(\alpha_1)+\dots+l(\alpha_i)=l-1\\ \alpha-\in\Lambda_{\alpha_1,\dots,\alpha_i}}}\frac{\partial G^1_{\alpha_1}}{\partial P_{k_1}}\cdots\frac{\partial G^1_{\alpha_i}}{\partial P_{k_i}}\\ &= \sum_{i=1}^{l-1}\frac{1}{i!}\sum_{k_1,\dots,k_i=1}^{n}\frac{\partial^i H_r}{\partial q_{k_1}\dots\partial q_{k_i}}\sum_{\substack{l(\alpha_1)+\dots+l(\alpha_i)=l-1\\ \pi(\alpha)-\in\Lambda_{\alpha_1,\dots,\alpha_i}}}\frac{\partial G^1_{\alpha_1}}{\partial P_{k_1}}\cdots\frac{\partial G^1_{\alpha_i}}{\partial P_{k_i}} = G^1_{\pi(\alpha)}, \end{aligned}$$

Case 2: Now consider any permutation π such that $\pi(l) = l-1$, $\pi(l-1) = l$, $(\alpha-)- = (\pi(\alpha)-)-$. Then we can write $\alpha = (i_1,\dots,i_{l-2},s,r)$ and $\pi(\alpha) = (i_1,\dots,i_{l-2},r,s)$, with $r = i_l \in \{0,\dots,m\}$ and $s = i_{l-1} \in \{0,\dots,m\}$. From (21) and since s is the "largest" number with respect to the partial order $\prec$ on $\alpha-$, we can write

$$\begin{aligned} G^1_\alpha &= \sum_{i=1}^{l-1}\frac{1}{i!}\sum_{k_1,\dots,k_i=1}^{n}\frac{\partial^i H_r}{\partial q_{k_1}\dots\partial q_{k_i}}\sum_{\substack{l(\alpha_1)+\dots+l(\alpha_i)=l-1\\ \alpha-\in\Lambda_{\alpha_1,\dots,\alpha_i}}}\frac{\partial G^1_{\alpha_1}}{\partial P_{k_1}}\cdots\frac{\partial G^1_{\alpha_i}}{\partial P_{k_i}}\\ &= \sum_{k_1=1}^{n}\frac{\partial H_r}{\partial q_{k_1}}\frac{\partial G^1_{((\alpha-)-)*(s)}}{\partial P_{k_1}}\\ &+ \sum_{i=2}^{l-1}\frac{1}{(i-1)!}\sum_{k_1,\dots,k_i=1}^{n}\frac{\partial^i H_r}{\partial q_{k_1}\dots\partial q_{k_i}}\frac{\partial H_s}{\partial P_{k_1}}\sum_{\substack{l(\alpha_2)+\dots+l(\alpha_i)=l-2\\ (\alpha-)-\in\Lambda_{\alpha_2,\dots,\alpha_i}}}\frac{\partial G^1_{\alpha_2}}{\partial P_{k_2}}\cdots\frac{\partial G^1_{\alpha_i}}{\partial P_{k_i}}\\ &+ \sum_{i=2}^{l-2}\frac{1}{(i-1)!}\sum_{j=1}^{l-i-1}\sum_{k_1,\dots,k_i=1}^{n}\frac{\partial^i H_r}{\partial q_{k_1}\dots\partial q_{k_i}}\sum_{\substack{l(\alpha_2)+\dots+l(\alpha_i)=l-2-j,\\ l(\alpha_1)=j,\quad (\alpha-)-\in\Lambda_{\alpha_1,\dots,\alpha_i}}}\frac{\partial G^1_{\alpha_1*(s)}}{\partial P_{k_1}}\cdots\frac{\partial G^1_{\alpha_i}}{\partial P_{k_i}} \end{aligned}$$

Using formula (23) for the first and the third terms, we get

$$
\begin{aligned}
G^1_\alpha = &\sum_{k_1=1}^{n} \frac{\partial H_r}{\partial q_{k_1}} \frac{\partial}{\partial P_{k_1}} \Bigg(\sum_{u=1}^{l-2} \frac{1}{u!} \sum_{c_1,\dots,c_u=1}^{n} \frac{\partial^u H_s}{\partial q_{c_1} \dots \partial q_{c_u}} \\
&\sum_{\substack{l(\beta_1)+\dots+l(\beta_u)=l-2 \\ (\alpha-)-\in\Lambda_{\beta_1,\dots,\beta_u}}} \frac{\partial G^1_{\beta_1}}{\partial P_{c_1}} \cdots \frac{\partial G^1_{\beta_u}}{\partial P_{c_u}} \Bigg) \\
&+ \sum_{i=2}^{l-1} \frac{1}{(i-1)!} \sum_{k_1,\dots,k_i=1}^{n} \frac{\partial^i H_r}{\partial q_{k_1} \dots \partial q_{k_i}} \frac{\partial H_s}{\partial P_{k_1}} \\
&\sum_{\substack{l(\alpha_2)+\dots+l(\alpha_i)=l-2 \\ (\alpha-)-\in\Lambda_{\alpha_2,\dots,\alpha_i}}} \frac{\partial G^1_{\alpha_2}}{\partial P_{k_2}} \cdots \frac{\partial G^1_{\alpha_i}}{\partial P_{k_i}} \\
&+ \sum_{i=2}^{l-2} \frac{1}{(i-1)!} \sum_{j=1}^{l-i-1} \sum_{k_1,\dots,k_i=1}^{n} \frac{\partial^i H_r}{\partial q_{k_1} \dots \partial q_{k_i}} \\
&\sum_{\substack{l(\alpha_2)+\dots+l(\alpha_i)=l-2-j, \\ l(\alpha_1)=j, \quad (\alpha-)-\in\Lambda_{\alpha_1,\dots,\alpha_i}}} \frac{\partial G^1_{\alpha_2}}{\partial P_{k_2}} \cdots \frac{\partial G^1_{\alpha_i}}{\partial P_{k_i}} \\
&\frac{\partial}{\partial P_{k_1}} \Bigg(\sum_{u=1}^{j} \frac{1}{u!} \sum_{c_1,\dots,c_u=1}^{n} \frac{\partial^u H_s}{\partial q_{c_1} \dots \partial q_{c_u}} \sum_{\substack{l(\beta_1)+\dots+l(\beta_u)=j \\ \alpha_1\in\Lambda_{\beta_1,\dots,\beta_u}}} \frac{\partial G^1_{\beta_1}}{\partial P_{c_1}} \cdots \frac{\partial G^1_{\beta_u}}{\partial P_{c_u}} \Bigg)
\end{aligned} \tag{26}
$$

By the product rule, we separate G^1_α into two sums denoted by T_1 and T_2 such that T_1 is formed with all terms that do not include differentiation of the Hamiltonian H_s with respect to P_i, for any $i = 1, \dots, n$. Thus $G^1_\alpha = T_1 + T_2$, with

$$
\begin{aligned}
T_1 = &\sum_{u=1}^{l-2} \frac{1}{u!} \sum_{k_1,c_1,\dots,c_u=1}^{n} \frac{\partial H_r}{\partial q_{k_1}} \frac{\partial^u H_s}{\partial q_{c_1} \dots \partial q_{c_u}} \sum_{\substack{l(\beta_1)+\dots+l(\beta_u)=l-2 \\ (\alpha-)-\in\Lambda_{\beta_1,\dots,\beta_u}}} \frac{\partial}{\partial P_{k_1}} \left(\frac{\partial G^1_{\beta_1}}{\partial P_{c_1}} \cdots \frac{\partial G^1_{\beta_u}}{\partial P_{c_u}} \right) \\
+ &\sum_{i=2}^{l-2} \sum_{j=1}^{l-i-1} \sum_{u=1}^{j} \frac{1}{u!(i-1)!} \sum_{\substack{k_1,\dots,k_i=1 \\ c_1,\dots,c_u=1}}^{n} \frac{\partial^i H_r}{\partial q_{k_1} \dots \partial q_{k_i}} \frac{\partial^u H_s}{\partial q_{c_1} \dots \partial q_{c_u}} \\
&\sum_{\substack{l(\alpha_2)+\dots+l(\alpha_i)=l-2-j, \\ l(\alpha_1)=j, \quad (\alpha-)-\in\Lambda_{\alpha_1,\dots,\alpha_i}}} \frac{\partial G^1_{\alpha_2}}{\partial P_{k_2}} \cdots \frac{\partial G^1_{\alpha_i}}{\partial P_{k_i}} \sum_{\substack{l(\beta_1)+\dots+l(\beta_u)=j \\ \alpha_1\in\Lambda_{\beta_1,\dots,\beta_u}}} \frac{\partial}{\partial P_{k_1}} \left(\frac{\partial G^1_{\beta_1}}{\partial P_{c_1}} \cdots \frac{\partial G^1_{\beta_u}}{\partial P_{c_u}} \right)
\end{aligned}
$$

After simple manipulations of the summation indexes, using (21) we get

$$
\begin{aligned}
T_1 = &\sum_{k_1,c_1=1}^{n} \frac{\partial H_r}{\partial q_{k_1}} \frac{\partial H_s}{\partial q_{c_1}} \frac{\partial^2 G^1_{(\alpha-)-}}{\partial P_{k_1} \partial P_{c_1}} \\
&+ \sum_{u=2}^{l-2} \frac{1}{u!} \sum_{k_1,c_1,\dots,c_u=1}^{n} \frac{\partial H_r}{\partial q_{k_1}} \frac{\partial^u H_s}{\partial q_{c_1} \dots \partial q_{c_u}} \sum_{\substack{l(\beta_1)+\dots+l(\beta_u)=l-2 \\ (\alpha-)-\in\Lambda_{\beta_1,\dots,\beta_u}}} \frac{\partial}{\partial P_{k_1}} \left(\frac{\partial G^1_{\beta_1}}{\partial P_{c_1}} \cdots \frac{\partial G^1_{\beta_u}}{\partial P_{c_u}} \right)
\end{aligned}
$$

$$+\sum_{i=2}^{l-2}\sum_{u=1}^{l-i-1}\frac{1}{(i-1)!u!}\sum_{\substack{k_1,\dots,k_i=1\\c_1,\dots,c_u=1}}^{n}\frac{\partial^i H_r}{\partial q_{k_1}\dots\partial q_{k_i}}\frac{\partial^u H_s}{\partial q_{c_1}\dots\partial q_{c_u}}\sum_{j=u}^{l-i-1}\sum_{\substack{l(\alpha_2)+\dots+l(\alpha_i)=l-2-j,\\ l(\alpha_1)=j,\quad (\alpha-)-\in\Lambda_{\alpha_1,\dots,\alpha_i}}}$$

$$\frac{\partial G^1_{\alpha_2}}{\partial P_{k_2}}\cdots\frac{\partial G^1_{\alpha_i}}{\partial P_{k_i}}\sum_{\substack{l(\beta_1)+\dots+l(\beta_u)=j\\ \alpha_1\in\Lambda_{\beta_1,\dots,\beta_u}}}\frac{\partial}{\partial P_{k_1}}\left(\frac{\partial G^1_{\beta_1}}{\partial P_{c_1}}\cdots\frac{\partial G^1_{\beta_u}}{\partial P_{c_u}}\right)$$

$$=\sum_{k_1,c_1=1}^{n}\frac{\partial H_r}{\partial q_{k_1}}\frac{\partial H_s}{\partial q_{c_1}}\frac{\partial^2 G^1_{(\alpha-)-}}{\partial P_{k_1}\partial P_{c_1}}$$

$$+\sum_{u=2}^{l-2}\frac{1}{u!}\sum_{k_1,c_1,\dots,c_u=1}^{n}\frac{\partial H_r}{\partial q_{k_1}}\frac{\partial^u H_s}{\partial q_{c_1}\dots\partial q_{c_u}}\sum_{\substack{l(\beta_1)+\dots+l(\beta_u)=l-2\\ (\alpha-)-\in\Lambda_{\beta_1,\dots,\beta_u}}}\frac{\partial}{\partial P_{k_1}}\left(\frac{\partial G^1_{\beta_1}}{\partial P_{c_1}}\cdots\frac{\partial G^1_{\beta_u}}{\partial P_{c_u}}\right)$$

$$+\sum_{i=2}^{l-2}\sum_{u=1}^{l-i-1}\frac{1}{u!(i-1)!}\sum_{\substack{k_1,\dots,k_i=1\\c_1,\dots,c_u=1}}^{n}\frac{\partial^i H_r}{\partial q_{k_1}\dots\partial q_{k_i}}\frac{\partial^u H_s}{\partial q_{c_1}\dots\partial q_{c_u}}$$

$$\sum_{\substack{l(\alpha_2)+\dots+l(\beta_u)=l-2\\ (\alpha-)-\in\Lambda_{\alpha_2,\dots,\alpha_i,\beta_1,\dots,\beta_u}}}\frac{\partial G^1_{\alpha_2}}{\partial P_{k_2}}\cdots\frac{\partial G^1_{\alpha_i}}{\partial P_{k_i}}\frac{\partial}{\partial P_{k_1}}\left(\frac{\partial G^1_{\beta_1}}{\partial P_{c_1}}\cdots\frac{\partial G^1_{\beta_u}}{\partial P_{c_u}}\right)$$

