

## ON GLOBAL ERROR OF SYMPLECTIC SCHEMES FOR STOCHASTIC HAMILTONIAN SYSTEMS

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**Abstract.** We investigate a first order weak symplectic numerical scheme for stochastic Hamiltonian systems. Given the solution  $(X_t)$  and a class of functions  $f$ , we derive the expansion of the global approximation error for the computed  $E(f(X_t))$  in powers of the discretization step size. The present study is an extension of the results obtained by Talay and Tubaro for the explicit Euler scheme. Based on the derived global error expansion, we construct an extrapolation method of the weak second order. The performance of the extrapolation method is demonstrated numerically for a model simulating oscillations of the particles in storage rings.

**Key words.** Stochastic Hamiltonian system, symplectic methods, numerical weak schemes, extrapolation method.

### 1. Introduction

In recent years, considerable progress has been made in the study of uncertainty quantification. It is known that for some practical problems in science and engineering, the effect due to random noise may lead to a significant change in the physical response. Hence, mathematical models based on a deterministic approach may not be sufficient, and the use of stochastic models has been receiving considerable attention. To take into account the random effect, the governing equations are usually represented by stochastic differential equations. In contrast to many efficient and robust numerical algorithms already developed for the deterministic differential equations, the progress on numerical methods for solving stochastic differential equations is less mature. The most common problems associated with computational algorithms for stochastic differential equations are the poor accuracy and poor convergence, especially when long time solutions are required. Hence, it is a challenging task to develop accurate and robust numerical schemes for stochastic differential equations.

The Euler method is a popular numerical method for solving differential equations, and the scheme has been extended to stochastic equations because of its simple implementation [3]. For stochastic Hamiltonian systems, symplectic schemes [5] are important computational methods that preserve the symplectic structure, and their accuracy does not deteriorate even for long time computations. In this paper, we focus on the application of the Euler method and a first order weak symplectic scheme for approximating the solution of stochastic Hamiltonian systems.

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

$$(1) \quad \begin{aligned} dP &= -\partial_Q H_0(P, Q)dt - \sum_{r=1}^m \partial_Q H_r(P, Q) \circ dw_t^r, \quad P(0) = p \\ dQ &= \partial_P H_0(P, Q)dt + \sum_{r=1}^m \partial_P H_r(P, Q) \circ dw_t^r, \quad Q(0) = q, \end{aligned}$$

where  $P, Q, p, q$  are  $n$ -dimensional column 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 SDE (1) is called a Stochastic Hamiltonian Systems (SHS) ([7]). Here and in the rest of this paper, for any function  $f$  defined on  $\mathbb{R}^n \times \mathbb{R}^n$ , we denote by  $\partial_P f$  the column vector with components  $(\partial f / \partial P_i), 1 \leq i \leq n$ , and similarly we let  $\partial_Q f$  denote the column vector with components  $(\partial f / \partial Q_i), 1 \leq i \leq n$ .

We denote the solution of the stochastic Hamiltonian system (SHS) (1) by  $X_t^{0, X_0} = \begin{pmatrix} P_t^{0; p, q} \\ Q_t^{0; p, q} \end{pmatrix}$ , where  $0 \leq t \leq T$  and  $X_0 = (p^T, q^T)^T$  is a random variable having moments of any order and independent of any increments  $W_t - W_s$  of the Wiener process  $W_t = (w_t^1, \dots, w_t^m)^T$ . It is known that if  $H_j, j = 0, \dots, m$  are sufficiently smooth, then  $X_t^{0, X_0}$  is a phase flow (diffeomorphism) almost sure ([4]).

The stochastic flow  $(p, q) \longrightarrow (P, Q)$  of the SHS (1) preserves the symplectic structure [7, Theorem 2.1] as follows:

$$(2) \quad dP \wedge dQ = dp \wedge dq,$$

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

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

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

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

Let divide the interval  $[0, T]$  in  $N$  subintervals with a uniform time step  $h = T/N$ . If the approximation  $\bar{X}_k^{0, X_0} = X_0, \bar{X}_k^{0, X_0} = (\bar{P}_k^{(0; p, q)}, \bar{Q}_k^{(0; p, q)}), k = 1, \dots, N$ , of the solution  $X_{t_k}^{0, X_0} = (P_{t_k}^{(0; p, q)}, Q_{t_k}^{(0; p, q)})$ , satisfies

$$(3) \quad |E[f(\bar{X}_k^{0, X_0})] - E[f(X_{t_k}^{0, X_0})]| \leq Kh^j,$$

for  $f$  from a sufficiently large class of functions, where  $t_k = kh \in [0, T]$  and the constant  $K > 0$  does not depend on  $k$  and  $h$ , then we say that  $\bar{X}_k^{0, X_0}$  approximate the solution  $X_{t_k}^{0, X_0}$  of (1) in the weak sense [5] with weak order of accuracy  $j$ .

To simplify the notation we define

$$(4) \quad G_{(r,r)} = \sum_{i=1}^n \frac{\partial H_r}{\partial Q_i} \frac{\partial H_r}{\partial P_i},$$

for  $r = 1, \dots, m$ . We consider the following weak method  $\bar{X}_k^{0, X_0} = (\bar{P}_k^{(0;p,q)}, \bar{Q}_k^{(0;p,q)})$ ,

$$(5) \quad \begin{aligned} \bar{P}_{k+1} &= \bar{P}_k - h \left( \partial_Q H_0 + \frac{1}{2} \sum_{r=1}^m \partial_Q G_{(r,r)} \right) - \sqrt{h} \sum_{r=1}^m \varsigma_{rk} \partial_Q H_r \\ \bar{Q}_{k+1} &= \bar{Q}_k + h \left( \partial_P H_0 + \frac{1}{2} \sum_{r=1}^m \partial_P G_{(r,r)} \right) + \sqrt{h} \sum_{r=1}^m \varsigma_{rk} \partial_P H_r \end{aligned}$$

where the random variables  $\varsigma_{rk}$  are mutually independent identically distributed according to the law,  $P(\varsigma_{rk} = \pm 1) = 1/2$ , and everywhere the arguments are  $(\bar{P}_{k+1}, \bar{Q}_k)$ . Under certain conditions regarding the Hamiltonians  $H_i$ ,  $i = 1, \dots, m$ , the implicit scheme (5) is well-defined, symplectic, and of weak order 1 (see Theorem 4.2 in [5] for  $\alpha = 1/2, \beta = 1$ ). Thus, for a smooth function  $f$  from  $\mathbb{R}^{2n} \rightarrow \mathbb{R}$ , for the global error

$$(6) \quad Err(T, h) = E[f(X_T^{0, X_0})] - E[f(\bar{X}_N^{0, X_0})]$$

there exists a positive constant  $C(T)$  independent of  $h$  such that

$$(7) \quad |Err(T, h)| \leq C(T)h.$$

In this work, we derive an error expansion for  $Err(T, h)$  of the form

$$(8) \quad Err(T, h) = e_1(T)h + O(h^2).$$

We investigate the proposed symplectic scheme (5), following the same approach and assuming similar conditions as reported in [9]. In [8], under less restrictive assumptions, the error expansion is derived for the implicit Euler scheme and a system with constant diffusion matrix. However, instead of the Euler scheme, we now focus on the fully implicit symplectic scheme and derive the expansion of the global error. The main challenge to lower the assumptions in the present study is the fact that in addition to non-constant diffusion coefficients for the SHS (1), the symplectic scheme (5) contains implicit terms in the stochastic part.

