Error Expansion for a Symplectic Scheme for Stochastic Hamiltonian Systems

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Abstract We consider a stochastic autonomous Hamiltonian system for which the flow preserves the symplectic structure. Numerical simulations show that for stochastic Hamiltonian systems symplectic schemes produce more accurate results for long term simulations than non-sysmplectic numerical schemes. We study the approximation error corresponding to a symplectic weak scheme of order one. A backward error analysis is done at the level of the Kolmogorov equation associated with the initial stochastic Hamiltonian system. We obtain an expansion of the error in terms of powers of the discretization step size and the solutions of the modified Kolmogorov equation.

Keywords Backward error analysis · Stochastic Hamiltonian systems
Kolmogorov equation · Weak symplectic scheme

1 Introduction

Numerical simulations [5, 9, 11] show that for stochastic Hamiltonian systems (SHS) symplectic schemes give more accurate results for long term simulation that non-symplectic schemes, but, to the best of our knowledge, no theoretical proof was done in the stochastic case. For a SHS and a first weak order symplectic scheme, in [2] we present an expansion of the global approximation error in powers of the discretization step size. Comparing this expansion with the global error expansion obtained in [13] for the Euler scheme (which has also weak order one), we justify the superior performance of the symplectic scheme for the simple linear SHS corresponding to the Kobo oscillator [2]. However, this justification can not be easily extended for general non-linear SHSs. Here we use backward error analysis to find an expansion of error for the symplectic scheme in terms of the powers of the discretization step size and the solutions of the modified Kolmogorov equation [3].

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Backward error analysis was successfully applied to study long term behavior of deterministic Hamiltonian systems [4]. Recently, backward error analysis was extended to stochastic differential equations (SDE). Modified SDEs associated with various numerical schemes are presented in [1, 10, 14]. A SDE defined on the n-dimensional torus and its approximation by the explicit Euler scheme are studied using backward error analysis in [3].

We follow the same approach as in [3], and we construct the modified equation not at the level of the SDE, but at the level of the associated Kolmogorov equation. Compared with [3] we consider a fully implicit scheme instead of an explicit one, and we consider a SHS with additive or multiplicative noise defined on R^{2n} instead of the compact n dimensional torus. Implicit numerical schemes are also considered in [6, 7], but for Langevin SDEs on R^n with additive noise. Studying the multiplicative noise case is more difficult, especially for a fully implicit numerical scheme.

In the next section we present some preliminary results regarding the solution of the SHS and the approximate solution given by the numerical scheme. The steps followed for the backward error analysis are included in Sect. 3. The last section contains the conclusions.

2 Assumptions and Preliminary Results

We introduce a few definitions and notations. We denote $N = \{1, 2, \ldots\}$, $N^* = \{1, 2, \ldots\}$ and for any $x = (x_1, \ldots, x_n)^T \in R^n$, $|x|$ represents the Euclidean norm.

For any multi-index $\alpha = (\alpha_1, \ldots, \alpha_r) \in N^r$ with length $|\alpha| = \alpha_1 + \cdots + \alpha_r$, let $\partial_\alpha = \frac{\partial^{|\alpha|}}{\partial_1^{\alpha_1} \cdots \partial_r^{\alpha_r}}$ denote the partial derivative of order $|\alpha|$.

We define the following space of functions with polynomial growth:

$$C^\infty_{pol}(R^{2n}) = \Big\{ f \in C^\infty(R^{2n}) \text{ such that } f \text{ and all its derivatives have polynomial growth} \Big\}$$

For any $k, l \in N$, we denote

$$C^l_k(R^{2n}) = \Big\{ f \in C^l(R^{2n}) : \text{ there exists } C_{l,k} > 0 \text{ such that for all } x \in R^{2n} \text{ and any index } \alpha \in N^{2n}, |\alpha| \le l, |\partial_\alpha f(x)| \le C_{l,k}(1 + |x|^{2k}) \Big\}.$$

On $C^l_k(R^{2n})$ we define [7] the norm $\|\cdot\|_{l,k}$ and the semi norm $|\cdot|_{l,k}$:

$$\|f\|_{l,k} = \sup_{\alpha, |\alpha| \le l} \frac{|\partial_\alpha f(x)|}{1 + |x|^{2k}}, \quad |f|_{l,k} = \sup_{\alpha, 1 \le |\alpha| \le l} \frac{|\partial_\alpha f(x)|}{1 + |x|^{2k}}. \tag{1}$$

Notice that if $\phi \in C^\infty_{pol}(R^{2n})$, then for all $d \in N$, there exists $r_d \in N$ such that $\phi \in C^d_{r_d}(R^{2n})$.