Using again the product rule and (21), we obtain

$$\begin{aligned}
T_1 = &\sum_{k_1,c_1=1}^{n}\frac{\partial H_r}{\partial q_{k_1}}\frac{\partial H_s}{\partial q_{c_1}}\frac{\partial^2 G^1_{(\alpha-)-}}{\partial P_{k_1}\partial P_{c_1}}+\sum_{u=2}^{l-2}\frac{1}{(u-1)!}\\
&\sum_{k_1,c_1,\dots,c_u=1}^{n}\frac{\partial H_r}{\partial q_{k_1}}\frac{\partial^u H_s}{\partial q_{c_1}\dots\partial q_{c_u}}\sum_{\substack{1\le l(\beta)\le l-1-u\\ R(\beta)\subseteq R((\alpha-)-)}}\frac{\partial^2 G^1_\beta}{\partial P_{k_1}\partial P_{c_1}}\\
&\sum_{\substack{l(\beta)+l(\gamma_1)\dots+l(\gamma_{u-1})=l-2\\ (\alpha-)-\in\Lambda_{\beta,\gamma_1\dots,\gamma_{u-1}}}}\frac{\partial G^1_{\gamma_1}}{\partial P_{c_2}}\cdots\frac{\partial G^1_{\gamma_{u-1}}}{\partial P_{c_u}}+\sum_{i=2}^{l-2}\frac{1}{(i-1)!}\\
&\sum_{c_1,k_1,\dots,k_i=1}^{n}\frac{\partial^i H_r}{\partial q_{k_1}\dots\partial q_{k_i}}\frac{\partial H_s}{\partial q_{c_1}}\sum_{\substack{1\le l(\beta)\le l-1-i\\ R(\beta)\subseteq R((\alpha-)-)}}\frac{\partial^2 G^1_\beta}{\partial P_{k_1}\partial P_{c_1}}\\
&\sum_{\substack{l(\beta)+l(\gamma_1)\dots+l(\gamma_{i-1})=l-2\\ (\alpha-)-\in\Lambda_{\beta,\gamma_1\dots,\gamma_{i-1}}}}\frac{\partial G^1_{\gamma_1}}{\partial P_{k_2}}\cdots\frac{\partial G^1_{\gamma_{i-1}}}{\partial P_{k_i}}+\sum_{i=2}^{l-3}\sum_{u=2}^{l-i-1}\frac{1}{(i-1)!(u-1)!}\\
&\sum_{\substack{k_1,\dots,k_i=1\\c_1,\dots,c_u=1}}^{n}\frac{\partial^i H_r}{\partial q_{k_1}\dots\partial q_{k_i}}\frac{\partial^u H_s}{\partial q_{c_1}\dots\partial q_{c_u}}\sum_{\substack{1\le l(\beta)\le l-i-u\\ R(\beta)\subseteq R((\alpha-)-)}}\frac{\partial^2 G^1_\beta}{\partial P_{k_1}\partial P_{c_1}}\\
&\sum_{\substack{l(\beta)+l(\gamma_1)+\dots+l(\gamma_{i+u-2})=l-2\\ (\alpha-)-\in\Lambda_{\beta,\gamma_1,\dots,\gamma_{i+u-2}}}}\frac{\partial G^1_{\gamma_1}}{\partial P_{k_2}}\cdots\frac{\partial G^1_{\gamma_{i-1}}}{\partial P_{k_i}}\frac{\partial G^1_{\gamma_i}}{\partial P_{c_2}}\cdots\frac{\partial G^1_{\gamma_{i+u-2}}}{\partial P_{c_u}}
\end{aligned}\tag{27}$$

Notice that by first summing with respect to u and then with respect to i, we can rewrite the last term of T_1 as

$$\sum_{u=2}^{l-3}\sum_{i=2}^{l-u-1}\frac{1}{(i-1)!(u-1)!}\sum_{\substack{k_1,\dots,k_i=1\\c_1,\dots,c_u=1}}^{n}\frac{\partial^i H_r}{\partial q_{k_1}\dots\partial q_{k_i}}\frac{\partial^u H_s}{\partial q_{c_1}\dots\partial q_{c_u}}\sum_{\substack{1\le l(\beta)\le l-i-u\\R(\beta)\subseteq R((\alpha-)-)}}\frac{\partial^2 G^1_\beta}{\partial P_{k_1}\partial P_{c_1}}$$
$$\sum_{\substack{l(\beta)+l(\gamma_1)+\dots+l(\gamma_{i+u-2})=l-2\\(\alpha-)-\in\Lambda_{\beta,\gamma_1,\dots,\gamma_{i+u-2}}}}\frac{\partial G^1_{\gamma_1}}{\partial P_{k_2}}\cdots\frac{\partial G^1_{\gamma_{i-1}}}{\partial P_{k_i}}\frac{\partial G^1_{\gamma_i}}{\partial P_{c_2}}\cdots\frac{\partial G^1_{\gamma_{i+u-2}}}{\partial P_{c_u}}$$

Thus if we switch s and r, the formula (27) for T_1 does not change. Hence, T_1 is symmetric in s and r.

From equation (26) and $G^1_\alpha = T_1 + T_2$, we have

$$T_2=\sum_{i=2}^{l-1}\frac{1}{(i-1)!}\sum_{k_1,\dots,k_i=1}^{n}\frac{\partial^i H_r}{\partial q_{k_1}\dots\partial q_{k_i}}\frac{\partial H_s}{\partial P_{k_1}}\sum_{\substack{l(\alpha_2)+\dots+l(\alpha_i)=l-2\\(\alpha-)-\in\Lambda_{\alpha_2,\dots,\alpha_i}}}\frac{\partial G^1_{\alpha_2}}{\partial P_{k_2}}\cdots\frac{\partial G^1_{\alpha_i}}{\partial P_{k_i}}$$
$$+\sum_{u=1}^{l-2}\frac{1}{u!}\sum_{k_1,c_1,\dots,c_u=1}^{n}\frac{\partial H_r}{\partial q_{k_1}}\frac{\partial^{u+1} H_s}{\partial P_{k_1}\partial q_{c_1}\dots\partial q_{c_u}}\sum_{\substack{l(\beta_1)+\dots+l(\beta_u)=l-2\\(\alpha-)-\in\Lambda_{\beta_1,\dots,\beta_u}}}\frac{\partial G^1_{\beta_1}}{\partial P_{c_1}}\cdots\frac{\partial G^1_{\beta_u}}{\partial P_{c_u}}$$
$$+\sum_{i=2}^{l-2}\sum_{j=1}^{l-i-1}\sum_{u=1}^{j}\frac{1}{(i-1)!u!}\sum_{\substack{k_1,\dots,k_i=1\\c_1,\dots,c_u=1}}^{n}\frac{\partial^i H_r}{\partial q_{k_1}\dots\partial q_{k_i}}\frac{\partial^{u+1} H_s}{\partial P_{k_1}\partial q_{c_1}\dots\partial q_{c_u}}$$
$$\sum_{\substack{l(\alpha_2)+\dots+l(\alpha_i)=l-2-j,\\l(\alpha_1)=j,\quad(\alpha-)-\in\Lambda_{\alpha_1,\dots,\alpha_i}}}\frac{\partial G^1_{\alpha_2}}{\partial P_{k_2}}\cdots\frac{\partial G^1_{\alpha_i}}{\partial P_{k_i}}\sum_{\substack{l(\beta_1)+\dots+l(\beta_u)=j\\\alpha_1\in\Lambda_{\beta_1,\dots,\beta_u}}}\frac{\partial G^1_{\beta_1}}{\partial P_{c_1}}\cdots\frac{\partial G^1_{\beta_u}}{\partial P_{c_u}}$$

Similarly as for T_1, using (21), we obtain

$$T_2=\sum_{i=1}^{l-2}\frac{1}{i!}\sum_{k_1,j_1\dots,j_i=1}^{n}\frac{\partial^{i+1} H_r}{\partial q_{k_1}\partial q_{j_1}\dots\partial q_{j_i}}\frac{\partial H_s}{\partial P_{k_1}}\sum_{\substack{l(\alpha_1)+\dots+l(\alpha_i)=l-2\\(\alpha-)-\in\Lambda_{\alpha_1,\dots,\alpha_i}}}\frac{\partial G^1_{\alpha_1}}{\partial P_{j_1}}\cdots\frac{\partial G^1_{\alpha_i}}{\partial P_{j_i}}$$
$$+\sum_{i=1}^{l-2}\frac{1}{i!}\sum_{k_1,j_1\dots,j_i=1}^{n}\frac{\partial H_r}{\partial q_{k_1}}\frac{\partial^{i+1} H_s}{\partial P_{k_1}\partial q_{j_1}\dots\partial q_{j_i}}\sum_{\substack{l(\beta_1)+\dots+l(\beta_i)=l-2\\(\alpha-)-\in\Lambda_{\beta_1,\dots,\beta_i}}}\frac{\partial G^1_{\beta_1}}{\partial P_{j_1}}\cdots\frac{\partial G^1_{\beta_i}}{\partial P_{j_i}}$$
$$+\sum_{i=2}^{l-2}\sum_{u=1}^{l-i-1}\frac{1}{(i-1)!u!}\sum_{\substack{k_1,\dots,k_i=1\\c_1,\dots,c_u=1}}^{n}\frac{\partial^i H_r}{\partial q_{k_1}\dots\partial q_{k_i}}\frac{\partial^{u+1} H_s}{\partial P_{k_1}\partial q_{c_1}\dots\partial q_{c_u}}$$
$$\sum_{\substack{l(\alpha_2)+\dots+l(\beta_u)=l-2\\(\alpha-)-\in\Lambda_{\alpha_2,\dots,\alpha_i,\beta_1,\dots,\beta_u}}}\frac{\partial G^1_{\alpha_2}}{\partial P_{k_2}}\cdots\frac{\partial G^1_{\alpha_i}}{\partial P_{k_i}}\frac{\partial G^1_{\beta_1}}{\partial P_{c_1}}\cdots\frac{\partial G^1_{\beta_u}}{\partial P_{c_u}}$$

Introducing a new summation with index $v = i + u - 1$ for the last term, we get

$$T_2 = \sum_{i=1}^{l-2} \frac{1}{i!} \sum_{k_1, j_1 \ldots, j_i = 1}^{n} \frac{\partial^{i+1} H_r}{\partial q_{k_1} q_{j_1} \ldots \partial q_{j_i}} \frac{\partial H_s}{\partial P_{k_1}} \sum_{\substack{l(\alpha_1)+\cdots+l(\alpha_i)=l-2 \\ (\alpha-)-\in\Lambda_{\alpha_1,\ldots,\alpha_i}}} \frac{\partial G^1_{\alpha_1}}{\partial P_{j_1}} \cdots \frac{\partial G^1_{\alpha_i}}{\partial P_{j_i}}$$

$$+ \sum_{i=1}^{l-2} \frac{1}{i!} \sum_{k_1, j_1 \ldots, j_i = 1}^{n} \frac{\partial H_r}{\partial q_{k_1}} \frac{\partial^{i+1} H_s}{\partial P_{k_1} \partial q_{j_1} \ldots \partial q_{j_i}} \sum_{\substack{l(\beta_1)+\cdots+l(\beta_i)=l-2 \\ (\alpha-)-\in\Lambda_{\beta_1,\ldots,\beta_i}}} \frac{\partial G^1_{\beta_1}}{\partial P_{j_1}} \cdots \frac{\partial G^1_{\beta_i}}{\partial P_{j_i}}$$

$$+ \sum_{v=2}^{l-2} \sum_{i=2}^{v} \frac{1}{(i-1)!(v-i+1)!} \sum_{k_1, j_1, \ldots, j_v = 1}^{n} \frac{\partial^i H_r}{\partial q_{k_1} \partial q_{j_1} \ldots \partial q_{j_{i-1}}} \frac{\partial^{v+2-i} H_s}{\partial P_{k_1} \partial q_{j_i} \ldots \partial q_{j_v}}$$

$$\sum_{\substack{l(\gamma_1)+\cdots+l(\gamma_v)=l-2 \\ (\alpha-)-\in\Lambda_{\gamma_1,\ldots,\gamma_v}}} \frac{\partial G^1_{\gamma_1}}{\partial P_{j_1}} \cdots \frac{\partial G^1_{\gamma_v}}{\partial P_{j_v}}$$