It is known that symplectic numerical schemes for Hamiltonian systems produce accurate results for long term simulations ([5], [1], [2]). Recall that in the weak formulation, both the Euler and the symplectic scheme (5) have the same order (i.e., order 1) of accuracy. The current work was motivated by the interest to provide a theoretical explanation for the excellent approximations obtained with the symplectic weak scheme (5), whereas the Euler method produces a very poor solution for the Kubo oscillator, which is a simple linear stochastic Hamiltonian system. As will be shown shortly in Section 4.1, a clear justification could be revealed by the derived global error expansions.

After presenting preliminary results in the next section, in Section 3 we derive the global error expansion (8) for the first order weak symplectic scheme (5). Section 4 illustrates some applications of the error expansion. First, using the present expansion (8) and the global error expansion for the Euler scheme given in [9], we explain the poor accuracy of the Euler scheme compared to the symplectic scheme (5) for the Kubo oscillator. Then, based on the global error expansion and applying an extrapolation method, we construct a second weak order scheme and we confirm numerically its accuracy. Conclusions and possible extensions of this approach to higher order symplectic schemes are discussed in Section 5.

## 2. Preliminary discussion

We assume that the coefficients of (1) are smooth enough to satisfy the following global Lipschitz condition,  $L_1 > 0$

$$(9) \quad \sum_{j=0}^m \left\| \begin{pmatrix} \partial_P H_j \\ \partial_Q H_j \end{pmatrix} (P, Q) - \begin{pmatrix} \partial_P H_j \\ \partial_Q H_j \end{pmatrix} (p, q) \right\| \leq L_1 (\|P - p\| + \|Q - q\|).$$

We also suppose that  $H_i$ ,  $i = 0, \dots, m$  are  $C^\infty$  functions, whose derivatives of any order are bounded. Under these conditions we know from Theorem 4.2 in [5] that the implicit scheme (5) is well defined and of the first weak order.

To simplify the notation, let denote

$$\begin{aligned} a &= -\partial_Q H_0 + \frac{1}{2} \sum_{r=1}^m \sum_{j=1}^n \left( \frac{\partial H_r}{\partial Q_j} \partial_Q \left( \frac{\partial H_r}{\partial P_j} \right) - \frac{\partial H_r}{\partial P_j} \partial_Q \left( \frac{\partial H_r}{\partial Q_j} \right) \right) \\ b &= \partial_P H_0 + \frac{1}{2} \sum_{r=1}^m \sum_{j=1}^n \left( -\frac{\partial H_r}{\partial Q_j} \partial_P \left( \frac{\partial H_r}{\partial P_j} \right) + \frac{\partial H_r}{\partial P_j} \partial_P \left( \frac{\partial H_r}{\partial Q_j} \right) \right) \\ \sigma^r &= -\partial_Q H_r, \quad \gamma^r = \partial_P H_r, \end{aligned}$$

where everywhere the arguments are  $(P, Q)$ , and  $a$ ,  $b$ ,  $\sigma^r$ ,  $\gamma^r$ ,  $r = 1, \dots, m$  are  $n$ -dimensional column vectors. Using the Ito stochastic integration, we rewrite the equations (1) as

$$(10) \quad dP = a(P, Q)dt + \sum_{r=1}^m \sigma^r(P, Q)dw_t^r, \quad P(0) = p$$

$$(11) \quad dQ = b(P, Q)dt + \sum_{r=1}^m \gamma^r(P, Q)dw_t^r, \quad Q(0) = q,$$

Let  $L$  be the differential operator associated with (10)-(11) given by

$$(12) \quad \begin{aligned} L &= \sum_{j=1}^n \left( a_j \frac{\partial}{\partial P_j} + b_j \frac{\partial}{\partial Q_j} \right) \\ &+ \frac{1}{2} \sum_{r=1}^m \sum_{i,j=1}^n \left( \sigma_i^r \sigma_j^r \frac{\partial^2}{\partial P_i \partial P_j} + \gamma_i^r \gamma_j^r \frac{\partial^2}{\partial Q_i \partial Q_j} + 2\sigma_i^r \gamma_j^r \frac{\partial^2}{\partial P_i \partial Q_j} \right) \end{aligned}$$

The weak Euler scheme for the system (10)-(11) has the form  $\tilde{X}_k^{0, X_0} = (\tilde{P}_k^{(0;p,q)}, \tilde{Q}_k^{(0;p,q)})$  where

$$(13) \quad \begin{aligned} \tilde{P}_{k+1} &= \tilde{P}_k + ha(\tilde{P}_k, \tilde{Q}_k) - \sqrt{h} \sum_{r=1}^m \sigma^r(\tilde{P}_k, \tilde{Q}_k) \varsigma_{rk} \\ \tilde{Q}_{k+1} &= \tilde{P}_k + hb(\tilde{P}_k, \tilde{Q}_k) - \sqrt{h} \sum_{r=1}^m \gamma^r(\tilde{P}_k, \tilde{Q}_k) \varsigma_{rk} \end{aligned}$$

where the random variables  $\varsigma_{rk}$  are mutually independent identically distributed according to the law,  $P(\varsigma_{rk} = \pm 1) = 1/2$  (see chapter 14.1 in [3]).

We define the class  $\mathcal{F}$  to be formed with the functions  $f$  defined on  $\mathbb{R}^{2n}$  for which there exists constants  $K > 0$  and  $\chi > 0$ , such that

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

for any  $x \in \mathbf{R}^{2n}$ . If  $f \in \mathcal{F}$ , then the function  $u(t, x) := E[f(X_T^{t,x})]$  verifies the equations

$$(14) \quad \frac{\partial u}{\partial t} + Lu = 0, \quad u(T, x) = f(x).$$

Notice that, we can express the global error as

$$(15) \quad Err(T, h) = E[u(0, X_0)] - E[u(T, \bar{X}_N^{0, X_0})].$$

For any multi-index  $\alpha = (\alpha_1, \dots, \alpha_r)$  with length  $|\alpha| = \alpha_1 + \dots + \alpha_r$ , let  $\partial_\alpha$  denote the partial derivative of order  $|\alpha|$ :

$$(16) \quad \frac{\partial^{|\alpha|}}{\partial_1^{\alpha_1} \dots \partial_r^{\alpha_r}}.$$

From Lemma 2 in [9], we have

**Lemma 2.1.** *For any multi-index  $\alpha$  there exist the constants  $k_\alpha(T) > 0$  and  $C_\alpha(T) > 0$  such that for any  $0 \leq t \leq T$*

$$(17) \quad |\partial_\alpha u(t, x)| \leq C_\alpha(T)(1 + |x|^{k_\alpha(T)}).$$

From the proof of Theorem 4.2 in [5], it is clear that for the scheme (5) we have:

**Lemma 2.2.** *For any integer  $k$  there exist a constant  $C_k > 0$  such that for any  $N$  and any integer  $0 \leq j \leq N$  we have*

$$(18) \quad E[|\bar{X}_j^{0, x_0}|^k] \leq \exp(c_k T).$$

### 3. Main results

**Theorem 3.1.** *For the first order symplectic weak scheme given in (5), the global error is given by*

$$(19) \quad Err(T, h) = -h \int_0^T E[\phi(s, X_s^{0, X_0})] ds + O(h^2),$$

for some smooth function  $\phi$ . Moreover, it is possible to obtain an expansion of the form

$$(20) \quad Err(T, h) = e_1(T)h + \dots + e_j(T)h^j + O(h^{j+1}).$$

*Proof.* The proof is similar with the proof of Theorem 1 in [9]. For simplicity we will give only the proof for  $j = 1$ . Let  $\bar{X}_0^{0, X_0} = X_0$ ,  $\bar{X}_k^{0, X_0} = (\bar{P}_k^{(0; p, q)}, \bar{Q}_k^{(0; p, q)})$ ,  $k = 1, \dots, N$  be the approximation obtained from scheme (5) starting at  $t = 0$  from  $X_0 = (p, q)^T$ . Using equation (15) we get

$$(21) \quad \begin{aligned} Err(T, h) &= E[u(0, X_0)] - E[u(h, \bar{X}_1^{0, X_0})] + E[u(h, \bar{X}_1^{0, X_0})] - E[u(2h, \bar{X}_2^{0, X_0})] \\ &+ \dots + E[u((N-1)h, \bar{X}_{N-1}^{0, X_0})] - E[u(T, \bar{X}_N^{0, X_0})] \end{aligned}$$

For any multi-index  $\alpha = (\alpha_1, \dots, \alpha_{2n})$  and any column vector  $x = (x_1, \dots, x_{2n})^T$  we denote  $\Delta x^\alpha := (\Delta x_1)^{\alpha_1} \dots (\Delta x_{2n})^{\alpha_{2n}}$ . We compute  $E[u(kh, \bar{X}_k^{0, X_0})] - E[u((k-1)h, \bar{X}_{k-1}^{0, X_0})]$ ,  $k = 1, \dots, N$  using the following Taylor expansion at the point  $\left( (k-1)h, \bar{X}_{k-1}^{0, X_0} \right)$ ,

1) $h, \bar{X}_{k-1}^{0, X_0}$ ):

$$\begin{aligned} u(t+h, x+\Delta x) &= u(t, x) + h \frac{\partial}{\partial t} u(t, x) + \frac{1}{2} h^2 \frac{\partial^2}{\partial t^2} u(t, x) + h \sum_{|\alpha|=1} \Delta x^\alpha \frac{\partial}{\partial t} (\partial_\alpha u(t, x)) \\ &\quad + \frac{h}{2} \sum_{|\alpha|=2} \Delta x^\alpha \frac{\partial}{\partial t} (\partial_\alpha u(t, x)) + \frac{h}{6} \sum_{|\alpha|=3} \Delta x^\alpha \frac{\partial}{\partial t} (\partial_\alpha u(t, x)) \\ &\quad + \frac{1}{|\alpha|!} \sum_{|\alpha|=1}^5 \Delta x^\alpha \partial_\alpha u(t, x) + O(h^3). \end{aligned}$$

To compute  $\Delta \bar{X}_{k-1}^{0, X_0} = \begin{pmatrix} \bar{P}_k - \bar{P}_{k-1} \\ \bar{Q}_k - \bar{Q}_{k-1} \end{pmatrix}$ , we use the Taylor expansions repeatedly in equations (5) (the calculations are similar with those reported in the proof of Theorem 4.2 in [5]). Using equations (12) and (14) we get, for any integer  $1 \leq k \leq N$

$$(22) \quad \begin{aligned} E[u(kh, \bar{X}_k^{0, X_0})] &= E[u((k-1)h, \bar{X}_{k-1}^{0, X_0})] + h^2 E \left[ \phi \left( (k-1)h, \bar{X}_{k-1}^{0, X_0} \right) \right] \\ &\quad + h^3 E[R_k]. \end{aligned}$$

Here the function  $\phi(t, x)$  is a sum of terms of the type  $g(x) \partial_\alpha u(t, x)$ , where  $\alpha$  is a multi-index and  $g \in \mathcal{F}$  (see Appendix for the exact formula for  $\phi$  when  $n = m = 1$ ). The remainder term  $E[R_k]$  is a sum of terms of the type

$$(23) \quad E[d(\bar{X}_{k-1}^{0, X_0}) \partial_\alpha u \left( (k-1)h, \bar{X}_{k-1}^{0, X_0} + \theta(\bar{X}_k^{0, X_0} - \bar{X}_{k-1}^{0, X_0}) \prod_{r=1}^m \zeta_{r(k-1)}^{j_r} \right)],$$

where  $d \in \mathcal{F}$  and  $\theta$  is a random variable taking values in  $(0, 1)$ . Thus from Lemma 2.1 and Lemma 2.2, there exists the real numbers  $C_1(T) > 0$ ,  $C_2(T) > 0$  independent of  $h$  such that for some positive integer  $s$ , for any  $t \in [0, T]$  and any  $x \in \mathbb{R}^{2n}$ , we have

$$(24) \quad |\phi(t, x)| \leq C_1(T)(1 + |x|^s),$$

and for any integer  $1 \leq k \leq N$ , we have

$$(25) \quad E \left[ \left| \phi \left( (k-1)h, \bar{X}_{k-1}^{0, X_0} \right) \right| \right] \leq C_2(T), \quad E[|R_k|] \leq C_2(T).$$

Replacing (22) in (21), we obtain

$$(26) \quad Err(T, h) = -h^2 \sum_{k=0}^{N-1} E \left[ \phi \left( kh, \bar{X}_k^{0, X_0} \right) \right] - h^3 \sum_{k=1}^N E[R_k].$$

Using (25) and  $T = hN$ , we rewrite

$$(27) \quad Err(T, h) = -h \left( h \sum_{k=0}^{N-1} E \left[ \phi \left( kh, \bar{X}_k^{0, X_0} \right) \right] \right) + h^2 \mathcal{R}_N,$$

and there exists a real number  $C(T) > 0$  independent of  $h$  such that  $|\mathcal{R}_N| \leq C(T)$ , and

$$(28) \quad h \sum_{k=0}^{N-1} E \left[ \left| \phi \left( kh, \bar{X}_k^{0, X_0} \right) \right| \right] \leq C(T).$$

Thus equation (27) implies that for any function  $f \in \mathcal{F}$ , there exists a real number  $c_1(T) > 0$  independent of  $h$ , such that

$$(29) \quad E[f(\bar{X}_T^{0,X_0})] = E[f(X_T^{0,X_0})] + R_T(h),$$

with  $|R_T(h)| \leq hc_1(T)$ . Hence from (24) we also have

$$(30) \quad E[\phi(t, \bar{X}_T^{0,X_0})] = E[\phi(t, X_T^{0,X_0})] + R'_T(h),$$

with  $|R'_T(h)| \leq hc(T)$  for some real number  $c(T) > 0$  independent of  $h$ . Finally, notice that

$$(31) \quad \begin{aligned} & \left| h \sum_{k=0}^{N-1} E \left[ \phi \left( kh, \bar{X}_k^{0,X_0} \right) \right] - \int_0^T E \left[ \phi \left( s, X_s^{0,X_0} \right) \right] ds \right| \leq \\ & h \sum_{k=0}^{N-1} \left| E \left[ \phi \left( kh, \bar{X}_k^{0,X_0} \right) \right] - E \left[ \phi \left( kh, X_{hk}^{0,X_0} \right) \right] \right| \\ & + \left| h \sum_{k=0}^{N-1} E \left[ \phi \left( kh, X_{hk}^{0,X_0} \right) \right] - \int_0^T E \left[ \phi \left( s, X_s^{0,X_0} \right) \right] ds \right| \end{aligned}$$