We consider the following stochastic Hamiltonian system

$$dP = -\partial_Q H_0(P, Q)dt - \sum_{r=1}^{m} \partial_Q H_r(P, Q) \circ dw_t^r, \quad P(0) = p$$
$$dQ = \partial_P H_0(P, Q)dt + \sum_{r=1}^{m} \partial_P H_r(P, Q) \circ dw_t^r, \quad Q(0) = q, \tag{2}$$

where P, Q, p, q are n-dimensional column vectors, w_t^r, $r = 1, \ldots, m$ are independent standard Wiener processes, and for any function f defined on $\mathrm{R}^n \times \mathrm{R}^n$, $\partial_P f$ and $\partial_Q f$ denote the column vectors with components $(\partial f/\partial P_i)$, $1 \le i \le n$ and $(\partial f/\partial Q_i)$, $1 \le i \le n$, respectively. The stochastic flow $(p, q) \longrightarrow (P, Q)$ of the SHS (2) preserves the symplectic structure [9]: $dP \wedge dQ = dp \wedge dq$, where the differential 2-form $dp \wedge dq = dp_1 \wedge dq_1 + \cdots + dp_n \wedge dq_n$.

The system (2) can be re-written in the Ito formulation:

$$dP = a(P, Q)dt + \sum_{r=1}^{m} \sigma^r(P, Q)dw_t^r, \quad P(0) = p \tag{3}$$

$$dQ = b(P, Q)dt + \sum_{r=1}^{m} \gamma^r(P, Q)dw_t^r, \quad Q(0) = q, \tag{4}$$

where

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

Here everywhere the arguments are (P, Q), and a, b, σ^r, γ^r, $r = 1, \ldots, m$ are $n-$dimensional column vectors.

The Kolmogorov generator $L(p, q, \partial_p, \partial_q)$ associated with the SHS (3)–(4) has the following form [12]

$$L(p, q, \partial_p, \partial_q)\phi(p, q) = \sum_{j=1}^{n}\left(a_j\frac{\partial}{\partial p_j}\phi(p, q) + b_j\frac{\partial}{\partial q_j}\phi(p, q)\right) + \frac{1}{2}\sum_{r=1}^{m}\sum_{i,j=1}^{n}\Bigg(\sigma_i^r\sigma_j^r \frac{\partial^2}{\partial p_i p_j}\phi(p, q) + \gamma_i^r\gamma_j^r\frac{\partial^2}{\partial q_i q_j}\phi(p, q) + 2\sigma_i^r\gamma_j^r\frac{\partial^2}{\partial p_i q_j}\phi(p, q)\Bigg), \phi \in C^\infty(\mathrm{R}^{2n})$$

Throughout the paper we make the same assumptions as in [12, 13]:

A1. The derivatives of any order of $H_i \in C^\infty$, $i = 1, \dots, m$ are bounded, and the derivative of any order $k \geq 2$ of $H_0 \in C^\infty$ are bounded.
A2. The operator L is uniformly elliptic: there exists a constant $\alpha > 0$ such that for all $x = (p, q)^T \in \mathrm{R}^{2n}$ we have

$$\alpha |x|^2 \leq \sum_{r=1}^{m} \sum_{i,j=1}^{n} \left(\sigma_i^r \sigma_j^r p_i p_j + \gamma_i^r \gamma_j^r q_i q_j + 2\sigma_i^r \gamma_j^r p_i q_j \right) \tag{5}$$

A3. There exists a constant $\beta > 0$ and a compact set K such that for all $x = (p, q)^T \in \mathrm{R}^{2n} - K$ we have $p \cdot a(x) + q \cdot b(x) \leq -\beta |x|^2$.