Notice that T_2 can be expressed as follows
(28)
$$T_2 = \sum_{v=1}^{l-2} \frac{1}{v!} \sum_{k_1, j_1, \ldots, j_v = 1}^{n} \frac{\partial^v}{\partial q_{j_1} \cdots \partial q_{j_v}} \left(\frac{\partial H_r}{\partial q_{k_1}} \frac{\partial H_s}{\partial P_{k_1}} \right) \sum_{\substack{l(\gamma_1)+\cdots+l(\gamma_v)=l-2 \\ (\alpha-)-\in\Lambda_{\gamma_1,\ldots,\gamma_v}}} \frac{\partial G^1_{\gamma_1}}{\partial P_{j_1}} \cdots \frac{\partial G^1_{\gamma_v}}{\partial P_{j_v}}.$$

Hence T_2 is symmetric with respect to s and r because $\frac{\partial H_r}{\partial q_{k_1}} \frac{\partial H_s}{\partial P_{k_1}} = \frac{\partial H_r}{\partial P_{k_1}} \frac{\partial H_s}{\partial q_{k_1}}$ for any $k_1 = 1, \ldots, n$.

Thus G^1_α is symmetric with respect to r and s, so we have $G^1_\alpha = G^1_{\pi(\alpha)}$.

Case3: For any arbitrary permutation π on $\{1, \ldots, l\}$ not in any of the previous two cases (i.e. $\pi(l) \neq l$ and either $\pi(l) \neq l-1$ or $\pi(l-1) \neq l$), let consider any multi-index $\alpha = (i_1, \ldots, i_{l-1}, i_l)$, $\pi(\alpha) = (i_{\pi(1)}, \ldots, i_{\pi(l-1)}, i_{\pi(l)})$ and denote $r = i_l$, $s = i_{\pi(l)}$. Since $\pi(l) \neq l$, we have $r \neq s$, and there exists $k \in \{1, \ldots, l-1\}$ such that $i_k = s$. We consider a permutation π_1 on $\{1, \ldots, l\}$ defined by $\pi_1(k) = l-1$, $\pi_1(l-1) = k$, $\pi_1(u) = u$, for $u = 1, \ldots, l$, $u \neq k$, $u \neq l-1$. Thus $\pi_1(\alpha) = (i_{\pi_1(1)}, \ldots, s, r)$, and from Cases 1 and 2, we know that $G^1_\alpha = G^1_{\pi_1(\alpha)} = G^1_{\alpha_1}$, where $\alpha_1 = (i_{\pi_1(1)}, \ldots, r, s)$. Notice that $\alpha_1 = (i_1, \ldots, i_{l-1}, \ldots, i_l, s)$, so we can obtain $\pi(\alpha)$ from α_1 by applying a permutation π_2 with $\pi_2(l) = l$. From Case 1, we have $G^1_{\alpha_1} = G^1_{\pi_2(\alpha_1)} = G^1_{\pi(\alpha)}$. Therefore, $G^1_\alpha = G^1_{\pi(\alpha)}$.

Putting together the previous three cases, we get $G^1_\alpha = G^1_{\pi(\alpha)}$ for any permutation π and any multi-index α with $l(\alpha) = l$. □

Given that the coefficients of the generating function S^2_ω are obtained by replacing q by p and P by Q in the recurrence (23), we can easily adapt the previous proof to show that the coefficients of S^2_ω are also invariant under permutations .

A similar result also holds for the coefficients of the generating function S^3_ω and it is based on formula (24).

Theorem 3.2. *For SHS preserving the Hamiltonian functions, the coefficients G^3_α of the generating function S^3_ω are invariant under permutations.*

Proof. The proof can be done by induction on the length of the multi-index α. For systems preserving the Hamiltonian functions the coefficients G^3_α of S^3_ω are invariant under the permutations on α, when $l(\alpha) = 2$ because for any $r_1, r_2 = 0, \ldots, m$, we have

$$G^3_{(r_1,r_2)} = \frac{1}{2}\sum_{k=1}^{n}\left(-\frac{\partial H_{r_2}}{\partial y_k}\frac{\partial H_{r_1}}{\partial y_{k+n}} + \frac{\partial H_{r_2}}{\partial y_{k+n}}\frac{\partial H_{r_1}}{\partial y_k}\right) = 0 = G^3_{(r_2,r_1)}. \tag{29}$$

We assume that $G^3_\alpha = G^3_{\pi(\alpha)}$ for any multi-index α with $l(\alpha) < l$ and for any permutation π on $\{1,\dots,l(\alpha)\}$. Let consider any multi-index α with $l(\alpha) = l$. We suppose that the components of the multi-index α are distinct, otherwise we rename the repeating ones with distinct subscripts. To prove that $G^3_\alpha = G^3_{\pi(\alpha)}$, we analyze the same three cases as in the proof of Theorem 3.1. The arguments for Cases 1 and 3 are similar, so we will present the details only for Case 2.

Let consider any permutation π such that $\pi(l) = l-1$, $\pi(l-1) = l$, $(\alpha-)- = (\pi(\alpha)-)-$, and denote $\alpha = (i_1,\dots,i_{l-2},s,r)$ and $\pi(\alpha) = (i_1,\dots,i_{l-2},r,s)$, with $r,s \in \{0,\dots,m\}$. Notice that for any $2n$- dimensional vector $v = (v_1,\dots,v_{2n})^T$, we have $J^{-1}v = (-v_{n+1},\dots,-v_{2n},v_1,\dots,v_n)^T$.

Since s is the "largest" number with respect to the partial order $\prec$ on $\alpha-$, from formulas (21) and (24) we get

$$\begin{aligned}
G^3_\alpha &= \sum_{i=1}^{l-1}\frac{1}{2^i i!}\sum_{k_1,\dots,k_i=1}^{2n}\frac{\partial^i H_r}{\partial y_{k_1}\dots\partial y_{k_i}}\sum_{\substack{l(\alpha_1)+\dots+l(\alpha_i)=l-1\\ \alpha-\in\Lambda_{\alpha_1,\dots,\alpha_i}}}(J^{-1}\nabla G^3_{\alpha_1})_{k_1}\dots(J^{-1}\nabla G^3_{\alpha_i})_{k_i}\\
&= \frac{1}{2}\sum_{k_1=1}^{n}\left(-\frac{\partial H_r}{\partial y_{k_1}}\frac{\partial G^3_{((\alpha-)-)*(s)}}{\partial y_{k_1+n}} + \frac{\partial H_r}{\partial y_{k_1+n}}\frac{\partial G^3_{((\alpha-)-)*(s)}}{\partial y_{k_1}}\right)\\
&+ \sum_{i=2}^{l-1}\frac{1}{2^i(i-1)!}\sum_{k1=1}^{n}\sum_{k_2,\dots,k_i=1}^{2n}\left(-\frac{\partial^i H_r}{\partial y_{k_1}\dots\partial y_{k_i}}\frac{\partial H_s}{\partial y_{k_1+n}} + \frac{\partial^i H_r}{\partial y_{k_1+n}\dots\partial y_{k_i}}\frac{\partial H_s}{\partial y_{k_1}}\right)\\
&\sum_{\substack{l(\alpha_2)+\dots+l(\alpha_i)=l-2\\ (\alpha-)-\in\Lambda_{\alpha_2,\dots,\alpha_i}}}(J^{-1}\nabla G^3_{\alpha_2})_{k_2}\dots(J^{-1}\nabla G^3_{\alpha_i})_{k_i} + \sum_{i=2}^{l-2}\frac{1}{2^i(i-1)!}\\
&\sum_{j=1}^{l-i-1}\sum_{k_1=1}^{n}\sum_{k_2,\dots,k_i=1}^{2n}\sum_{\substack{l(\alpha_2)+\dots+l(\alpha_i)=l-2-j,\\ l(\alpha_1)=j,\quad (\alpha-)-\in\Lambda_{\alpha_1,\dots,\alpha_i}}}(J^{-1}\nabla G^3_{\alpha_2})_{k_2}\dots(J^{-1}\nabla G^3_{\alpha_i})_{k_i}\\
&\left(-\frac{\partial^i H_r}{\partial y_{k_1}\dots\partial y_{k_i}}\frac{\partial G^3_{\alpha_1*(s)}}{\partial y_{k_1+n}} + \frac{\partial^i H_r}{\partial y_{k_1+n}\dots\partial y_{k_i}}\frac{\partial G^3_{\alpha_1*(s)}}{\partial y_{k_1}}\right)
\end{aligned}$$

Using formula (24) for the first and the third terms, we get

$$\begin{aligned}
G^3_\alpha &= \frac{1}{2}\sum_{k_1=1}^{n}\sum_{u=1}^{l-2}\frac{1}{2^u u!}\Bigg(-\frac{\partial H_r}{\partial y_{k_1}}\frac{\partial}{\partial y_{k_1+n}}\Bigg(\sum_{c_1,\dots,c_u=1}^{2n}\frac{\partial^u H_s}{\partial y_{c_1}\dots\partial y_{c_u}}\\
&\sum_{\substack{l(\beta_1)+\dots+l(\beta_u)=l-2\\ (\alpha-)-\in\Lambda_{\beta_1,\dots,\beta_u}}}(J^{-1}\nabla G^3_{\beta_1})_{c_1}\dots(J^{-1}\nabla G^3_{\beta_u})_{c_u}\Bigg)+\frac{\partial H_r}{\partial y_{k_1+n}}\\
&\frac{\partial}{\partial y_{k_1}}\Bigg(\sum_{c_1,\dots,c_u=1}^{2n}\frac{\partial^u H_s}{\partial y_{c_1}\dots\partial y_{c_u}}\sum_{\substack{l(\beta_1)+\dots+l(\beta_u)=l-2\\ (\alpha-)-\in\Lambda_{\beta_1,\dots,\beta_u}}}(J^{-1}\nabla G^3_{\beta_1})_{c_1}\dots(J^{-1}\nabla G^3_{\beta_u})_{c_u}\Bigg)\Bigg)
\end{aligned}$$

$$+\sum_{i=2}^{l-1}\frac{1}{2^i(i-1)!}\sum_{k1=1}^{n}\sum_{k_2,\dots,k_i=1}^{2n}\left(-\frac{\partial^i H_r}{\partial y_{k_1}\dots\partial y_{k_i}}\frac{\partial H_s}{\partial y_{k_1+n}}+\frac{\partial^i H_r}{\partial y_{k_1+n}\dots\partial y_{k_i}}\frac{\partial H_s}{\partial y_{k_1}}\right)$$
$$\sum_{\substack{l(\alpha_2)+\dots+l(\alpha_i)=l-2\\(\alpha-)-\in\Lambda_{\alpha_2,\dots,\alpha_i}}}(J^{-1}\nabla G^3_{\alpha_2})_{k_2}\dots(J^{-1}\nabla G^3_{\alpha_i})_{k_i}$$
$$+\sum_{i=2}^{l-2}\frac{1}{2^i(i-1)!}\sum_{j=1}^{l-i-1}\sum_{u=1}^{j}\frac{1}{2^u u!}\sum_{k_1=1}^{n}\sum_{k_2,\dots,k_i=1}^{2n}\sum_{\substack{l(\alpha_2)+\dots+l(\alpha_i)=l-2-j,\\l(\alpha_1)=j,\quad(\alpha-)-\in\Lambda_{\alpha_1,\dots,\alpha_i}}}(J^{-1}\nabla G^3_{\alpha_2})_{k_2}$$
$$\dots(J^{-1}\nabla G^3_{\alpha_i})_{k_i}\Bigg(-\frac{\partial^i H_r}{\partial y_{k_1}\dots\partial y_{k_i}}\frac{\partial}{\partial y_{k_1+n}}\Bigg(\sum_{c_1,\dots,c_u=1}^{2n}\frac{\partial^u H_s}{\partial y_{c_1}\dots\partial y_{c_u}}$$
$$\sum_{\substack{l(\beta_1)+\dots+l(\beta_u)=j\\\alpha_1\in\Lambda_{\beta_1,\dots,\beta_u}}}(J^{-1}\nabla G^3_{\beta_1})_{c_1}\dots(J^{-1}\nabla G^3_{\beta_u})_{c_u}\Bigg)+\frac{\partial^i H_r}{\partial y_{k_1+n}\dots\partial y_{k_i}}$$
$$\frac{\partial}{\partial y_{k_1}}\Bigg(\sum_{c_1,\dots,c_u=1}^{2n}\frac{\partial^u H_s}{\partial y_{c_1}\dots\partial y_{c_u}}\sum_{\substack{l(\beta_1)+\dots+l(\beta_u)=j\\\alpha_1\in\Lambda_{\beta_1,\dots,\beta_u}}}(J^{-1}\nabla G^3_{\beta_1})_{c_1}\dots(J^{-1}\nabla G^3_{\beta_u})_{c_u}\Bigg)\Bigg)$$