Thus, using (30),  $T = Nh$  and the fact that the function  $s \rightarrow E[\phi(s, X_s^{0,X_0})]$  has a continuous first derivative, we get

$$(32) \quad \left| h \sum_{k=0}^{N-1} E \left[ \phi \left( kh, \bar{X}_k^{0,X_0} \right) \right] - \int_0^T E \left[ \phi \left( s, X_s^{0,X_0} \right) \right] ds \right| = O(h).$$

Replacing in (27), the equation (19) is derived.  $\square$

#### 4. Applications

In this section, we report numerical simulations and present a new second weak order scheme constructed using the Romberg extrapolation method.

**4.1. Numerical tests.** In [6] the Kubo oscillator based on the following SDEs in the sense of Stratonovich is used to demonstrate the advantage of using the stochastic symplectic scheme (5) instead of the Euler scheme (13) for long time computations. The mathematical model for the Kubo oscillator is given by:

$$(33) \quad \begin{aligned} dP &= -aQdt - \sigma Q \circ dw_t, & P(0) &= p_0, \\ dQ &= aPdt + \sigma P \circ dw_t, & Q(0) &= q_0, \end{aligned}$$

where  $a$  and  $\sigma$  are constants. Even though this is a simple linear system, the Euler method produces a very poor result compared to the symplectic scheme. It should be noted that both numerical schemes have the same order of accuracy.

With  $n = m = 1$ , the Hamiltonian functions are given by

$$(34) \quad H_0(P(t), Q(t)) = a \frac{P(t)^2 + Q(t)^2}{2}, \quad H_1(P(t), Q(t)) = \sigma \frac{P(t)^2 + Q(t)^2}{2}.$$

Replacing in (4) we have  $G_{(1,1)}(P(t), Q(t)) = \sigma^2 P(t)Q(t)$ . Since (33) is a linear system, the expectations can be computed analytically and we have

$$(35) \quad E(P_T^{t;p,q}) = e^{-\frac{\sigma^2(T-t)}{2}} (\cos(a(T-t))p - \sin(a(T-t))q)$$

$$(36) \quad E(Q_T^{t;p,q}) = e^{-\frac{\sigma^2(T-t)}{2}} (\sin(a(T-t))p + \cos(a(T-t))q).$$

Let the values of the parameters be  $a = 2$ ,  $\sigma = 0.2$ , and the initial values be  $p_0 = 1$ ,  $q_0 = 0$ . The time step is taken as  $h = 2^{-5}$ . In Fig. 1, we compare the estimations obtained using the explicit Euler scheme and the first-order weak symplectic scheme

(5). The numerical results are compared for Monte Carlo simulations using 100000 samples. It is clear that the Euler scheme fails even after a short term simulation.

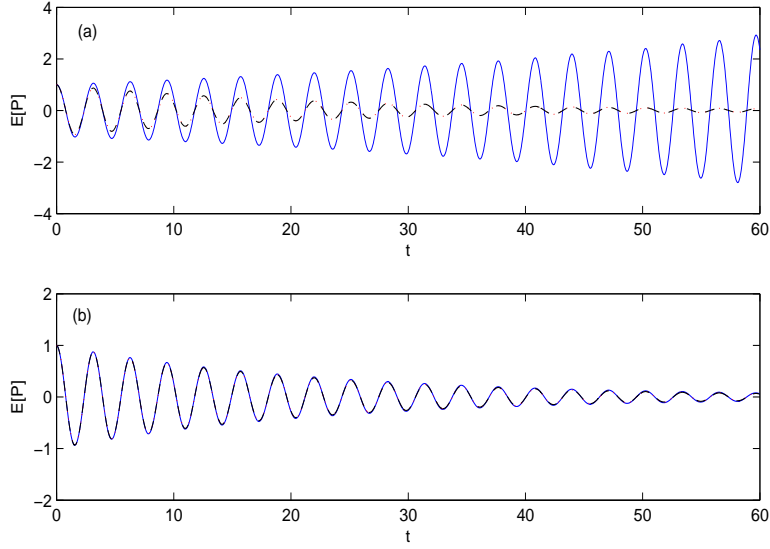


FIGURE 1. The expected value of  $P(t)$  (a) Exact value (red dashed line), Euler weak scheme (blue solid line) (b): Exact value (red dashed line), first order symplectic weak scheme (blue solid line)

By comparing the error expansions for the Euler scheme and the symplectic scheme (5), the results presented in Fig. 1 are justified. Consider

$$(37) \quad f\left((P_t^{0;p_0,q_0}, Q_t^{0;p_0,q_0})^T\right) = P_t^{0;p_0,q_0},$$

then  $u(t, (p, q)^T) = E(P_T^{t;p,q})$  is given in equation (35). For the symplectic scheme (5), from Theorem 3.1 we get

$$(38) \quad e_1(T) = - \int_0^T E[\phi(s, (P_s^{0;p_0,q_0}, Q_s^{0;p_0,q_0})^T)] ds.$$

Using the formula in appendix for  $\phi$ , for  $\sigma = 0.2$  and  $a = 2$ , we have

$$(39) \quad e_1(T) = \exp(-0.02T) \left( -p_0 \sin(2T) - 0.0004T p_0 \cos(2T) + 0.0004T q_0 \sin(2T) \right).$$

For the Euler scheme, the first order term in the global error expansion [9] is given by

$$(40) \quad e_1^e(T) = - \int_0^T E[\psi_e(s, (P_s^{0;p_0,q_0}, Q_s^{0;p_0,q_0})^T)] ds,$$