Notice that assumption A1 implies that we have a Lipschitz condition, i.e. there exists $L_1 > 0$ such that for all $X = (P, Q)^T, x = (p, q)^T \in \mathrm{R}^{2n}$ we have

$$\sum_{j=0}^{m} \left| \left(\partial_P H_j, \partial_Q H_j\right)^T (X) - \left(\partial_p H_j, \partial_q H_j\right)^T (x) \right| \leq L_1 |X - x|. \tag{6}$$

2.1 Results Regarding the Solution of the Stochastic Hamiltonian System

Proceeding as in Proposition 3.1 in [12], under the assumptions A1-A3 we can prove the following result regarding the solution $\left(X^{0,x_0}(t)\right) = \left((P(t, p_0, q_0), Q(t, p_0, q_0))^T\right)$ of the SHS (2) with the initial condition $x_0 = (p_0, q_0)^T \in \mathrm{R}^{2n}$.

Lemma 1 *The Markov process $\left(X^{0,x_0}(t)\right)$ is ergodic. The unique invariant probability measure μ has finite moments of any order and a density $\rho \geq 0$. Moreover, for any $k \in \mathrm{N}$ there exist $C_k, \gamma_k > 0$ such that for any $x_0 = (p_0, q_0)^T \in \mathrm{R}^{2n}$, and any $t \geq 0$ we have:*

$$E(|X^{0,x_0}(t)|^k) \leq C_k \left(1 + |x_0|^k \exp(-\gamma_k t)\right). \tag{7}$$

We consider any function $\phi \in C_{pol}^\infty(\mathrm{R}^{2n})$, and for all $x = (p, q)^T \in \mathrm{R}^{2n}$ and all $t > 0$ we define $u(t, p, q) := E[\phi(X^{0,x}(t)]$. Notice that Lemma 1 implies that u is well defined. It is well known [12] that $u(t, p, q)$ is a classical solution of the Kolmogorov equation

$$\frac{du}{dt}(t, p, q) = Lu(t, p, q), \quad u(0, p, q) = \phi(p, q), (p, q)^T \in \mathrm{R}^{2n}, t > 0. \tag{8}$$

For any function $f \in C_{pol}^\infty(\mathrm{R}^{2n})$ we denote the average

$$< f > := \int f(x) d\mu(x)$$

The results included in the following lemma show the exponential convergence of u and its derivatives and are essential for the backward error analysis presented in this paper. The proof is an extension of the proof of Theorem 3.4 in [12], based on Theorem 2.5 in [8].

Lemma 2 *Let $k \in \mathrm{N}$, $k \geq 1$, and $\phi \in C^{\infty}_{pol}(\mathrm{R}^{2n}) \cap C^{k+n+1}_{r_{k+n+1}}(\mathrm{R}^{2n})$, $r_{k+n+1} \in \mathrm{N}$. Then there exist $\gamma_k > 0$, $C_k > 0$ and $l_k \in \mathrm{N}$ such that $l_k > r_{k+n+1}$ and for any $0 < \gamma < \gamma_k$ and all $t \geq 0$ we have*

$$|u(t,x)|_{k,l_k} \leq C_k \, \|\phi - <\phi>\|_{k+n+1, r_{k+n+1}} \exp(-\gamma t). \tag{9}$$

$$\|u(t,x) - <\phi>\|_{0,l_0} \leq C_0 \, \|\phi - <\phi>\|_{n+1, r_{n+1}} \exp(-\gamma t). \tag{10}$$

2.2 Results Regarding the Symplectic Scheme

We consider the following one-step approximation [9] for the system (2):

$$P_{k+1} = P_k - h \left(\partial_Q H_0 + \frac{1}{2} \sum_{r=1}^{m} \partial_Q G_{(r,r)} \right) - \sqrt{h} \sum_{r=1}^{m} \varsigma_{rk} \partial_Q H_r, \quad P_0 = p_0 \tag{11}$$

$$Q_{k+1} = Q_k + h \left(\partial_P H_0 + \frac{1}{2} \sum_{r=1}^{m} \partial_P G_{(r,r)} \right) + \sqrt{h} \sum_{r=1}^{m} \varsigma_{rk} \partial_P H_r \quad Q_0 = q_0 \tag{12}$$

where $G_{(r,r)} = \sum_{i=1}^{n} \frac{\partial H_r}{\partial Q_i} \frac{\partial H_r}{\partial P_i}$, the random variables ς_{rk} are mutually independent identically distributed according to the law, $\mathrm{P}(\varsigma_{rk} = \pm 1) = 1/2$, and everywhere the arguments are (P_{k+1}, Q_k).