As in the proof of Theorem 3.1, we separate into $G^3_\alpha = T_1 + T_2$ with

$$T_1=\sum_{u=1}^{l-2}\frac{1}{2^{u+1}u!}\sum_{k_1=1}^{n}\sum_{c_1,\dots,c_u=1}^{2n}\frac{\partial^u H_s}{\partial y_{c_1}\dots\partial y_{c_u}}$$
$$\sum_{\substack{l(\beta_1)+\dots+l(\beta_u)=l-2\\(\alpha-)-\in\Lambda_{\beta_1,\dots,\beta_u}}}\Bigg(-\frac{\partial H_r}{\partial y_{k_1}}\frac{\partial}{\partial y_{k_1+n}}\left((J^{-1}\nabla G^3_{\beta_1})_{c_1}\dots(J^{-1}\nabla G^3_{\beta_u})_{c_u}\right)$$
$$+\frac{\partial H_r}{\partial y_{k_1+n}}\frac{\partial}{\partial y_{k_1}}\left((J^{-1}\nabla G^3_{\beta_1})_{c_1}\dots(J^{-1}\nabla G^3_{\beta_u})_{c_u}\right)\Bigg)$$
$$+\sum_{i=2}^{l-2}\sum_{j=1}^{l-i-1}\sum_{u=1}^{j}\frac{1}{2^{u+i}u!(i-1)!}\sum_{k_1=1}^{n}\sum_{\substack{k_2,\dots,k_i=1\\c_1,\dots,c_u=1}}^{2n}\frac{\partial^u H_s}{\partial y_{c_1}\dots\partial y_{c_u}}$$
$$\sum_{\substack{l(\alpha_2)+\dots+l(\alpha_i)=l-2-j,\\l(\alpha_1)=j,\quad(\alpha-)-\in\Lambda_{\alpha_1,\dots,\alpha_i}}}(J^{-1}\nabla G^3_{\alpha_2})_{k_2}\dots(J^{-1}\nabla G^3_{\alpha_i})_{k_i}$$
$$\sum_{\substack{l(\beta_1)+\dots+l(\beta_u)=j\\\alpha_1\in\Lambda_{\beta_1,\dots,\beta_u}}}\Bigg(-\frac{\partial^i H_r}{\partial y_{k_1}\dots\partial y_{k_i}}\frac{\partial}{\partial y_{k_1+n}}\left((J^{-1}\nabla G^3_{\beta_1})_{c_1}\dots(J^{-1}\nabla G^3_{\beta_u})_{c_u}\right)$$
$$+\frac{\partial^i H_r}{\partial y_{k_1+n}\dots\partial y_{k_i}}\frac{\partial}{\partial y_{k_1}}\left((J^{-1}\nabla G^3_{\beta_1})_{c_1}\dots(J^{-1}\nabla G^3_{\beta_u})_{c_u}\right)\Bigg)$$

After simple manipulations of the summation indexes, using (21) we get

$$T_1=\frac{1}{2^2}\sum_{k_1=1}^{n}\sum_{c_1=1}^{2n}\frac{\partial H_s}{\partial y_{c_1}}\left(-\frac{\partial H_r}{\partial y_{k_1}}\frac{\partial(J^{-1}\nabla G^3_{(\alpha-)-})_{c_1}}{\partial y_{k_1+n}}+\frac{\partial H_r}{\partial y_{k_1+n}}\frac{\partial(J^{-1}\nabla G^3_{(\alpha-)-})_{c_1}}{\partial y_{k_1}}\right)$$

$$+\sum_{u=2}^{l-2}\frac{1}{2^{u+1}u!}\sum_{k_1=1}^{n}\sum_{c_1,\dots,c_u=1}^{2n}\frac{\partial^u H_s}{\partial y_{c_1}\dots\partial y_{c_u}}$$

$$\sum_{\substack{l(\beta_1)+\dots+l(\beta_u)=l-2\\(\alpha-)-\in\Lambda_{\beta_1,\dots,\beta_u}}}\Bigg(-\frac{\partial H_r}{\partial y_{k_1}}\frac{\partial}{\partial y_{k_1+n}}\left((J^{-1}\nabla G^3_{\beta_1})_{c_1}\dots(J^{-1}\nabla G^3_{\beta_u})_{c_u}\right)$$

$$+\frac{\partial H_r}{\partial y_{k_1+n}}\frac{\partial}{\partial y_{k_1}}\left((J^{-1}\nabla G^3_{\beta_1})_{c_1}\dots(J^{-1}\nabla G^3_{\beta_u})_{c_u}\right)\Bigg)$$

$$+\sum_{i=2}^{l-2}\sum_{u=1}^{l-i-1}\frac{1}{2^{u+i}u!(i-1)!}\sum_{k_1=1}^{n}\sum_{\substack{k_2,\dots,k_i=1\\c_1,\dots,c_u=1}}^{2n}\frac{\partial^u H_s}{\partial y_{c_1}\dots\partial y_{c_u}}$$

$$\sum_{\substack{l(\alpha_2)+\dots+l(\beta_u)=l-2\\(\alpha-)-\in\Lambda_{\alpha_2,\dots,\alpha_i,\beta_1,\dots,\beta_u}}}(J^{-1}\nabla G^3_{\alpha_2})_{k_2}\dots(J^{-1}\nabla G^3_{\alpha_i})_{k_i}$$

$$\left(-\frac{\partial^i H_r}{\partial y_{k_1}\dots\partial y_{k_i}}\frac{\partial}{\partial y_{k_1+n}}\left((J^{-1}\nabla G^3_{\beta_1})_{c_1}\dots(J^{-1}\nabla G^3_{\beta_u})_{c_u}\right)\right.$$

$$\left.+\frac{\partial^i H_r}{\partial y_{k_1+n}\dots\partial y_{k_i}}\frac{\partial}{\partial y_{k_1}}\left((J^{-1}\nabla G^3_{\beta_1})_{c_1}\dots(J^{-1}\nabla G^3_{\beta_u})_{c_u}\right)\right)$$

From (21) and the product rule, we obtain

$$T_1=\frac{1}{2^2}\sum_{k_1,c_1=1}^{n}\left(\frac{\partial H_r}{\partial y_{k_1}}\frac{\partial H_s}{\partial y_{c_1}}\frac{\partial^2 G^3_{(\alpha-)-}}{\partial y_{k_1+n}\partial y_{c_1+n}}+\frac{\partial H_r}{\partial y_{k_1+n}}\frac{\partial H_s}{\partial y_{c_1+n}}\frac{\partial^2 G^3_{(\alpha-)-}}{\partial y_{k_1}\partial y_{c_1}}\right.$$

$$\left.-\frac{\partial H_r}{\partial y_{k_1}}\frac{\partial H_s}{\partial y_{c_1+n}}\frac{\partial^2 G^3_{(\alpha-)-}}{\partial y_{k_1+n}\partial y_{c_1}}-\frac{\partial H_r}{\partial y_{k_1+n}}\frac{\partial H_s}{\partial y_{c_1}}\frac{\partial^2 G^3_{(\alpha-)-}}{\partial y_{k_1}\partial y_{c_1+n}}\right)$$

$$+\sum_{u=2}^{l-2}\frac{1}{2^{u+1}(u-1)!}\sum_{k_1,c_1=1}^{n}\sum_{c_2,\dots,c_u=1}^{2n}\sum_{\substack{1\le l(\beta)\le l-1-u\\R(\beta)\subseteq R((\alpha-)-)}}\left(\frac{\partial H_r}{\partial y_{k_1}}\frac{\partial^u H_s}{\partial y_{c_1}\dots\partial y_{c_u}}\frac{\partial^2 G^3_\beta}{\partial y_{k_1+n}\partial y_{c_1+n}}\right.$$

$$+\frac{\partial H_r}{\partial y_{k_1+n}}\frac{\partial^u H_s}{\partial y_{c_1+n}\dots\partial y_{c_u}}\frac{\partial^2 G^3_\beta}{\partial y_{k_1}\partial y_{c_1}}-\frac{\partial H_r}{\partial y_{k_1+n}}\frac{\partial^u H_s}{\partial y_{c_1}\dots\partial y_{c_u}}\frac{\partial^2 G^3_\beta}{\partial y_{k_1}\partial y_{c_1+n}}-\frac{\partial H_r}{\partial y_{k_1}}$$

$$\left.\frac{\partial^u H_s}{\partial y_{c_1+n}\dots\partial y_{c_u}}\frac{\partial^2 G^3_\beta}{\partial y_{k_1+n}\partial y_{c_1}}\right)\sum_{\substack{l(\beta)+l(\gamma_1)\dots+l(\gamma_{u-1})=l-2\\(\alpha-)-\in\Lambda_{\beta,\gamma_1\dots,\gamma_{u-1}}}}(J^{-1}\nabla G^3_{\gamma_1})_{c_2}\dots(J^{-1}\nabla G^3_{\gamma_{u-1}})_{c_u}$$

$$+\sum_{i=2}^{l-2}\frac{1}{2^{i+1}(i-1)!}\sum_{k_1,c_1=1}^{n}\sum_{k_2,\dots,k_i=1}^{2n}\sum_{\substack{1\le l(\beta)\le l-1-i\\R(\beta)\subseteq R((\alpha-)-)}}\left(\frac{\partial^i H_r}{\partial y_{k_1}\dots\partial y_{k_i}}\frac{\partial H_s}{\partial y_{c_1}}\frac{\partial^2 G^3_\beta}{\partial y_{k_1+n}\partial y_{c_1+n}}\right.$$

$$+\frac{\partial^i H_r}{\partial y_{k_1+n}\dots\partial y_{k_i}}\frac{\partial H_s}{\partial y_{c_1+n}}\frac{\partial^2 G^3_\beta}{\partial y_{k_1}\partial y_{c_1}}-\frac{\partial^i H_r}{\partial y_{k_1+n}\dots\partial y_{k_i}}\frac{\partial H_s}{\partial y_{c_1}}\frac{\partial^2 G^3_\beta}{\partial y_{k_1}\partial y_{c_1+n}}$$

$$\left.-\frac{\partial^i H_r}{\partial y_{k_1}\dots\partial y_{k_i}}\frac{\partial H_s}{\partial y_{c_1+n}}\frac{\partial^2 G^3_\beta}{\partial y_{k_1+n}\partial y_{c_1}}\right)\sum_{\substack{l(\beta)+l(\gamma_1)\dots+l(\gamma_{i-1})=l-2\\(\alpha-)-\in\Lambda_{\beta,\gamma_1\dots,\gamma_{i-1}}}}(J^{-1}\nabla G^3_{\gamma_1})_{k_2}\dots$$

$$(J^{-1}\nabla G^3_{\gamma_{i-1}})_{k_i} + \sum_{i=2}^{l-3}\sum_{u=2}^{l-i-1} \frac{1}{2^{u+i}(i-1)!(u-1)!} \sum_{k_1,c_1=1}^{n} \sum_{\substack{k_2,\dots,k_i=1\\ c_2,\dots,c_u=1}}^{2n}$$

$$\sum_{\substack{1\le l(\beta)\le l-i-u\\ R(\beta)\subseteq R((\alpha-)-)}} \left(\frac{\partial^i H_r}{\partial y_{k_1}\dots\partial y_{k_i}} \frac{\partial^u H_s}{\partial y_{c_1}\dots\partial y_{c_u}} \frac{\partial^2 G^3_\beta}{\partial y_{k_1+n}\partial y_{c_1+n}} + \frac{\partial^i H_r}{\partial y_{k_1+n}\dots\partial y_{k_i}} \right.$$

$$\frac{\partial^u H_s}{\partial y_{c_1+n}\dots\partial y_{c_u}} \frac{\partial^2 G^3_\beta}{\partial y_{k_1}\partial y_{c_1}} - \frac{\partial^i H_r}{\partial y_{k_1}\dots\partial y_{k_i}} \frac{\partial^u H_s}{\partial y_{c_1+n}\dots\partial y_{c_u}} \frac{\partial^2 G^3_\beta}{\partial y_{k_1+n}\partial y_{c_1}}$$

$$\left. - \frac{\partial^i H_r}{\partial y_{k_1+n}\dots\partial y_{k_i}} \frac{\partial^u H_s}{\partial y_{c_1}\dots\partial y_{c_u}} \frac{\partial^2 G^3_\beta}{\partial y_{k_1}\partial y_{c_1+n}} \right) \sum_{\substack{l(\beta)+l(\gamma_1)+\dots+l(\gamma_{i+u-2})=l-2\\ (\alpha-)-\in\Lambda_{\beta,\gamma_1,\dots,\gamma_{i+u-2}}}}$$

$$(J^{-1}\nabla G^3_{\gamma_1})_{k_2}\cdots(J^{-1}\nabla G^3_{\gamma_{i-1}})_{k_i}(J^{-1}\nabla G^3_{\gamma_i})_{c_2}\cdots(J^{-1}\nabla G^3_{\gamma_{i+u-2}})_{c_u}$$