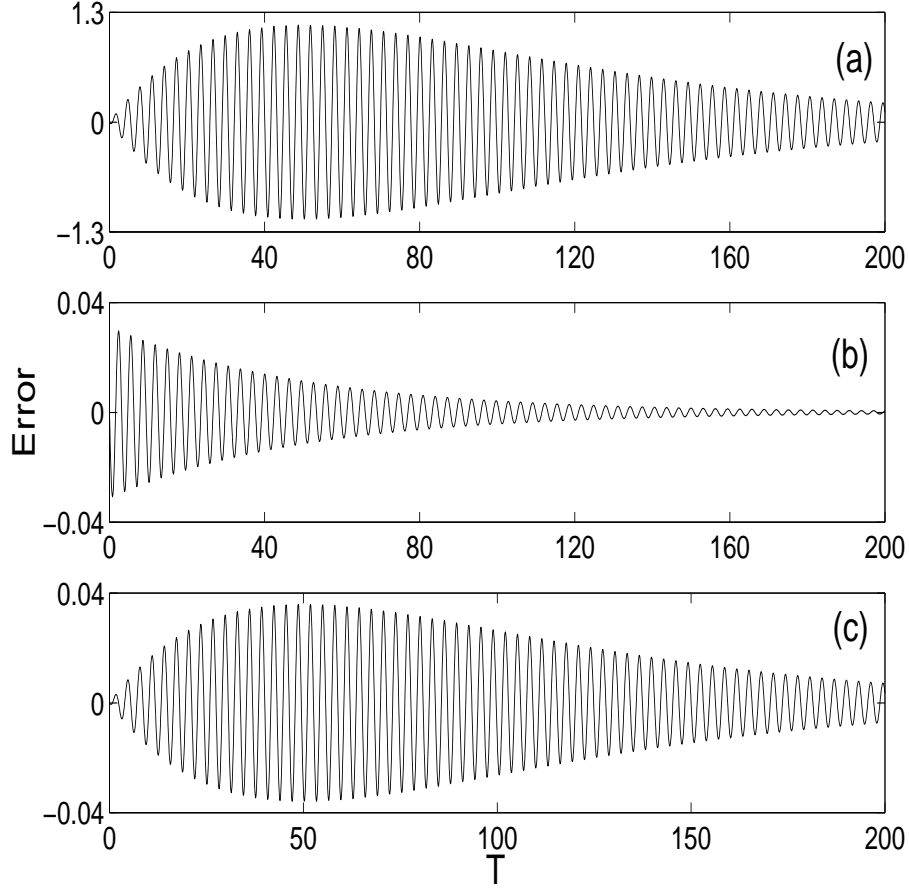


FIGURE 2. Global error first order term (a)  $e_1^e(T)h$  for  $h = 2^{-5}$ , (b)  $e_1(T)h$  for  $h = 2^{-5}$  (c)  $e_1^e(T)h$  for  $h = 2^{-10}$

and applying the equation (9) in [9] for the formula for  $\psi_e$  with  $\sigma = 0.2$  and  $a = 2$ , we get

$$(41) \quad e_1^e(T) = \exp(-0.02T)T \left( -2p_0 \cos(2T) + 2q_0 \sin(2T) + 0.04p_0 \sin(2T) + 0.04q_0 \cos(2T) \right).$$

In Fig. 2 we plot the graphs of  $e_1(T)h$  and  $e_1^e(T)h$  for  $p_0 = 1$ ,  $q_0 = 0$  and two values of the time step  $h$ . With  $h = 2^{-5}$ , the amplitude of error based on the Euler scheme  $e_1^e(T)h$  increases very rapidly to values larger than 1, and when  $T > 80$ , the error is oscillating around 0 with a decreasing amplitude (see Fig. 2 a). In contrast, the error for the symplectic scheme  $e_1(T)h$  oscillates around 0 with a fast decaying amplitude, the maximum error appears at the beginning with amplitude less than 0.03 (see Fig. 2 b). The error behaviors explains the results given in Fig. 1.

It is interesting to note that the error profile is independent of the time step  $h$ . Fig. 2 c displays the Euler error with  $h = 2^{-10}$ . Comparing the errors illustrated in Fig. 2 a and Fig. 2 c, the profiles are essentially identical but the maximum error

is reduced from 1.3 for  $h = 2^{-5}$  to less than 0.04 when  $h = 2^{-10}$ . Clearly, the Euler scheme will produce solutions as accurate as those resulted from the symplectic scheme when a finer time step is adopted.

**4.2. Extrapolation method.** Following the idea introduced in [9], we now apply the global error expansion in Theorem 3.1 to construct numerical results of order  $h^2$  from results of the first weak order scheme (5).

Let  $\bar{X}_k^{0,X_0}(h)$  and  $\bar{X}_k^{0,X_0}(h/2)$  be the approximations obtained from the symplectic first weak order scheme (5) with time steps  $h$  and  $h/2$ , respectively. Then using (19) it is easy to verify that for the new approximation

$$(42) \quad \bar{Y}_k^{0,X_0}(h) = 2E \left[ f \left( \bar{X}_k^{0,X_0}(h/2) \right) \right] - E \left[ f \left( \bar{X}_k^{0,X_0}(h) \right) \right]$$

we have

$$(43) \quad E[f(X_T^{0,X_0})] - \bar{Y}_N^{0,X_0}(h) = O(h^2).$$

In [1] we propose a symplectic second weak order scheme for the SHS (1). Compared with the second order approximation given by extrapolation (42), the second order symplectic scheme in [1] requires the computation of several extra partial derivatives of the Hamiltonians and the generation of more random variables if  $m > 1$ . Therefore, the second order symplectic scheme requires more calculations and the computing time than those needed based on the extrapolation formula(42). However, it is not obvious whether the approximation (42) has the desirable property of preserving the symplectic structure for any general function  $f$ .

We illustrate numerically the performance of the extrapolation (42) for the following SHS modeling the oscillations of the particles in storage rings ([6]):

$$(44) \quad \begin{aligned} dP &= -\beta^2 \sin Q dt - \sigma_1 \cos Q \circ dw_t^1 - \sigma_2 \sin Q \circ dw_t^2, \\ dQ &= P dt. \end{aligned}$$

Notice that

$$(45) \quad \begin{aligned} H_0(P, Q) &= -\beta^2 \cos Q + P^2/2 = U(Q) + V(P), \quad H_1(Q) = \sigma_1 \sin Q, \\ H_2(Q) &= -\sigma_2 \cos Q, \quad G_{1,1}(P, Q) = G_{2,2}(P, Q) = 0. \end{aligned}$$

Hence, the system (44) is a SHS with separable Hamiltonians [5]. The symplectic first order scheme (5) and the symplectic second order scheme in [1] are explicit.

The mean energy  $E[e(P, Q)]$  of the system (44) is defined ([5]) as

$$(46) \quad e(P, Q) = P^2/2 - \beta^2 \cos(Q).$$

If  $\sigma_1 = \sigma_2$  we have ([5])

$$(47) \quad E \left[ e \left( P_t^{0;p,q}, Q_t^{0;p,q} \right) \right] = e(p, q) + \frac{\sigma^2}{2} t.$$

A Monte Carlo simulation is performed for the parameters  $\sigma_1 = \sigma_2 = 0.3$ ,  $\beta = 4$ , the initial values  $p_0 = 1$ ,  $q_0 = 0$ , and  $t = 200$ . We estimate the 95% confidence intervals for  $E \left[ e \left( P_t^{0;p_0,q_0}, Q_t^{0;p_0,q_0} \right) \right]$  as

$$(48) \quad \bar{e}(t; 0, p_0, q_0) \pm 1.96 \frac{s_e(t; 0, p_0, q_0)}{\sqrt{M}},$$

where  $M$  is the number of independent realizations in the Monte Carlo simulations,  $\bar{e}(t; 0, p_0, q_0)$  is the sample average and  $s_e(t; 0, p_0, q_0)$  is the sample standard deviation (see also formula 7.7 in [5]). In addition to the weak schemes errors, we also have the Monte Carlo error, but the margin of error in the confidence intervals (48) reflects the Monte Carlo error only.