Notice that the first equation (11) is implicit. Let denote $\delta := \sqrt{h}$ and $F(p,q) = \big(H_0(p,q) + \frac{1}{2} \sum_{r=1}^{m} G_{(r,r)}(p,q)\big)$. Then we can reformulate the scheme (11)–(12) as follows:

$$P_{k+1} = P_k - \delta^2 \partial_Q F(P_{k+1}, Q_k) - \delta \sum_{r=1}^{m} \varsigma_{rk} \partial_Q H_r(P_{k+1}, Q_k) \tag{13}$$

$$Q_{k+1} = Q_k + \delta^2 \partial_P F(P_{k+1}, Q_k) + \delta \sum_{r=1}^{m} \varsigma_{rk} \partial_P H_r(P_{k+1}, Q_k) \tag{14}$$

Using the Lipschitz condition (6) and proceeding as in the proof of Theorem 4.6.1 in [9] we can show that the scheme (13)–(14) is well defined:

Lemma 3 *There exist $h_{01} > 0$, $C > 0$ such that for any $0 < h \leq h_{01}$ and any $(p,q)^t \in \mathrm{R}^{2n}$ there exists a unique $z \in \mathrm{R}^n$ such that $z = p - h\partial_q F(z,q) - \sqrt{h} \sum_{r=1}^{m} \varsigma_{rk} \partial_q H_r(z,q)$ which satisfies $|z - p| \leq C(1 + |p|)\sqrt{h}$.*

Moreover, Theorem 4.6.1 in [9] shows that implicit method (13)–(14) is symplectic and of first weak order: for any $T > 0$, and any $\phi \in C^{\infty}_{pol}(\mathrm{R}^{2n})$ we have

$$|E(\phi(P_k, Q_k)) - E(\phi(X^{0,x_0}(kh)))| \le c(\phi, T)h, k = 0, \dots, \lfloor T/h \rfloor, c(\phi, T) > 0. \quad (15)$$

We define the function ϕ_δ which associate to $(q, p) \in \mathrm{R}^{2n}$ the solution $z = (z_1, z_2)^T \in \mathrm{R}^{2n}$ of $f(\delta, q, p, z_1, z_2) = 0$, where

$$f(\delta, q, p, z) = \begin{bmatrix} z_1 - p + \delta^2 \partial_q F(z_1, q) + \delta \sum_{r=1}^m \varsigma_r \partial_q H_r(z_1, q) \\ z_2 - q - \delta^2 \partial_p F(z_1, q) - \delta \sum_{r=1}^m \varsigma_r \partial_p H_r(z_1, q) \end{bmatrix} \quad (16)$$

where the random variables ς_r are mutually independent identically distributed according to the law, $\mathrm{P}(\varsigma_r = \pm 1) = 1/2$, Since the scheme (13)–(14) is well defined, the function ϕ_δ is also well defined for any $\delta \in (0, \sqrt{h_{01}})$. Using A1 it is easy to show that there exists $h_{03} \le h_{01}$ such that $\partial_z f(\delta, q, p, z) = I - B(\delta, p, q, z)$ where $\|B(\delta, p, q, z)\| < 1$ for any $(\delta, p, q, z) \in (0, \sqrt{h_{03}}) \times \mathrm{R}^{2n} \times \mathrm{R}^{2n}$. Thus, $\partial_z f(\delta, q, p, z)$ is invertible, and from the Implicit Functions Theorem we obtain that the function defined by $(\delta, p, q) \to \phi_\delta(p, q)$ is C^∞ on a neighborhood of each point of $(0, \sqrt{h_{03}}) \times \mathrm{R}^{2n}$.

Following the same approach as in the proof of Proposition 7.1 in [12] we can show that the moments of the approximating process (P_k, Q_k) satisfy a similar property with (7):

Lemma 4 *There exist $0 < h_{02} \le h_{01}$ such that the symplectic scheme (11)–(12) with any initial condition $(p, q)^t \in \mathrm{R}^{2n}$ and any $0 < h \le h_{02}$ satisfies for any $l \in \mathrm{N}^*$*

$$E_{p,q}(|P_k|^{2l} + |Q_k|^{2l}) \le C_l \left(1 + (|p|^{2l} + |q|^{2l}) \exp(-\alpha_l kh)\right), \quad C_l > 0, \alpha_l > 0. \quad (17)$$

3 Asymptotic Expansion of the Weak Error

Using a Taylor expansion and the fact that u is a solution of the Kolmogorov equation (8) we obtain the following expansion.