Notice that the previous formula does not change by switching r and s. Hence, T_1 is symmetric in r and s.

The difference $T_2 = G^3_\alpha - T_1$ is given by

$$T_2 = \sum_{i=2}^{l-1} \frac{1}{2^i(i-1)!} \sum_{k1=1}^{n} \sum_{k_2,\dots,k_i=1}^{2n} \left(-\frac{\partial^i H_r}{\partial y_{k_1}\dots\partial y_{k_i}} \frac{\partial H_s}{\partial y_{k_1+n}} + \frac{\partial^i H_r}{\partial y_{k_1+n}\dots\partial y_{k_i}} \frac{\partial H_s}{\partial y_{k_1}} \right)$$

$$\sum_{\substack{l(\alpha_2)+\dots+l(\alpha_i)=l-2\\ (\alpha-)-\in\Lambda_{\alpha_2,\dots,\alpha_i}}} (J^{-1}\nabla G^3_{\alpha_2})_{k_2}\dots(J^{-1}\nabla G^3_{\alpha_i})_{k_i}$$

$$+ \sum_{u=1}^{l-2} \frac{1}{2^{u+1}u!} \sum_{k_1=1}^{n} \sum_{c_1,\dots,c_u=1}^{2n} \left(-\frac{\partial H_r}{\partial y_{k_1}} \frac{\partial^{u+1} H_s}{\partial y_{k_1+n}\partial y_{c_1}\dots\partial y_{c_u}} + \frac{\partial H_r}{\partial y_{k_1+n}} \frac{\partial^{u+1} H_s}{\partial y_{k_1}\partial y_{c_1}\dots\partial y_{c_u}} \right)$$

$$\sum_{\substack{l(\beta_1)+\dots+l(\beta_u)=l-2\\ (\alpha-)-\in\Lambda_{\beta_1,\dots,\beta_u}}} (J^{-1}\nabla G^3_{\beta_1})_{c_1}\dots(J^{-1}\nabla G^3_{\beta_u})_{c_u}$$

$$+ \sum_{i=2}^{l-2}\sum_{j=1}^{l-i-1}\sum_{u=1}^{j} \frac{1}{2^{u+i}(i-1)!u!} \sum_{k_1=1}^{n} \sum_{\substack{k_2,\dots,k_i=1\\ c_1,\dots,c_u=1}}^{2n} \left(-\frac{\partial^i H_r}{\partial y_{k_1}\dots\partial y_{k_i}} \frac{\partial^{u+1} H_s}{\partial y_{k_1+n}\partial y_{c_1}\dots\partial y_{c_u}} \right.$$

$$\left. + \frac{\partial^i H_r}{\partial y_{k_1+n}\dots\partial y_{k_i}} \frac{\partial^{u+1} H_s}{\partial y_{k_1}\partial y_{c_1}\dots\partial y_{c_u}} \right) \sum_{\substack{l(\alpha_2)+\dots+l(\alpha_i)=l-2-j,\\ l(\alpha_1)=j,\quad (\alpha-)-\in\Lambda_{\alpha_1,\dots,\alpha_i}}} (J^{-1}\nabla G^3_{\alpha_2})_{k_2}\dots$$

$$(J^{-1}\nabla G^3_{\alpha_i})_{k_i} \sum_{\substack{l(\beta_1)+\dots+l(\beta_u)=j\\ \alpha_1\in\Lambda_{\beta_1,\dots,\beta_u}}} (J^{-1}\nabla G^3_{\beta_1})_{c_1}\dots(J^{-1}\nabla G^3_{\beta_u})_{c_u}$$

Introducing new summation indexes $j = i - 1$ for the first term, and $v = i + u - 1$ for the last term and using (21), we obtain

$$T_2 = \sum_{j=1}^{l-2} \frac{1}{2^{j+1} j!} \sum_{k1=1}^{n} \sum_{c_1,\ldots,c_j=1}^{2n} \Big(-\frac{\partial^j H_r}{\partial y_{k_1} \ldots \partial y_{c_j}} \frac{\partial H_s}{\partial y_{k_1+n}} + \frac{\partial^j H_r}{\partial y_{k_1+n} \ldots \partial y_{c_j}} \frac{\partial H_s}{\partial y_{k_1}} \Big) \sum_{\substack{l(\alpha_1)+\cdots+l(\alpha_j)=l-2 \\ (\alpha-)-\in\Lambda_{\alpha_1,\ldots,\alpha_j}}} (J^{-1}\nabla G^3_{\alpha_1})_{c_1} \ldots (J^{-1}\nabla G^3_{\alpha_j})_{c_j}$$

$$+ \sum_{u=1}^{l-2} \frac{1}{2^{u+1} u!} \sum_{k_1=1}^{n} \sum_{c_1,\ldots,c_u=1}^{2n} \Big(-\frac{\partial H_r}{\partial y_{k_1}} \frac{\partial^{u+1} H_s}{\partial y_{k_1+n} \partial y_{c_1} \ldots \partial y_{c_u}} + \frac{\partial H_r}{\partial y_{k_1+n}} \frac{\partial^{u+1} H_s}{\partial y_{k_1} \partial y_{c_1} \ldots \partial y_{c_u}} \Big) \sum_{\substack{l(\beta_1)+\cdots+l(\beta_u)=l-2 \\ (\alpha-)-\in\Lambda_{\beta_1,\ldots,\beta_u}}} (J^{-1}\nabla G^3_{\beta_1})_{c_1} \ldots (J^{-1}\nabla G^3_{\beta_u})_{c_u}$$

$$+ \sum_{v=2}^{l-2} \sum_{i=2}^{v} \frac{1}{2^{v+1}(i-1)!(v-i+1)!} \sum_{k_1=1}^{n} \sum_{j_1,\ldots,j_v=1}^{2n} \Big(-\frac{\partial^i H_r}{\partial y_{k_1} \partial y_{j_1} \ldots \partial y_{j_{i-1}}} \frac{\partial^{v+2-i} H_s}{\partial y_{k_1+n} \partial y_{j_i} \ldots \partial y_{j_v}} + \frac{\partial^i H_r}{\partial y_{k_1+n} \partial y_{j_1} \ldots \partial y_{j_{i-1}}} \frac{\partial^{v+2-i} H_s}{\partial y_{k_1} \partial y_{j_i} \ldots \partial y_{j_v}} \Big) \sum_{\substack{l(\gamma_1)+\cdots+l(\gamma_v)=l-2 \\ (\alpha-)-\in\Lambda_{\gamma_1,\ldots,\gamma_v}}} (J^{-1}\nabla G^3_{\gamma_1})_{j_1} \cdots (J^{-1}\nabla G^3_{\gamma_v})_{j_v}$$

Notice that $T_2 = 0$ because $\frac{\partial H_r}{\partial y_{k_1}} \frac{\partial H_s}{\partial y_{k_1+n}} = \frac{\partial H_r}{\partial y_{k_1+n}} \frac{\partial H_s}{\partial y_{k_1}}$ for any $k_1 = 1, \ldots, n$ and T_2 can be expressed as follows

$$T_2 = \sum_{v=1}^{l-2} \frac{1}{2^{v+1} v!} \sum_{k_1=1}^{n} \sum_{j_1,\ldots,j_v=1}^{2n} \frac{\partial^v}{\partial y_{j_1} \cdots \partial y_{j_v}} \Big(-\frac{\partial H_r}{\partial y_{k_1}} \frac{\partial H_s}{\partial y_{k_1+n}} + \frac{\partial H_r}{\partial y_{k_1+n}} \frac{\partial H_s}{\partial y_{k_1}} \Big) \sum_{\substack{l(\gamma_1)+\cdots+l(\gamma_v)=l-2 \\ (\alpha-)-\in\Lambda_{\gamma_1,\ldots,\gamma_v}}} (J^{-1}\nabla G^3_{\gamma_1})_{j_1} \cdots (J^{-1}\nabla G^3_{\gamma_v})_{j_v}$$

Thus $G^3_\alpha = T_1$ is symmetric with respect to s and r □

4. Symplectic schemes

In this section, we apply the generating function method and the special properties of the coefficients G^i_α, $i = 1, 2, 3$ to construct symplectic schemes for SHS preserving the Hamiltonian functions. Taking advantage of the invariance under permutations of the coefficients G^i_α, $i = 1, 2, 3$, we propose high-order strong and weak symplectic schemes that are computationally attractive.

4.1. Symplectic strong schemes. Let define $\mathcal{A}_\gamma = \{\alpha : l(\alpha) + n(\alpha) \leq 2\gamma\}$, where $n(\alpha)$ is the number of zero components of the multi-index α. Symplectic schemes that have mean square order of convergence k can be constructed using the equations (12)-(14) and truncations of the appropriate generating functions S^i_ω, $i = 1, 2, 3$, according to the indexes $\alpha \in \mathcal{A}_k$. Since these schemes are implicit, the Stratonovich stochastic integrals should be approximated by bounded random variables ([11]).

In [4] we proposed first-order schemes for the SHS (1) based on truncations of the generating function S^i_ω, $i = 1, 3$, according to $\mathcal{A}_1$. Let $0 < h < 1$ be a small time step, and for any multi-index α let denote by J_α the multiple Stratonovich integral $J_{\alpha;0,h}$ defined in (16). To construct second-order schemes, we employ the following truncations according to $\mathcal{A}_2$:

$$\begin{aligned} S^i_\omega \approx{} & G^i_{(0)} J_{(0)} + \sum_{r=1}^{m} \Big(G^i_{(r)} J_{(r)} + G^i_{(0,r)} J_{(0,r)} + G^i_{(r,0)} J_{(r,0)} \Big) + G^i_{(0,0)} J_{(0,0)} \\ & + \sum_{r,j=1}^{m} G^i_{(r,j)} J_{(r,j)} + \sum_{r,j,k=1}^{m} G^i_{(r,j,k)} J_{(r,j,k)} + \sum_{r,j,k,s=1}^{m} G^i_{(r,j,k,s)} J_{(r,j,k,s)} \\ & + \sum_{r,j=1}^{m} \Big(G^i_{(r,j,0)} J_{(r,j,0)} + G^i_{(0,r,j)} J_{(0,r,j)} + G^i_{(r,0,j)} J_{(r,0,j)} \Big), \end{aligned} \tag{30}$$

for any $i = 1, 2, 3$.