TABLE 1. 95% confidence intervals for  $E(e(P_{200}^{0;1,0}, Q_{200}^{0;1,0}))$ 

$h$	$M$	scheme (5)	approx. (42)	2nd order symplectic scheme
0.1	$10^5$	$-6.229 \pm 0.059$	$-6.585 \pm 0.123$	$-7.147 \pm 0.055$
0.05	$10^5$	$-6.419 \pm 0.057$	$-6.529 \pm 0.127$	$-6.609 \pm 0.057$
0.01	$4 \cdot 10^6$	$-6.501 \pm 0.009$	$-6.503 \pm 0.02$	$-6.502 \pm 0.0098$

The extrapolation technique can also be applied using the results from the Euler scheme. However, the Euler scheme needs a smaller time step  $h < 2^{-10}$  to converge for the system (44). Hence, we do not consider using the Euler scheme in this study.

The experiments presented in Table 1 demonstrate that the extrapolation approximation produces more accurate results than the first and second order symplectic schemes for larger values of  $h$  ( $h = 0.1$ , and  $h = 0.05$ ). For  $h \leq 0.01$ , the sample averages  $\bar{e}(200; 0, 1, 0)$  corresponding to any of the three methods considered in Table 1 are in very good agreement with the exact solution  $E[e(P_{200}^{0;1,0}, Q_{200}^{0;1,0})] = -6.5$  obtained from (47). Moreover, the results presented here are similar with those obtained for the symplectic schemes (7.3) and (7.5) in [5] (see Table 1 in [5]).

## 5. Conclusions

In this paper, we present a global error expansion for a symplectic, implicit first weak order scheme for a stochastic Hamiltonian system. Our work is an extension of the study of the global error expansion for the explicit and implicit Euler schemes reported in [9] and [8]. Unlike the Euler schemes, the symplectic implicit first weak order scheme contains implicit terms also in the stochastic part.

The global error expansion in Theorem 3.1 offer a justification for the extrapolation technique that can be applied to construct a second error scheme from the first order scheme (5). The numerical simulations reported in this paper confirm that this new method produces accurate results and provides saving in computing time compared to using a second order symplectic weak scheme directly. Moreover, in general, if the expectation in equation (19) can be computed, we can use the global error expansion to estimate the time step  $h$  such that the numerical scheme will approximate the solution within a given precision.

The approach followed here can be also applied to determine the leading error coefficients in the global error expansion for any of the higher order implicit symplectic weak schemes presented in [1], but the complexity of the calculations increases with the scheme order (see also Theorem 14.6.1 in [3]).

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## Appendix

$$\begin{aligned}
\phi(t, (P, Q)^T) &= \frac{1}{2} \frac{\partial^2 u(t, (P, Q)^T)}{\partial t^2} + e_{tp}((P, Q)^T) \frac{\partial^2 u(t, (P, Q)^T)}{\partial t \partial P} \\
&+ e_{tq}((P, Q)^T) \frac{\partial^2 u(t, (P, Q)^T)}{\partial t \partial Q} + e_{tpp}((P, Q)^T) \frac{\partial^3 u(t, (P, Q)^T)}{\partial t \partial^2 P} \\
&+ e_{tqq}((P, Q)^T) \frac{\partial^3 u(t, (P, Q)^T)}{\partial t \partial^2 Q} + e_{tpq}((P, Q)^T) \frac{\partial^3 u(t, (P, Q)^T)}{\partial t \partial P \partial Q} \\
&+ e_p((P, Q)^T) \frac{\partial u(t, (P, Q)^T)}{\partial P} + e_q((P, Q)^T) \frac{\partial u(t, (P, Q)^T)}{\partial Q} \\
&+ e_{pp}((P, Q)^T) \frac{\partial^2 u(t, (P, Q)^T)}{\partial^2 P} + e_{qq}((P, Q)^T) \frac{\partial^2 u(t, (P, Q)^T)}{\partial^2 Q} \\
&+ e_{pq}((P, Q)^T) \frac{\partial^2 u(t, (P, Q)^T)}{\partial P \partial Q} + e_{ppp}((P, Q)^T) \frac{\partial^3 u(t, (P, Q)^T)}{\partial^3 P} \\
&+ e_{qqq}((P, Q)^T) \frac{\partial^3 u(t, (P, Q)^T)}{\partial^3 Q} + e_{ppq}((P, Q)^T) \frac{\partial^3 u(t, (P, Q)^T)}{\partial^2 P \partial Q} \\
&+ e_{pqq}((P, Q)^T) \frac{\partial^3 u(t, (P, Q)^T)}{\partial^2 Q \partial P} + e_{pppp}((P, Q)^T) \frac{\partial^4 u(t, (P, Q)^T)}{\partial^4 P} \\
&+ e_{qqqq}((P, Q)^T) \frac{\partial^4 u(t, (P, Q)^T)}{\partial^4 Q} + e_{ppqq}((P, Q)^T) \frac{\partial^4 u(t, (P, Q)^T)}{\partial^2 P \partial^2 Q} \\
&+ e_{pppq}((P, Q)^T) \frac{\partial^4 u(t, (P, Q)^T)}{\partial^3 P \partial Q} + e_{pqqq}((P, Q)^T) \frac{\partial^4 u(t, (P, Q)^T)}{\partial P \partial^3 Q}
\end{aligned}$$

The formulas for the coefficients are the following (everywhere the arguments are  $(P, Q)^T$ ):

$$(49) \quad e_{tp} = -\frac{\partial H_0}{\partial Q} - \frac{1}{2} \frac{\partial G_{11}}{\partial Q} + \frac{\partial H_1}{\partial Q} \frac{\partial^2 H_1}{\partial P \partial Q},$$

$$(50) \quad e_{tq} = \frac{\partial H_0}{\partial P} + \frac{1}{2} \frac{\partial G_{11}}{\partial P} - \frac{\partial H_1}{\partial Q} \frac{\partial^2 H_1}{\partial^2 P}$$

$$(51) \quad e_{tpp} = \frac{1}{2} \frac{\partial^2 H_1}{\partial^2 Q}, \quad e_{tqq} = \frac{1}{2} \frac{\partial^2 H_1}{\partial^2 P}, \quad e_{tpq} = -\frac{\partial H_1}{\partial P} \frac{\partial H_1}{\partial Q}$$

$$\begin{aligned}
(52) \quad e_{pp} &= \frac{1}{8} \left( \frac{\partial G_{11}}{\partial Q} \right)^2 + \frac{1}{2} \frac{\partial G_{11}}{\partial Q} \frac{\partial H_0}{\partial Q} + \frac{1}{2} \left( \frac{\partial H_0}{\partial Q} \right)^2 \\
&- \frac{\partial H_1}{\partial Q} \frac{\partial^2 H_1}{\partial P \partial Q} \frac{\partial G_{11}}{\partial Q} - 2 \frac{\partial H_1}{\partial Q} \frac{\partial^2 H_1}{\partial P \partial Q} \frac{\partial H_0}{\partial Q} - \left( \frac{\partial H_1}{\partial Q} \right)^2 \frac{\partial^2 H_0}{\partial P \partial Q} \\
&- \frac{1}{2} \left( \frac{\partial H_1}{\partial Q} \right)^2 \frac{\partial^2 G_{11}}{\partial P \partial Q} + \frac{9}{2} \left( \frac{\partial H_1}{\partial Q} \right)^2 \left( \frac{\partial^2 H_1}{\partial P \partial Q} \right)^2 + \frac{3}{2} \frac{\partial^3 H_1}{\partial^2 P \partial Q} \left( \frac{\partial H_1}{\partial Q} \right)^3
\end{aligned}$$