Proposition 1 *Let consider any $N \in \mathrm{N}$ and any $\phi \in C^\infty_{pol}(\mathrm{R}^{2n}) \cap C^{2N+n+3}_{r_{2N+n+3}}(\mathrm{R}^{2n})$, $r_{2N+n+3} \in \mathrm{N}$. There exist $c(N) > 0$ and $l_N \in \mathrm{N}$, $l_N > r_{2N+n+3}$ such that for all $h > 0$ and $(p, q)^T \in \mathrm{R}^{2\mathrm{n}}$ we have*

$$|u(h, p, q) - \sum_{k=0}^N \frac{h^k}{k!} L^k \phi(p, q)| \le c(N) h^{N+1} \|\phi - <\phi>\|_{2N+3+n, r_{2N+3+n}} (1 + |p|^{2l_N} + |q|^{2l_N}) \quad (18)$$

Let $h_0 = \min\{h_{02}, h_{03}\}$. We study the first step of the approximating process (P_k, Q_k), and later we will use the Markov property to extend the results at all steps. The following result gives an expansion for the symplectic scheme, similar with the expansion (18).

Proposition 2 *For any $k \in \mathrm{N}$ there exists an operator A_k of order $2k$ with coefficients in $C^\infty_{pol}(\mathrm{R}^{2n})$ such that for any $N \in \mathrm{N}$ and any $\phi \in C^\infty_{pol}(\mathrm{R}^{2n}) \cap C^{2N+2}_{r_{2N+2}}(\mathrm{R}^{2n})$, $r_{2N+2} \in \mathrm{N}$, there exist $C_N > 0$ and $l_N \in \mathrm{N}$ such that for all $0 < h \leq h_0$ and $(p, q)^T \in \mathrm{R}^{2n}$ we have $A_0 = I$, $A_1 = L$, and*

$$|E(\phi(Q_1, P_1)) - \sum_{k=0}^{N} h^k A_k(p, q)\phi(p, q)| \leq C_N h^{N+1}(1 + |p|^{2l_N} + |q|^{2l_N})|\phi|_{2N+2, r_{2N+2}}$$

Proof Firstly we use Taylor expansions to obtain expansions for P_1 and Q_1 (see also the proof of Lemma 3.4 in [6]). Then the proof can be done using the same approach as in the proof of Proposition 3.2 in [6].

3.1 The Modified Generator

Following the same approach as in [3], we want to construct a formal series $\mathscr{L} = L + hL_1 + \cdots + h^k L_k + \cdots$ such that formally the solution $v(h, p, q)$ of the equation

$$\partial_t v(t, p, q) = \mathscr{L} v(t, p, q), t > 0, \quad v(0, p, q) = \phi(p, q), (p, q)^T \in \mathrm{R}^{2n},$$

coincides in the sense of asymptotic expansion with the transition semigroup $E(\phi(P_1, Q_1))$ studied in Proposition 2. In order to have

$$\exp(h\mathscr{L})\phi = \phi + \sum_{k \geq 1} h^k A_k \phi$$

we define the L_k operator as

$$L_k = A_{k+1} + \sum_{l=1}^{k} \frac{B_l}{l!} \sum_{k_1+\cdots+k_{l+1}=k-l} L_{k_1} \ldots L_{k_l} A_{k_{l+1}+1} \tag{19}$$

B_l are the Bernoulli numbers and L_k is an operator of order $2k + 2$ with coefficients in $C^\infty_{pol}(\mathrm{R}^{2n})$ and $L_k 1 = 0$. We also have

$$A_k = \sum_{l=1}^{k} \frac{1}{l!} \sum_{k_1+\cdots+k_l=k-l} L_{k_1} \ldots L_{k_l}. \tag{20}$$

We define the modified generator

$$L^{(N)} = L + \sum_{k=1}^{N} h^k L_k, \quad N \in \mathrm{N}^*. \tag{21}$$

Since we do not know if the modified equation

$$\partial_t v^{(N)}(t,p,q) = L^{(N)} v^{(N)}(t,p,q),\, t > 0, \quad v^{(N)}(0,p,q) = \phi(p,q),\, (p,q)^T \in \mathrm{R}^{2\mathrm{n}},$$

has a solution, we construct an approximate solution associated to (21).