Using (22), we obtain

$$J_{(0)} J_{(r)} = \sum_{\beta \in \Lambda_{(0),(r)}} J_\beta = J_{(0,r)} + J_{(r,0)} \tag{31}$$

$$J_{(0)} J_{(r,r)} = \sum_{\beta \in \Lambda_{(0),(r,r)}} J_\beta = J_{(0,r,r)} + J_{(r,r,0)} + J_{(r,0,r)} \tag{32}$$

$$J_{(0)} J_{(r)} J_{(j)} = \sum_{\beta \in \Lambda_{(0),(r),(j)}} J_\beta = J_{(0,r,j)} + \ldots + J_{(j,r,0)} \tag{33}$$

$$J_{(r)} J_{(j)} = \sum_{\beta \in \Lambda_{(r),(j)}} J_\beta = J_{(r,j)} + J_{(j,r)} \tag{34}$$

$$J_{(j)} J_{(r,r)} = \sum_{\beta \in \Lambda_{(j),(r,r)}} J_\beta = J_{(j,r,r)} + J_{(r,r,j)} + J_{(r,j,r)} \tag{35}$$

$$J_{(j)} J_{(0,0)} = \sum_{\beta \in \Lambda_{(j),(r,r)}} J_\beta = J_{(j,0,0)} + J_{(0,0,j)} + J_{(0,j,0)} \tag{36}$$

$$J_{(r,r)} J_{(j,j)} = \sum_{\beta \in \Lambda_{(r,r),(j,j)}} J_\beta = J_{(r,r,j,j)} + \ldots + J_{(j,j,r,r)} \tag{37}$$

$$J_{(j)} J_{(r,r,r)} = \sum_{\beta \in \Lambda_{(j),(r,r,r)}} J_\beta = J_{(j,r,r,r)} + J_{(r,r,j,r)} + J_{(r,j,r,r)} + J_{(r,r,r,j)} \tag{38}$$

$$J_{(k)} J_{(r)} J_{(j)} = \sum_{\beta \in \Lambda_{(k),(r),(j)}} J_\beta = J_{(k,r,j)} + \ldots + J_{(j,r,k)} \tag{39}$$

$$J_{(k)} J_{(j)} J_{(r,r)} = \sum_{\beta \in \Lambda_{(k),(j),(r,r)}} J_\beta = J_{(k,j,r,r)} + \ldots + J_{(r,j,k,r)} \tag{40}$$

$$J_{(s)} J_{(k)} J_{(r)} J_{(j)} = \sum_{\beta \in \Lambda_{(s),(k),(r),(j)}} J_\beta = J_{(s,k,r,j)} + \ldots + J_{(j,r,k,s)}, \tag{41}$$

for any distinct positive integers r, j, k, $s = 1, \ldots, m$. The previous equations and Propositions 3.1 and 3.2 give us the following truncations of the generating functions S^i_ω, $i = 1, 2, 3$:

$$
\begin{aligned}
S^i_\omega \approx\ & G^i_{(0)} J_{(0)} + \sum_{r=1}^{m} \Big(G^i_{(r)} J_{(r)} + G^i_{(r,r)} J_{(r,r)} + G^i_{(0,r)} J_{(0)} J_{(r)} \Big) \\
& + G^i_{(0,0)} J_{(0,0)} + \sum_{r=1}^{m} \Big(G^i_{(r,r,0)} J_{(r,r)} J_{(0)} + G^i_{(r,r,r)} J_{(r,r,r)} + G^i_{(r,r,r,r)} J_{(r,r,r,r)} \Big) \\
& + \sum_{r=1}^{m-1} \sum_{j=r+1}^{m} \Big(G^i_{(r,j)} J_{(r)} J_{(j)} + G^i_{(r,r,j,j)} J_{(r,r)} J_{(j,j)} + G^i_{(0,r,j)} J_{(0)} J_{(r)} J_{(j)} \Big) \\
& + \sum_{r,j=1, r\neq j}^{m} \Big(G^i_{(r,r,j)} J_{(r,r)} J_{(j)} + G^i_{(r,r,r,j)} J_{(r,r,r)} J_{(j)} \Big) \\
& + \sum_{r=1}^{m-2} \sum_{j=r+1}^{m-1} \sum_{k=j+1}^{m} G^i_{(r,j,k)} J_{(r)} J_{(j)} J_{(k)} \\
& + \sum_{k=1}^{m-1} \sum_{j=k+1}^{m} \sum_{\substack{r=1,\\ r\neq k, r\neq j}}^{m} G^i_{(r,r,j,k)} J_{(r,r)} J_{(j)} J_{(k)} \\
& + \sum_{r=1}^{m-3} \sum_{j=r+1}^{m-2} \sum_{k=j+1}^{m-1} \sum_{s=k+1}^{m} G^i_{(r,j,k,s)} J_{(r)} J_{(j)} J_{(k)} J_{(s)}.
\end{aligned} \tag{42}
$$

Notice that to construct second-order symplectic schemes for SHS preserving Hamiltonian functions, we need to generate only the stochastic integrals $J_{(0)}$, $J_{(0,0)}$, $J_{(r)}$, $J_{(r,r)}$, $J_{(r,r,r)}$, and $J_{(r,r,r,r)}$, $r = 1, \dots, m$. To ensure that these implicit schemes are well-defined, we proceed as in [11], and to generate the stochastic integrals instead of the independent random variables $\xi(r) \sim N(0,1)$, $r = 1, \dots, m$, we use the bounded random variables $\xi_h(r)$:

$$
\xi_h(r) = \begin{cases} -A_h & \text{if } \xi(r) < -A_h \\ \xi(r) & \text{if } |\xi(r)| \le A_h \\ A_h & \text{if } \xi(r) > A_h, \end{cases} \tag{43}
$$

where $0 < h < 1$ is a small time step and $A_h = 2\sqrt{2|\ln h|}$. Hence, we apply the following approximations for the stochastic integrals:

$$
\begin{aligned}
& J_{(0)} = h, \quad J_{(0,0)} = \frac{h^2}{2}, \quad J_{(r)} = \sqrt{h}\xi_h(r), \\
& J_{(r,r)} = \frac{h\xi_h^2(r)}{2}, \quad J_{(r,r,r)} = \frac{h^{3/2}\xi_h^3(r)}{6}, \quad J_{(r,r,r,r)} = \frac{h^2\xi_h^4(r)}{24}.
\end{aligned} \tag{44}
$$

For example, for $m = 1$ (i.e. the SHS with one noise), using (12) and (42), the symplectic mean square second-order scheme based on the truncation of the generating function S^1_ω is given by:

$$
(45)\quad \begin{aligned}
P_i(l+1) &= P_i(l) - \Big(\frac{\partial G^1_{(0)}}{\partial Q_i}h + \frac{\partial G^1_{(1)}}{\partial Q_i}\sqrt{h}\xi_{h,l} + \frac{\partial G^1_{(0,0)}}{\partial Q_i}\frac{h^2}{2} + \frac{\partial G^1_{(1,1)}}{\partial Q_i}\frac{h\xi^2_{h,l}}{2} \\
&+ \frac{\partial G^1_{(1,0)}}{\partial Q_i}\xi_{h,l}h^{\frac{3}{2}} + \frac{\partial G^1_{(1,1,1)}}{\partial Q_i}\frac{h^{\frac{3}{2}}\xi^3_{h,l}}{6} + \frac{\partial G^1_{(1,1,0)}}{\partial Q_i}\frac{\xi^2_{h,l}h^2}{2} + \frac{\partial G^1_{(1,1,1,1)}}{\partial Q_i}\frac{h^2\xi^4_{h,l}}{24}\Big) \\
Q_i(l+1) &= Q_i(l) + \Big(\frac{\partial G^1_{(0)}}{\partial P_i}h + \frac{\partial G^1_{(1)}}{\partial P_i}\sqrt{h}\xi_{h,l} + \frac{\partial G^1_{(0,0)}}{\partial P_i}\frac{h^2}{2} + \frac{\partial G^1_{(1,1)}}{\partial P_i}\frac{h\xi^2_{h,l}}{2} \\
&+ \frac{\partial G^1_{(1,0)}}{\partial P_i}\xi_{h,l}h^{\frac{3}{2}} + \frac{\partial G^1_{(1,1,1)}}{\partial P_i}\frac{h^{\frac{3}{2}}\xi^3_{h,l}}{6} + \frac{\partial G^1_{(1,1,0)}}{\partial P_i}\frac{\xi^2_{h,l}h^2}{2} + \frac{\partial G^1_{(1,1,1,1)}}{\partial P_i}\frac{h^2\xi^4_{h,l}}{24}\Big),
\end{aligned}
$$

where everywhere the arguments are $(P(l+1), Q(l))$, and the random variables $\xi_{h,l}$ are generated independently at each step l according to (43).

For the coefficients of S^3_ω, a simple calculation shows that $G^3_{(r_1,r_2)} = 0$ for any $r_1, r_2 = 0, 1$ and $G^3_{(1,1,1,1)} = 0$. Hence, using (14), when $m = 1$ the second-order midpoint symplectic scheme can be expressed by

$$
(46)\quad \begin{aligned}
Y_{l+1} &= Y_l + J^{-1}\nabla G^3_{(0)}(Y_{l+\frac{1}{2}})h + J^{-1}\nabla G^3_{(1)}(Y_{l+\frac{1}{2}})\sqrt{h}\xi_{h,l} \\
&+ J^{-1}\nabla G^3_{(1,1,1)}(Y_{l+\frac{1}{2}})\frac{h^{\frac{3}{2}}\xi^3_{h,l}}{6} + J^{-1}\nabla G^3_{(1,1,0)}(Y_{l+\frac{1}{2}})\frac{\xi^2_{h,l}h^2}{2}
\end{aligned}
$$

where $Y_{l+\frac{1}{2}} = (Y_{l+1} + Y_l)/2$, $Y_l = \big(P^T(l), Q^T(l)\big)^T$, and the random variables $\xi_{h,l}$ are generated independently at each time step l according to (43).

Since the schemes (45) and (46) are based on the generating functions, we can easily prove that they are symplectic (see also the proof of Theorem 3.1 in [11]). Analogously with Theorem 5.3 in [4], the convergence with mean square order two can be proved under appropriate conditions using repeated Taylor expansions and Theorem 1.1 in [9].

4.2. Symplectic weak schemes. To obtain a k-order symplectic weak scheme, we replace in (15) the Stratonovich integrals J_α by the Ito integrals using the equation (18), and we truncate the series to include only Ito integrals with multi-indexes α such that $l(\alpha) \leq k$, $k = 1, 2, 3$ ([1]). Replacing in (18), we get $J_{(0)} = I_{(0)}$, $J_{(i)} = I_{(i)}$, $J_{(0,0)} = I_{(0,0)}$, $J_{(0,i)} = I_{(0,i)}$, $J_{(i,0)} = I_{(i,0)}$, $J_{(i,0,j)} = I_{(i,0,j)}$, $J_{(i,0,i)} = I_{(i,0,i)}$, $J_{(i,j)} = I_{(i,j)}$, $J_{(k,0,0)} = I_{(k,0,0)}$, $J_{(0,k,0)} = I_{(0,k,0)}$, $J_{(0,0,k)} = I_{(0,0,k)}$, $J_{(i,j,i)} = I_{(i,j,i)}$

$$
(47)\quad \begin{aligned}
&J_{(i,i)} = I_{(i,i)} + \frac{1}{2}I_{(0)}, \quad J_{(i,i,j)} = I_{(i,i,j)} + \frac{1}{2}I_{(0,j)} \\
&J_{(j,i,i)} = I_{(j,i,i)} + \frac{1}{2}I_{(j,0)}, \quad J_{(i,i,0)} = I_{(i,i,0)} + \frac{1}{2}I_{(0,0)}, \\
&J_{(0,i,i)} = I_{(0,i,i)} + \frac{1}{2}I_{(0,0)}, \quad J_{(i,i,i)} = I_{(i,i,i)} + \frac{1}{2}\big(I_{(0,i)} + I_{(i,0)}\big) \\
&J_{(i,i,j,j)} = I_{(i,i,j,j)} + \frac{1}{2}\big(I_{(0,j,j)} + I_{(i,i,0)}\big) + \frac{1}{4}I_{(0,0)}, \\
&J_{(i,i,i,i)} = I_{(i,i,i,i)} + \frac{1}{2}\big(I_{(0,i,i)} + I_{(i,0,i)} + I_{(i,i,0)}\big) + \frac{1}{4}I_{(0,0)},
\end{aligned}
$$

for any $i \neq j$, $i, j = 1, \ldots, m$. Thus, for a second-order weak scheme, we apply the following approximation for the generating functions S_ω^i, $i = 1, 2, 3$:

$$
\begin{aligned}
S_\omega^i \approx & \left(G_{(0)}^i + \frac{1}{2} \sum_{k=1}^m G_{(k,k)}^i \right) I_{(0)} + \sum_{k=1}^m G_{(k)}^i I_{(k)} \\
& + \left(G_{(0,0)}^i + \frac{1}{2} \sum_{k=1}^m (G_{(k,k,0)}^i + G_{(0,k,k)}^i) + \frac{1}{4} \sum_{k,j=1}^m G_{(k,k,j,j)}^i \right) I_{(0,0)} \\
& + \sum_{k=1}^m \left(\left(G_{(0,k)}^i + \frac{1}{2} \sum_{j=1}^m G_{(j,j,k)}^i \right) I_{(0,k)} + \left(G_{(k,0)}^i + \frac{1}{2} \sum_{j=1}^m G_{(k,j,j)}^i \right) I_{(k,0)} \right) \\
& + \sum_{j,k=1}^m G_{(j,k)}^i I_{(j,k)}.
\end{aligned} \tag{48}
$$