$$\begin{aligned}
e_p &= \frac{\partial^2 H_0}{\partial P \partial Q} \frac{\partial H_0}{\partial Q} + \frac{1}{2} \frac{\partial^2 H_0}{\partial P \partial Q} \frac{\partial G_{11}}{\partial Q} + \frac{1}{4} \frac{\partial^2 G_{11}}{\partial P \partial Q} \frac{\partial G_{11}}{\partial Q} \\
&+ \frac{1}{2} \frac{\partial^2 G_{11}}{\partial P \partial Q} \frac{\partial H_0}{\partial Q} - \left( \frac{\partial^2 H_1}{\partial P \partial Q} \right)^2 \frac{\partial H_0}{\partial Q} - \frac{\partial^2 H_1}{\partial P \partial Q} \frac{\partial H_1}{\partial Q} \frac{\partial^2 G_{11}}{\partial P \partial Q} \\
(53) \quad &- \frac{1}{2} \left( \frac{\partial^2 H_1}{\partial P \partial Q} \right)^2 \frac{\partial G_{11}}{\partial Q} - \frac{1}{4} \left( \frac{\partial H_1}{\partial Q} \right)^2 \frac{\partial^3 G_{11}}{\partial^2 P \partial Q} - 2 \frac{\partial^2 H_1}{\partial P \partial Q} \frac{\partial H_1}{\partial Q} \frac{\partial^2 H_0}{\partial P \partial Q} \\
&- \frac{1}{2} \left( \frac{\partial H_1}{\partial Q} \right)^2 \frac{\partial^3 H_0}{\partial^2 P \partial Q} - \frac{\partial^3 H_1}{\partial^2 P \partial Q} \frac{\partial H_1}{\partial Q} \frac{\partial H_0}{\partial Q} - \frac{1}{2} \frac{\partial^3 H_1}{\partial^2 P \partial Q} \frac{\partial H_1}{\partial Q} \frac{\partial G_{11}}{\partial Q} \\
&+ \frac{9}{2} \frac{\partial^2 H_1}{\partial P \partial Q} \frac{\partial^3 H_1}{\partial^2 P \partial Q} \left( \frac{\partial H_1}{\partial Q} \right)^2 + 3 \left( \frac{\partial^2 H_1}{\partial P \partial Q} \right)^3 \frac{\partial H_1}{\partial Q} + \frac{1}{2} \frac{\partial^4 H_0}{\partial^3 P \partial Q} \left( \frac{\partial H_1}{\partial Q} \right)^3
\end{aligned}$$

$$\begin{aligned}
e_q &= -\frac{1}{2} \frac{\partial^2 H_0}{\partial^2 P} \frac{\partial G_{11}}{\partial Q} - \frac{1}{2} \frac{\partial^2 G_{11}}{\partial^2 P} \frac{\partial H_0}{\partial Q} - \frac{1}{4} \frac{\partial^2 G_{11}}{\partial^2 P} \frac{\partial G_{11}}{\partial Q} \\
&- \frac{\partial^2 H_0}{\partial^2 P} \frac{\partial H_0}{\partial Q} + \frac{\partial^2 H_1}{\partial^2 P} \frac{\partial^2 H_1}{\partial P \partial Q} \frac{\partial H_0}{\partial Q} + \frac{1}{2} \frac{\partial^2 H_1}{\partial^2 P} \frac{\partial^2 H_1}{\partial P \partial Q} \frac{\partial G_{11}}{\partial Q} \\
(54) \quad &+ \frac{1}{2} \frac{\partial^3 H_0}{\partial^3 P} \left( \frac{\partial H_1}{\partial Q} \right)^2 + \frac{1}{2} \frac{\partial^2 H_1}{\partial^2 P} \frac{\partial H_1}{\partial Q} \frac{\partial^2 G_{11}}{\partial P \partial Q} + \frac{\partial^2 H_1}{\partial^2 P} \frac{\partial H_1}{\partial Q} \frac{\partial^2 H_0}{\partial P \partial Q} \\
&+ \frac{\partial^2 H_0}{\partial^2 P} \frac{\partial H_1}{\partial Q} \frac{\partial^2 H_1}{\partial P \partial Q} + \frac{1}{2} \frac{\partial^2 G_{11}}{\partial^2 P} \frac{\partial H_1}{\partial Q} \frac{\partial^2 H_1}{\partial P \partial Q} + \frac{1}{2} \frac{\partial^3 H_1}{\partial^3 P} \frac{\partial H_1}{\partial Q} \frac{\partial G_{11}}{\partial Q} \\
&+ \frac{1}{4} \frac{\partial^3 G_{11}}{\partial^3 P} \left( \frac{\partial H_1}{\partial Q} \right)^2 + \frac{\partial^3 H_1}{\partial^3 P} \frac{\partial H_1}{\partial Q} \frac{\partial H_0}{\partial Q} - \frac{3}{2} \frac{\partial^2 H_1}{\partial^2 P} \frac{\partial^3 H_1}{\partial^2 P \partial Q} \left( \frac{\partial H_1}{\partial Q} \right)^2 \\
&- \frac{1}{2} \frac{\partial^4 H_1}{\partial^4 P} \left( \frac{\partial H_1}{\partial Q} \right)^3 - 3 \frac{\partial^3 H_1}{\partial^3 P} \left( \frac{\partial H_1}{\partial Q} \right)^2 \frac{\partial^2 H_1}{\partial P \partial Q} - 3 \frac{\partial^2 H_1}{\partial^2 P} \left( \frac{\partial^2 H_1}{\partial P \partial Q} \right)^2 \frac{\partial H_1}{\partial Q}
\end{aligned}$$

$$\begin{aligned}
e_{qq} &= \frac{1}{8} \left( \frac{\partial G_{11}}{\partial P} \right)^2 + \frac{1}{2} \frac{\partial G_{11}}{\partial P} \frac{\partial H_0}{\partial P} + \frac{1}{2} \left( \frac{\partial H_0}{\partial P} \right)^2 \\
(55) \quad &- \frac{1}{2} \frac{\partial G_{11}}{\partial P} \frac{\partial^2 H_1}{\partial^2 P} \frac{\partial H_1}{\partial Q} - \frac{\partial^2 H_1}{\partial^2 P} \frac{\partial H_1}{\partial Q} \frac{\partial H_0}{\partial P} - \frac{\partial H_1}{\partial P} \frac{\partial^2 H_1}{\partial^2 P} \frac{\partial H_0}{\partial Q} \\
&- \frac{1}{2} \frac{\partial H_1}{\partial P} \frac{\partial^2 G_{11}}{\partial^2 P} \frac{\partial H_1}{\partial Q} - \frac{\partial H_1}{\partial P} \frac{\partial^2 H_0}{\partial^2 P} \frac{\partial H_1}{\partial Q} - \frac{1}{2} \frac{\partial H_1}{\partial P} \frac{\partial^2 H_1}{\partial^2 P} \frac{\partial G_{11}}{\partial Q} \\
&+ \frac{3}{2} \left( \frac{\partial^2 H_1}{\partial^2 P} \right)^2 \left( \frac{\partial H_1}{\partial Q} \right)^2 + 3 \frac{\partial H_1}{\partial P} \frac{\partial^2 H_1}{\partial^2 P} \frac{\partial H_1}{\partial Q} \frac{\partial^2 H_1}{\partial P \partial Q} + \frac{3}{2} \frac{\partial H_1}{\partial P} \frac{\partial^3 H_1}{\partial^3 P} \left( \frac{\partial H_1}{\partial Q} \right)^2
\end{aligned}$$