Proposition 3 *Let* $\phi \in C^{\infty}_{pol}(\mathrm{R}^{2n})$. *For all* $k \in \mathrm{N}$ *there exist functions* $v_k(t,\cdot) \in C^{\infty}_{pol}(\mathrm{R}^{2n})$ *defined for all* $t \geq 0$ *such that* $v_0(0,\cdot) = \phi(\cdot)$, $v_k(0,\cdot) = 0$, $k \geq 1$, *and*

$$\partial_t v_k(t,p,q) - L v_k(t,p,q) = \sum_{l=1}^{k} L_l v_{k-l}(t,p,q), \quad t \geq 0. \tag{22}$$

Moreover, for all $k \in \mathrm{N}$, $j \in \mathrm{N}^*$ *there exist* $\gamma_{k,j} > 0$ *and positive integers* $\alpha_{k,j}$ *and* $l_{k,0}$ *such that for all* $t \geq 0$ *we have*

$$|v_k(t)|_{j,\alpha_{k,j}} \leq Q_{k,j}(t) e^{-\gamma_{k,j} t} \|\phi- <\phi> \|_{j+(n+1)(k+1)+4k,\, r_{j+(n+1)(k+1)+4k}}, \tag{23}$$

$$\|v_k(t)\|_{0,l_{k,0}} \leq C_{0,k} \|\phi- <\phi> \|_{(n+1)(k+1)+4k,\, r_{(n+1)(k+1)+4k}}, \tag{24}$$

Here $Q_{k,j} : [0,\infty) \to [0,\infty)$ *are polynomial functions with positive coefficients and the constants* $C_{0,k}$ *do not depend on* t.

Proof The proof is similar with the proof of Theorem 4.1 in [6]. Inequalities (23)–(24) are a consequence of the results presented in Lemma 2.

For any $N \geq 0$, we define the approximate solution of the modified flow as:

$$v^{(N)}(t,p,q) = \sum_{k=0}^{N} h^k v_k(t,p,q). \tag{25}$$

We can easily show that for all $t \geq 0$ we have

$$\partial_t v^{(N)}(t,p,q) = L^{(N)} v^{(N)}(t,p,q) - R^{(N)}(t,p,q), \quad v^{(N)}(0,p,q) = \phi(p,q), \tag{26}$$

where

$$R^{(N)}(t,p,q) = \sum_{i=N+1}^{2N} h^i \sum_{k=i-N}^{N} L_k v_{i-k} \tag{27}$$

is of order $O(h^{N+1})$. The following result can be proved similarly with Theorem 4.1 in [3].

Proposition 4 *Let $\phi \in C^\infty_{pol}(\mathbb{R}^{2n})$. For any $N \in \mathbb{N}^*$ there exist $C_N > 0$ and l_N, $k_{2N+2} \in \mathbb{N}$ such that for all $t \geq 0$, $0 < h \leq h_0$, $(p, q) \in \mathbb{R}^{2n}$ we have*

$$\left|E(v^{(N)}(t, P_1, Q_1) - v^{(N)}(t+h, p, q))\right| \leq h^{N+1} C_N (1 + |p|^{2l_N} + |q|^{2l_N}) \sup_{\substack{s\in[0,h]\\ k=0,\dots,N}} |v_k(t+s, \cdot)|_{2N+2, k_{2N+2}}. \tag{28}$$

3.2 Main Result

We now study the long time behavior of the numerical solution. We obtain an expansion similar with the one for the exact solution, given in Proposition 1.

Theorem 1 *Let $N \in \mathbb{N}$ be fixed, and let (P_k, Q_k) be the discrete process defined by the symplectic scheme. Let $0 < h \leq h_0$, $\alpha_N = 6N + 8 + (n+1)(N+2)$ and $\phi \in C^\infty_{pol}(\mathbb{R}^{2n}) \cap C^{\alpha_N}_{r_{\alpha_N}}$. Then there exist $C_N > 0$ and $l_N \in \mathbb{N}$ such that for all $k \in \mathbb{N}$*

$$|E(\phi(P_k, Q_k)) - v^{(N)}(kh, p, q)| \leq h^{N+1} C_N (1 + |p|^{2l_N} + |q|^{2l_N}) \|\phi - <\phi>\|_{\alpha_N, r_{\alpha_N}}.$$