Using Propositions 3.1 and 3.2 together with equations (31) and (34), we get:

$$
\begin{aligned}
S_\omega^i \approx & \left(G_{(0)}^i + \frac{1}{2} \sum_{k=1}^m G_{(k,k)}^i \right) I_{(0)} + \sum_{k=1}^m G_{(k)}^i I_{(k)} \\
& + \left(G_{(0,0)}^i + \sum_{k=1}^m \left(G_{(k,k,0)}^i + \frac{1}{4} G_{(k,k,k,k)}^i \right) + \frac{1}{2} \sum_{k=1}^{m-1} \sum_{j=k+1}^m G_{(k,k,j,j)}^i \right) I_{(0,0)} \\
& + \sum_{k=1}^m \left(G_{(0,k)}^i + \frac{1}{2} \sum_{j=1}^m G_{(j,j,k)}^i \right) I_{(0)} I_{(k)} + \sum_{k=1}^m G_{(k,k)}^i I_{(k,k)} \\
& + \sum_{k=1}^{m-1} \sum_{j=k+1}^m G_{(k,j)}^i I_{(k)} I_{(j)}.
\end{aligned} \tag{49}
$$

For a weak scheme, we can generate the noise increments more efficiently than for a strong scheme. Hence proceeding as in section 14.2 of [7] to simulate the stochastic integrals $I_{(k)}$, $k = 1, \ldots, m$, we generate independent random variable $\sqrt{h}\zeta_{k,l}$, $k = 1, \ldots, m$ at each time step l with the following discrete distribution

$$
P(\zeta_{k,l} = \pm\sqrt{3}) = \frac{1}{6}, \quad P(\zeta_{k,l} = 0) = \frac{2}{3}. \tag{50}
$$

The moments of $\zeta_{k,l}$ are equal up to order 5 with the moments of the normal distribution $N(0, 1)$, so we obtain the scheme based on S_ω^1:

$$
\begin{aligned}
P_i(l+1) = & P_i(l) - h \frac{\partial G_{(0)}^1}{\partial Q_i} - h^{1/2} \sum_{k=1}^m \zeta_{k,l} \frac{\partial G_{(k)}^1}{\partial Q_i} - \frac{h^2}{2} \Bigg(\frac{\partial G_{(0,0)}^1}{\partial Q_i} \\
& + \sum_{k=1}^m \left(\frac{\partial G_{(k,k,0)}^1}{\partial Q_i} + \frac{1}{4} \frac{\partial G_{(k,k,k,k)}^1}{\partial Q_i} \right) + \frac{1}{2} \sum_{k=1}^{m-1} \sum_{j=k+1}^m \frac{\partial G_{(k,k,j,j)}^1}{\partial Q_i} \Bigg) \\
& - \frac{h}{2} \sum_{k=1}^m \zeta_{k,l}^2 \frac{\partial G_{(k,k)}^1}{\partial Q_i} - \frac{h}{2} \sum_{k=1}^{m-1} \sum_{j=k+1}^m \frac{\partial G_{(k,j)}^1}{\partial Q_i} \zeta_{k,l} \zeta_{j,l} \\
& - h^{3/2} \sum_{k=1}^m \zeta_{k,l} \left(\frac{\partial G_{(0,k)}^1}{\partial Q_i} + \frac{1}{2} \sum_{j=1}^m \frac{\partial G_{(j,j,k)}^1}{\partial Q_i} \right),
\end{aligned} \tag{51}
$$

$$
\begin{aligned}
Q_i(l+1) &= Q_i(l) + h\frac{\partial G^1_{(0)}}{\partial P_i} + h^{1/2}\sum_{k=1}^m \zeta_{k,l}\frac{\partial G^1_{(k)}}{\partial P_i} + \frac{h^2}{2}\Bigg(\frac{\partial G^1_{(0,0)}}{\partial P_i} \\
&+ \sum_{k=1}^m\left(\frac{\partial G^1_{(k,k,0)}}{\partial P_i} + \frac{1}{4}\frac{\partial G^1_{(k,k,k,k)}}{\partial P_i}\right) + \frac{1}{2}\sum_{k=1}^{m-1}\sum_{j=k+1}^m \frac{\partial G^1_{(k,k,j,j)}}{\partial P_i}\Bigg) \\
&+ \frac{h}{2}\sum_{k=1}^m \zeta^2_{k,l}\frac{\partial G^1_{(k,k)}}{\partial P_i} + \frac{h}{2}\sum_{k=1}^{m-1}\sum_{j=k+1}^m \frac{\partial G^1_{(k,j)}}{\partial P_i}\zeta_{k,l}\zeta_{j,l} \\
&+ h^{3/2}\sum_{k=1}^m \zeta_{k,l}\left(\frac{\partial G^1_{(0,k)}}{\partial P_i} + \frac{1}{2}\sum_{j=1}^m \frac{\partial G^1_{(j,j,k)}}{\partial P_i}\right),
\end{aligned} \tag{52}
$$

where $i = 1, \dots, n$, and everywhere the arguments are $(P(l+1), Q(l))$. In Theorem 1 in [1], we prove that the scheme based on the one-step approximation (51)-(52) is symplectic and of weak order two.

Similarly we can construct symplectic schemes of weak order three based on the following approximations of the generating functions S^i_ω, $i = 1, 2, 3$ (see also section 3 in [1]):

$$
\begin{aligned}
S^i_\omega &\approx \left(G^i_{(0)} + \frac{1}{2}\sum_{k=1}^m G^i_{(k,k)}\right) I_{(0)} + \Bigg(G^i_{(0,0)} + \frac{1}{2}\sum_{k=1}^m (G^i_{(k,k,0)} + G^i_{(0,k,k)}) \\
&+ \frac{1}{4}\sum_{k,j=1}^m G^i_{(k,k,j,j)}\Bigg) I_{(0,0)} + \sum_{k=1}^m \Bigg(\left(G^i_{(0,k)} + \frac{1}{2}\sum_{j=1}^m G^i_{(j,j,k)}\right) I_{(0,k)} \\
&+ \left(G^i_{(k,0)} + \sum_{j=1}^m \frac{1}{2} G^i_{(k,j,j)}\right) I_{(k,0)}\Bigg) + \sum_{k=1}^m G^i_{(k)} I_{(k)} \\
&+ \sum_{k,j=1}^m G^i_{(k,j)} I_{(k,j)} + \Bigg(G^i_{(0,0,0)} + \frac{1}{2}\sum_{k=1}^m \left(G^i_{(k,k,0,0)} + G^i_{(0,k,k,0)} + G^i_{(0,0,k,k)}\right) \\
&+ \frac{1}{4}\sum_{k,j=1}^m \left(G^i_{(k,k,j,j,0)} + G^i_{(0,k,k,j,j)} + G^i_{(k,k,0,j,j)}\right) + \frac{1}{8}\sum_{k,j,l=1}^m G^i_{(k,k,j,j,l,l)}\Bigg) I_{(0,0,0)} \\
&+ \sum_{k=1}^m \Bigg(G^i_{(0,0,k)} + \frac{1}{2}\sum_{j=1}^m \left(G^i_{(j,j,0,k)} + G^i_{(0,j,j,k)}\right) + \frac{1}{4}\sum_{j,l=1}^m G^i_{(j,j,l,l,k)}\Bigg) I_{(0,0,k)} \\
&+ \sum_{k=1}^m \Bigg(G^i_{(0,k,0)} + \frac{1}{2}\sum_{j=1}^m \left(G^i_{(j,j,k,0)} + G^i_{(0,k,j,j)}\right) + \frac{1}{4}\sum_{j,l=1}^m G^i_{(j,j,k,l,l)}\Bigg) I_{(0,k,0)} \\
&+ \sum_{k=1}^m \Bigg(G^i_{(k,0,0)} + \frac{1}{2}\sum_{j=1}^m \left(G^i_{(k,j,j,0)} + G^i_{(k,0,j,j)}\right) + \frac{1}{4}\sum_{j,l=1}^m G^i_{(k,j,j,l,l)}\Bigg) I_{(k,0,0)} \\
&+ \sum_{k,j=1}^m \Bigg(\left(G^i_{(k,j,0)} + \frac{1}{2}\sum_{l=1}^m G^i_{(k,j,l,l)}\right) I_{(k,j,0)} + \left(G^i_{(0,k,j)} + \frac{1}{2}\sum_{l=1}^m G^i_{(l,l,k,j)}\right) I_{(0,k,j)} \\
&+ \left(G^i_{(k,0,j)} + \frac{1}{2}\sum_{l=1}^m G^i_{(k,l,l,j)}\right) I_{(k,0,j)}\Bigg) + \sum_{k,j,l=1}^m G^i_{(k,j,l)} I_{(k,j,l)}.
\end{aligned}
$$

Using Propositions 3.1 and 3.2, equations (31)-(36), (39) and (47), the previous approximation becomes

$$
\begin{aligned}
S_\omega^i \approx & \left(G^i_{(0)} + \frac{1}{2}\sum_{k=1}^m G^i_{(k,k)}\right) I_{(0)} + \sum_{k=1}^m G^i_{(k)} I_{(k)} \\
& + \left(G^i_{(0,0)} + \sum_{k=1}^m \left(G^i_{(k,k,0)} + \frac{1}{4} G^i_{(k,k,k,k)}\right) + \frac{1}{2}\sum_{k=1}^{m-1}\sum_{j=k+1}^m G^i_{(k,k,j,j)}\right) I_{(0,0)} \\
& + \sum_{k=1}^m \left(G^i_{(0,k)} + \frac{1}{2}\sum_{j=1}^m G^i_{(j,j,k)}\right) I_{(0)} I_{(k)} + \sum_{k=1}^m G^i_{(k,k)} I_{(k,k)} \\
& + \sum_{k=1}^{m-1}\sum_{j=k+1}^m G^i_{(k,j)} I_{(k)} I_{(j)} + \left(G^i_{(0,0,0)} + \frac{3}{2}\sum_{k=1}^m G^i_{(k,k,0,0)}\right. \\
& \left. + \frac{3}{4}\sum_{k,j=1}^m G^i_{(k,k,j,j,0)} + \frac{1}{8}\sum_{k,j,l=1}^m G^i_{(k,k,j,j,l,l)}\right) I_{(0,0,0)} \\
& + \sum_{k=1}^m \left(G^i_{(0,0,k)} + \sum_{j=1}^m G^i_{(j,j,0,k)} + \frac{1}{4}\sum_{j,l=1}^m G^i_{(j,j,l,l,k)}\right) I_{(0,0)} I_{(k)} \\
& + \sum_{k=1}^{m-1}\sum_{j=k+1}^m \left(G^i_{(k,j,0)} + \frac{1}{2}\sum_{l=1}^m G^i_{(k,j,l,l)}\right) I_{(k)} I_{(j)} I_{(0)} \\
& + \sum_{k=1}^m \left(G^i_{(k,k,0)} + \frac{1}{2}\sum_{l=1}^m G^i_{(k,k,l,l)}\right)\left(I_{(k,k)} I_{(0)} + \frac{1}{2} I^2_{(0)} - I_{(0,0)}\right) \\
& + \sum_{k=1}^{m-2}\sum_{j=k+1}^{m-1}\sum_{l=j+1}^m G^i_{(k,j,l)} I_{(k)} I_{(j)} I_{(l)} + \sum_{k=1}^m G^i_{(k,k,k)} I_{(k,k,k)} \\
& + \sum_{k=1}^{m-1}\sum_{j=k+1}^m G^i_{(k,k,j)} I_{(k,k)} I_{(j)}.
\end{aligned}
\tag{53}
$$

We can now obtain third-order symplectic weak schemes based on one of the equations (12)-(14) and the approximation (53) of the corresponding generating functions S^i_ω, $i = 1, 2, 3$. Notice that we only need to generate the multiple stochastic integrals $I_{(k)}$, $I_{(k,k)}$, $I_{(k,k,k)}$, $k = 0, \ldots, m$. At each time step l, we can generate the stochastic integrals $I_{(k)}$, $k = 1, \ldots, m$, as independent random variable $\sqrt{h}\xi_{k,l}$, $k = 1, \ldots, m$, with the following discrete distribution (see the scheme (10.36) in [9])

$$
P(\xi_{k,l} = 0) = \frac{1}{3}, \quad P(\xi_{k,l} = \pm 1) = \frac{3}{10}, \quad P(\xi_{k,l} = \pm\sqrt{6}) = \frac{1}{30}, \tag{54}
$$

$I_{(k,k)}$, as $h\xi^2_{k,l}/2 - h/2$, and $I_{(k,k,k)}$, as $h\sqrt{h}\xi^3_{k,l}/6 - h^{3/2}\xi_{k,l}/2$, $k = 1, \ldots, m$. Under appropriate assumptions regarding the functions H_r, $r = 0, \ldots, m$, we can prove the convergence of the schemes with weak order three proceeding as in [1], using Theorem 4.1 in [10] and repeated Taylor expansions.