$$(56) \quad e_{ppp} = -\frac{1}{2} \left( \frac{\partial H_1}{\partial Q} \right)^2 \frac{\partial H_0}{\partial Q} - \frac{1}{4} \left( \frac{\partial H_1}{\partial Q} \right)^2 \frac{\partial G_{11}}{\partial Q} + \frac{3}{2} \left( \frac{\partial H_1}{\partial Q} \right)^3 \frac{\partial^2 H_1}{\partial P \partial Q}$$

$$(57) \quad e_{qqq} = \frac{1}{2} \left( \frac{\partial H_1}{\partial P} \right)^2 \frac{\partial H_0}{\partial P} + \frac{1}{4} \left( \frac{\partial H_1}{\partial P} \right)^2 \frac{\partial G_{11}}{\partial P} - \frac{3}{2} \left( \frac{\partial H_1}{\partial P} \right)^2 \frac{\partial^2 H_1}{\partial^2 P} \frac{\partial H_1}{\partial Q}$$

$$\begin{aligned}
(58) \quad e_{pq} &= \left( \frac{\partial H_1}{\partial Q} \right)^2 \frac{\partial^2 H_0}{\partial^2 P} + \frac{1}{2} \frac{\partial G_{11}}{\partial P} \frac{\partial H_1}{\partial Q} \frac{\partial^2 H_1}{\partial P \partial Q} + \frac{1}{2} \frac{\partial H_1}{\partial P} \frac{\partial^2 H_1}{\partial P \partial Q} \frac{\partial G_{11}}{\partial Q} \\
&+ \frac{\partial H_0}{\partial P} \frac{\partial H_1}{\partial Q} \frac{\partial^2 H_1}{\partial P \partial Q} + \frac{1}{2} \frac{\partial H_1}{\partial P} \frac{\partial H_1}{\partial Q} \frac{\partial^2 G_{11}}{\partial P \partial Q} + \frac{1}{2} \left( \frac{\partial H_1}{\partial Q} \right)^2 \frac{\partial^2 G_{11}}{\partial^2 P} \\
&+ \frac{\partial H_1}{\partial P} \frac{\partial^2 H_1}{\partial P \partial Q} \frac{\partial H_0}{\partial Q} + \frac{\partial^2 H_1}{\partial^2 P} \frac{\partial H_1}{\partial Q} \frac{\partial G_{11}}{\partial Q} + 2 \frac{\partial^2 H_1}{\partial^2 P} \frac{\partial H_1}{\partial Q} \frac{\partial H_0}{\partial Q} \\
&+ \frac{\partial H_1}{\partial P} \frac{\partial H_1}{\partial Q} \frac{\partial^2 H_0}{\partial P \partial Q} - \frac{3}{2} \left( \frac{\partial H_1}{\partial Q} \right)^3 \frac{\partial^3 H_1}{\partial^3 P} - \frac{3}{2} \frac{\partial H_1}{\partial P} \frac{\partial^3 H_1}{\partial^2 P \partial Q} \left( \frac{\partial H_1}{\partial Q} \right)^2 \\
&- 3 \frac{\partial H_1}{\partial P} \left( \frac{\partial^2 H_1}{\partial P \partial Q} \right)^2 \frac{\partial H_1}{\partial Q} - 6 \frac{\partial^2 H_1}{\partial^2 P} \left( \frac{\partial H_1}{\partial Q} \right)^2 \frac{\partial^2 H_1}{\partial P \partial Q} - \frac{1}{2} \frac{\partial G_{11}}{\partial P} \frac{\partial H_0}{\partial Q} \\
&- \frac{1}{2} \frac{\partial H_0}{\partial P} \frac{\partial G_{11}}{\partial Q} - \frac{\partial H_0}{\partial P} \frac{\partial H_0}{\partial Q} - \frac{1}{4} \frac{\partial G_{11}}{\partial P} \frac{\partial G_{11}}{\partial Q}
\end{aligned}$$

$$\begin{aligned}
(59) \quad e_{ppq} &= \frac{1}{2} \frac{\partial H_1}{\partial P} \frac{\partial H_1}{\partial Q} \frac{\partial G_{11}}{\partial Q} + \frac{\partial H_1}{\partial P} \frac{\partial H_1}{\partial Q} \frac{\partial H_0}{\partial Q} + \frac{1}{2} \left( \frac{\partial H_1}{\partial Q} \right)^2 \frac{\partial H_0}{\partial P} \\
&+ \frac{1}{4} \left( \frac{\partial H_1}{\partial Q} \right)^2 \frac{\partial G_{11}}{\partial P} - \frac{3}{2} \left( \frac{\partial H_1}{\partial Q} \right)^3 \frac{\partial^2 H_1}{\partial^2 P} - 3 \frac{\partial H_1}{\partial P} \left( \frac{\partial H_1}{\partial Q} \right)^2 \frac{\partial^2 H_1}{\partial P \partial Q}
\end{aligned}$$

$$\begin{aligned}
(60) \quad e_{pqq} &= -\frac{1}{2} \frac{\partial H_1}{\partial P} \frac{\partial H_1}{\partial Q} \frac{\partial G_{11}}{\partial P} - \frac{\partial H_1}{\partial P} \frac{\partial H_1}{\partial Q} \frac{\partial H_0}{\partial P} - \frac{1}{2} \left( \frac{\partial H_1}{\partial P} \right)^2 \frac{\partial H_0}{\partial Q} \\
&- \frac{1}{4} \left( \frac{\partial H_1}{\partial P} \right)^2 \frac{\partial G_{11}}{\partial Q} + \frac{3}{2} \left( \frac{\partial H_1}{\partial P} \right)^2 \frac{\partial^2 H_1}{\partial P \partial Q} \frac{\partial H_1}{\partial Q} + 3 \frac{\partial H_1}{\partial P} \left( \frac{\partial H_1}{\partial Q} \right)^2 \frac{\partial^2 H_1}{\partial^2 P}
\end{aligned}$$

$$(61) \quad e_{pppp} = \frac{1}{8} \left( \frac{\partial H_1}{\partial Q} \right)^4, \quad e_{qqqq} = \frac{1}{8} \left( \frac{\partial H_1}{\partial P} \right)^4, \quad e_{ppqq} = \frac{3}{8} \left( \frac{\partial H_1}{\partial P} \right)^2 \left( \frac{\partial H_1}{\partial Q} \right)^2$$

$$(62) \quad e_{pppq} = -\frac{1}{2} \frac{\partial H_1}{\partial P} \left( \frac{\partial H_1}{\partial Q} \right)^3, \quad e_{pqqq} = -\frac{1}{2} \frac{\partial H_1}{\partial Q} \left( \frac{\partial H_1}{\partial P} \right)^3$$

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