Proof Let $t_k = kh$. By the Markov property of (P_k, Q_k) we have

$$\begin{aligned}
&|E(\phi(P_k, Q_k) - v^{(N+1)}(t_k, p, q)| = |E(v^{(N+1)}(0, P_k, Q_k)) - v^{(N+1)}(t_k, p, q)| = \\
&\left|E\left(\sum_{j=0}^{k-1} E\left(v^{(N+1)}(t_j, P_{k-j}, Q_{k-j}) - v^{(N+1)}(t_{j+1}, P_{k-j-1}, Q_{k-j-1})\middle| P_{k-j-1}, Q_{k-j-1}\right)\right)\right| \\
&\leq \sum_{j=0}^{k-1}\left|E\Big(E\Big(v^{(N+1)}\left(t_j, P_1(P_{k-j-1}, Q_{k-j-1}), Q_1(P_{k-j-1}, Q_{k-j-1})\right) - v^{(N+1)}(t_{j+1},\right. \\
&\left. P_{k-j-1}, Q_{k-j-1})\Big| P_{k-j-1}, Q_{k-j-1}\Big)\Big)\right|,
\end{aligned}$$

where $(P_1(p, q), Q_1(p, q))$ is the first step of the scheme (11)–(12) when the initial condition is (p, q). Using inequalities (17), (23), and (28), with $t = t_j$, $j = 0, \dots, k-1$, we deduce that there exist positive integers l_N, k_N such that

$$\begin{aligned}
\|E(v^{(N+1)}(0, P_k, Q_k) - v^{(N+1)}(t_k, p, q)\|_{0,l_N} &\leq h^{N+2} c \sum_{j=0}^{k-1} \sup_{\substack{s\in[0,h]\\ i=0,\dots,N+1}} |v_i(t_j + s, \cdot)|_{2N+4, k_N} \\
&\leq h^{N+2} c \|\phi - <\phi>\|_{\alpha_N, r_{\alpha_N}} \sum_{j=0}^{k-1} Q_{2N+4}(t_j) e^{-\lambda_{2N+4} t_j} \\
&\leq h^{N+2} c \|\phi - <\phi>\|_{\alpha_N, r_{\alpha_N}} \sum_{j=0}^{k-1} e^{-\tilde{\lambda}_{2N+4} t_j},
\end{aligned}$$

where $c > 0$, $0 < \tilde{\lambda}_{2N+4} < \lambda_{2N+4}$ and Q_{2N+4} is a polynomial function with positive coefficients. Notice that for a fixed constant $\lambda > 0$ we have

$$\sum_{j=0}^{k-1} e^{-\lambda t_j} \le \frac{1}{1 - e^{-\lambda h}} \le \frac{c_1}{h},$$

where the constant c_1 depends on λ and h_0. Hence, using the previous inequality and (24) we get

$$\begin{aligned}
&\|E(\phi(P_k, Q_k) - v^{(N)}(t_k, p, q)\|_{0,l_N} = \|E(v^{(N+1)}(0, P_k, Q_k) - v^{(N+1)}(t_k, p, q) \\
&+ h^{N+1} v_{N+1}(t_k, p, q)\|_{0,l_N} \le h^{N+1} c_2 \|\phi - < \phi > \|_{\alpha_N, r_{\alpha_N}} + h^{N+1} \|v_{N+1}(t_k, p, q)\|_{0,l_N} \\
&\le h^{N+1} c_2 \|\phi - < \phi > \|_{\alpha_N, r_{\alpha_N}} + h^{N+1} C_{0,N+1} \|\phi - < \phi > \|_{(n+1)(N+2)+4(N+1), r_{\alpha_N}} \\
&\le h^{N+1} C_N \|\phi - < \phi > \|_{\alpha_N, r_{\alpha_N}}
\end{aligned}$$

4 Conclusions and Future Work

We have presented a weak backward error analysis for a SHS system and a symplectic scheme of first weak order. The main tools are the exponential convergence to equilibrium of the solution of the Kolmogorov equation, and the uniform ellipticity of the associated operator. We plan to do a backward error analysis under less restrictive assumptions. The main difficulty is that the symplectic schemes are fully implicit, and for SDEs with multiplicative noise and unbounded coefficients, methods from Malliavin calculus are needed.

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