5. Numerical simulations

In this section we illustrate numerically the performance of the strong and weak symplectic methods for SHSs preserving the Hamiltonian functions. We consider the Kubo oscillator:

$$(55)\qquad \begin{aligned} dP &= -aQdt - \sigma Q \circ dw_t, \quad P(0) = p, \\ dQ &= aPdt + \sigma P \circ dw_t, \quad Q(0) = q. \end{aligned}$$

Given the special form of the linear system (55), it is easy to verify that the Poisson bracket of the Hamiltonian functions $H^{(0)}$ and $H^{(1)}$ vanishes, so $H^{(0)}$ and $H^{(1)}$ conserve along the phase flow of the system. For the following numerical simulations the values of the parameters are $a = 2$, $\sigma = 0.3$, and we let the initial values be $p = 1$, $q = 0$.

The superior performance for long term simulations of symplectic strong schemes compared to non-symplectic schemes is shown in [11], [1]. Here we consider five types of stochastic strong symplectic schemes: the schemes based on S^1_ω with mean square order 0.5, 1 and 2, and the mean square first- and second-order schemes based on S^3_ω. The linear system (55) can be solved analytically and the solution is given by the following equations

$$(56)\qquad \begin{aligned} P(T;0,p,q) &= \cos{(aT + \sigma w_T)}p + \sin{(aT + \sigma w_T)}q \\ Q(T;0,p,q) &= -\sin{(aT + \sigma w_T)}p + \cos{(aT + \sigma w_T)}q. \end{aligned}$$

Hence, we can compute the error associated with the proposed symplectic schemes. Our attention here will focus on comparing the efficiency in terms of the accuracy and the CPU time required for various numerical schemes.

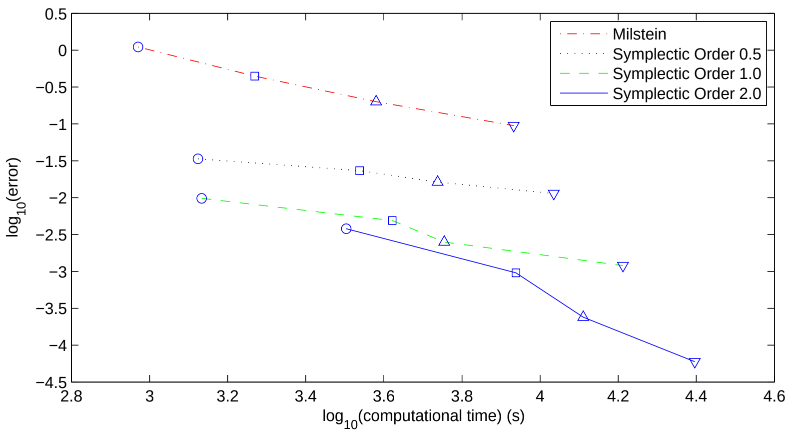

FIGURE 1. Computing time v.s. error for Milstein scheme and different types of symplectic strong S^1_ω schemes with various time step for $T = 100$ with 10^5 samples, ◯: $h = 0.004$; □: $h = 0.002$; △: $h = 0.001$, ▽: $h = 0.0005$.

It is usually difficult to implement the symplectic schemes of mean square order two or higher because it requires the simulation of many multiple stochastic integrals. However, for SHSs preserving the Hamiltonian functions, the higher order symplectic schemes such as (45) and (46) have a simpler form due to the invariance of the coefficients under permutations (see theorems 3.1 and 3.2).

Fig. 1 and Fig. 2 clearly confirm that the higher order strong schemes are more efficient than the lower order schemes. To achieve a similar level of accuracy, a larger step size can be employed in a higher order scheme and this could lead to a saving in the computing time.

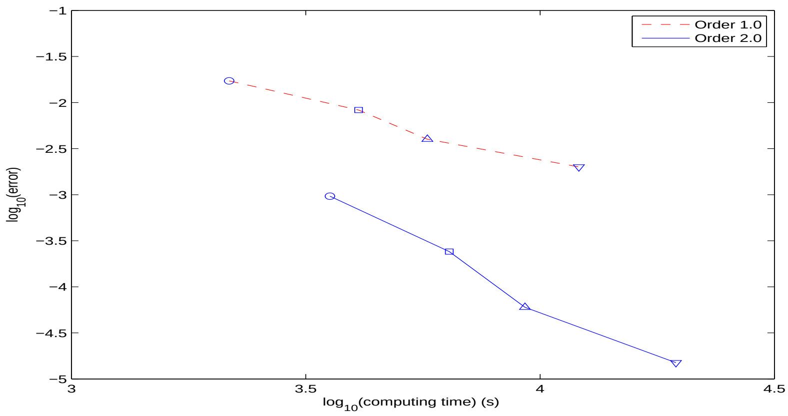

FIGURE 2. Computing time v.s. error for different types of symplectic strong S^3_ω schemes with various time step for $T = 100$ with 10^5 samples, ◯: $h = 0.004$; □: $h = 0.002$; △: $h = 0.001$, ▽: $h = 0.0005$

For example, Fig. 1 shows that the error of the second order S^1_w scheme with $h = 0.004$ and the error of the first order S^1_w scheme with finer $h = 0.002$ are 0.0038 and 0.0049. However, the computing time required for the second order scheme is about 3200 seconds which is less than the 4180 seconds needed for the first order schemes. In Fig. 2, we observe that the error for the first order S^3_w scheme with $h = 0.0005$ is larger that that resulted from the second order S^3_w with a much larger step size $h = 0.004$. More importantly, the computing time required for the first and second order schemes are 12100 and 3560 seconds, respectively. Thus, a considerable reduction in computing time is achieved using a higher order scheme.

In Fig. 1 we have also included a non-symplectic scheme, namely the mean square first order Milstein scheme (see Chapter 10.3 in [7]). There is no doubt to conclude that the symplectic schemes offer a significant improvement in accuracy, but without a substantial increase in the computing time. For example, for $h = 0.001$, the error of the Milstein scheme is 0.2, more than 50 - 80 times larger than the corresponding errors of the first order symplectic schemes (which are 0.004 for the scheme based on S^3_w and 0.0025 for the scheme based on S^1_w). The computing time for the first order symplectic schemes based on S^1_ω and S^3_ω are 5684 seconds and 5747 seconds respectively, compared with 3804 seconds for the Milstein scheme.Thus, a remarkable improvement in accuracy is obtained using the symplectic schemes with an acceptable computing time.

In Table 1, we compare several symplectic and non-symplectic weak schemes. Since the system (55) is linear, it is easy to verify that we have

$$E(P(T;0,p,q) = e^{-\frac{\sigma^2 T}{2}}(\cos{(aT)}p - \sin{(aT)}q) \tag{57}$$

$$E(Q(T;0,p,q) = e^{-\frac{\sigma^2 T}{2}}(\sin{(aT)}p + \cos{(aT)}q). \tag{58}$$

We run a Monte Carlo simulation and estimate the 95% confidence intervals for $E(P(t;0,p,q))$ as

$$\bar{P}(t;0,p,q) \pm 1.96\frac{s_P(t;0,p,q)}{\sqrt{M}}, \tag{59}$$

TABLE 1. $E[P(T)]$ from various schemes for $a = 2$, $\sigma = 0.3$ and $T = 100$

Numerical Method	time step	95% confidence interval	computational time (s)
weak Euler scheme	$h = 0.01$	0.0049 ± 0.0010	904
	$h = 0.001$	0.007 ± 0.0017	9010
weak 2nd order Taylor scheme	$h = 0.01$	0.0048 ± 0.0014	4650
	$h = 0.001$	0.0055 ± 0.0014	46100
weak S^1_ω 1st order scheme	$h = 0.01$	0.006 ± 0.0013	873
	$h = 0.001$	0.0057 ± 0.0013	13492
weak S^1_ω 2nd order scheme	$h = 0.01$	0.0033 ± 0.0014	4526
	$h = 0.001$	0.0051 ± 0.0014	44624
weak S^3_ω 1st order scheme	$h = 0.01$	0.0056 ± 0.0013	1085
	$h = 0.001$	0.0056 ± 0.0013	12735
weak S^3_ω 2nd order scheme	$h = 0.01$	0.0046 ± 0.0013	2816
	$h = 0.001$	0.0055 ± 0.0014	30356

where $M = 10^6$ is the number of independent realizations in the Monte Carlo simulations, $\bar{P}(t; 0, p, q)$ is the sample average and $s_P(t; 0, p, q)$ is the sample standard deviation (see also formula 7.7 in [10]). In addition to the weak scheme error, we also have the Monte Carlo error, but the margin of error in the confidence intervals (59) reflects the Monte Carlo error only. In [4] we show that the Euler scheme requires a much smaller time step h to converge than the symplectic schemes, and it fails for $h = 2^{-5}$, so here we consider $h = 0.01$ and $h = 0.001$ (see also [2] for a study of the global error).

Replacing $T = 100$ in (57) we get $E[P(100; 0, 1, 0)] = 0.0056$. From the numerical results reported in Table 1 for $T = 100$, we notice that, with one exception, the confidence intervals include the exact value 0.0056. Moreover, the weak 2nd order symplectic schemes require less computational time than the weak 2nd order Taylor scheme. This can be explained by the fact that for the system (55), the 2nd order Taylor scheme includes the stochastic integrals $I_{(0,1)}$, $I_{(0,2)}$, $I_{(1,0)}$, $I_{(2,0)}$, $I_{(1,2)}$, $I_{(2,1)}$, in addition to the multiple stochastic integrals included in the 2nd order symplectic schemes.

Due to the invariance under permutations proved in Theorems 3.1 and 3.2, for any SHS (1) preserving the Hamiltonian functions, the stochastic integrals included in a k-order weak symplectic scheme based on the generating functions S^i_ω, $i = 1, 2, 3$ are $\{I_\alpha | l(\alpha) = 1, \ldots, k, \alpha = (j, \ldots, j), j = 0, \ldots, m\}$. On the other hand, a k-order weak Taylor scheme contains the stochastic integrals $\{I_\alpha | l = l(\alpha) = 1, \ldots, k, \alpha = (j_1, \ldots, j_l), j_i = 0, \ldots, m, i = 1, \ldots, l\}$. Thus, the computational advantage of the weak symplectic schemes compared with the weak Taylor schemes for SHS (1) preserving the Hamiltonian functions increases with the order k, because simulating multiple stochastic integrals of higher order is both mathematically difficult and time consuming.

6. Conclusions

We propose strong and weak symplectic schemes for the special class of stochastic Hamiltonian systems preserving the Hamiltonian functions. Following an approach based on the generating function method, the important contribution of the present work is to prove that the coefficients of the generating functions are invariant under permutations for stochastic Hamiltonian systems preserving Hamiltonian functions. This invariance property is the crucial factor leading to the successful construction of computationally efficient high order symplectic schemes.

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