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LONG-TERM ANALYSIS OF STOCHASTIC HAMILTONIAN SYSTEMS UNDER TIME DISCRETIZATIONS*

RAFFAELE D'AMBROSIO† AND STEFANO DI GIOVACCHINO†

Abstract. In this paper, we focus our investigation on providing long-term estimates of the Hamiltonian deviation computed along numerical approximations to the solutions of stochastic Hamiltonian systems, of both Itô and Stratonovich types. It is well known that the expected Hamiltonian of an Itô Hamiltonian system with additive noise exhibits a linear drift in time [C. Chen et al., *Adv. Comput. Math.*, 46 (2020), 27], while the Hamiltonian function is conserved along the exact flow of a Stratonovich Hamiltonian system [T. Misawa, *Japan J. Indust. Appl. Math.*, 17 (2000), pp. 119–128; T. Misawa, *Math. Probl. Eng.*, 2010 (2010), 384937]. Here, we focus our attention on providing modified differential equations associated to suitable discretizations for the above problems, by means of weak backward error analysis arguments [K. C. Zygalakis, *SIAM J. Sci. Comput.*, 33 (2011), pp. 102–130]. Then, long-term estimates are provided for both Itô and Stratonovich Hamiltonian systems, revealing the presence of parasitic terms affecting the overall conservation accuracy. Finally, selected numerical experiments are provided to confirm the theoretical analysis.

Key words. stochastic Hamiltonian systems, modified differential equations, symplectic methods, energy-preserving numerical methods, weak backward error analysis

MSC codes. 65C30, 65P10, 60H10

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1. Introduction and background.

Stochastic geometric numerical integration is attracting wide interest in the current research on numerics for stochastic differential equations (SDEs), in both the Itô and Stratonovich settings [2, 7, 8, 9, 11, 12, 13, 14, 16, 25, 27, 28, 29, 30, 31, 33]. Specifically, we focus our attention on stochastic Hamiltonian problems [8, 9, 11, 14, 25, 27, 28, 29, 30, 33], which are used to provide a suitable stochastic generalization of classical mechanics that reconciles its Hamiltonian nature (strictly related to the canonical character of evolution equations) with the nondifferentiability of the Wiener process (describing stochastic effects visible, for instance, in the statistical independence of the future from the past and irreversibility of the time arrow, as well as in the intrinsically random effects exhibited by quantum mechanics in the context of the theory of diffusions) [5, 6, 24, 32].

For a given positive integer m, let $q, p \in \mathbb{R}^m$ be the generalized coordinates of a physical system to which we associate a sufficiently smooth general Hamiltonian function $H : \mathbb{R}^{2m} \to \mathbb{R}$. Moreover, for a fixed $T > 0$ and a fixed positive integer d, we consider a probability space $(\Omega, \mathcal{F}, \mathbb{P})$ with normal filtration $(\mathcal{F}_t)_{t\in[0,T]}$, and denote by $W : [0,T] \times \Omega \to \mathbb{R}^d$ a standard $(\mathcal{F}_t)_{t\in[0,T]}$-Brownian motion, with continuous sample paths on $(\Omega, \mathcal{F}, \mathbb{P})$.

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†Department of Information Engineering and Computer Science and Mathematics, University of L'Aquila, L'Aquila, 67100, Italy (raffaele.dambrosio@univaq.it, stefano.digiovacchino@graduate.univaq.it).

1.1. Stochastic Hamiltonian systems of Itô type. Given a nonseparable general Hamiltonian function, we consider the stochastic Hamiltonian system of Itô type [11]:

$$\begin{cases} \mathrm{d}q(t) = \nabla_p H(q(t),p(t))\mathrm{d}t, \\ \mathrm{d}p(t) = -\nabla_q H(q(t),p(t))\mathrm{d}t + \Sigma \mathrm{d}W(t), \end{cases} \tag{1.1}$$

where $\Sigma \in \mathbb{R}^{m\times d}$, whose generic element is denoted by σ_{ij} for $i = 1,2,\dots,m$ and $j = 1,2,\dots,d$. Moreover, we assume that the initial datum (q_0,p_0) of the system (1.1) provides an initial Hamiltonian of finite expectation, i.e., $\mathbb{E}[H(q_0,p_0)] < \infty$. We note that if the matrix Σ is the zero matrix, the stochastic Hamiltonian system (1.1) recasts the deterministic Hamiltonian system whose Hamiltonian is conserved along its exact flow.

It is well known that the Itô stochastic version (1.4) of a deterministic Hamiltonian system does not preserve the Hamiltonian function, nor its expected value. Indeed, using Itô's lemma, the following trace equation for the expectation of the Hamiltonian at time $t \in [0,T]$ is established [9]:

$$\mathbb{E}\left[H(q(t),p(t))\right] = \mathbb{E}\left[H(q_0,p_0)\right] + \frac{1}{2}\sum_{i=1}^{d} \bar{\sigma}_i^2 \int_0^t \mathbb{E}\left[\nabla_{pp}^{ii} H(q(s),p(s))\right]\mathrm{d}s, \tag{1.2}$$

where we have denoted by $\bar{\sigma}_i$ the diagonal element on the ith row of the matrix $\Sigma^{\mathsf{T}}\Sigma$, $i = 1,\dots,d$, and by $\nabla_{pp}^{ii}H$ the element in position (i,i) of the Hessian matrix associated to the function H with respect to p.

Equation (1.2) reveals that one cannot expect a conservative structure for an Itô stochastic Hamiltonian system. In the case of separable Hamiltonian functions of type

$$H(q,p) = \frac{1}{2}\sum_{i=1}^{m} p_i^2 + V(q), \tag{1.3}$$

depending on a suitable smooth potential $V : \mathbb{R}^m \to \mathbb{R}$, the corresponding stochastic Hamiltonian system of Itô type (1.1) reads

$$\begin{cases} \mathrm{d}q(t) = p(t)\mathrm{d}t, \\ \mathrm{d}p(t) = -\nabla_q V(q(t))\mathrm{d}t + \Sigma \mathrm{d}W(t). \end{cases} \tag{1.4}$$

Correspondingly, (1.2) assumes a more compact form [9, 11],

$$\mathbb{E}\left[H(q(t),p(t))\right] = \mathbb{E}\left[H(q_0,p_0)\right] + \frac{1}{2}\mathrm{Tr}\left(\Sigma^{\mathsf{T}}\Sigma\right)t, \tag{1.5}$$

and reveals that, for the Hamiltonian system (1.4), the expectation of the Hamiltonian function (1.3) grows linearly in time and the growth rate depends on the trace of the matrix $\Sigma^{\mathsf{T}}\Sigma$. In the remainder of this paper, for the Itô case, we focus on the separable version (1.4), where the Hamiltonian (1.3) can be physically interpreted as the sum of kinetic and potential energy terms and its expectation obeys the compact trace equation (1.5).

Several contributions regarding the numerics for stochastic Hamiltonian systems are detectable in the existing literature, for instance, [2, 8, 9, 11, 14, 28, 32, 33] and references therein. Some of these contributions aimed to construct numerical methods able to retain the trace equation (1.5) along the discretized dynamics and, for specific numerical schemes, they showed that

$$\mathbb{E}\left[H(q_n,p_n)\right] = \mathbb{E}\left[H(q_0,p_0)\right] + \frac{1}{2}\mathrm{Tr}\left(\Sigma^{\mathsf{T}}\Sigma\right)t_n, \tag{1.6}$$

where $t_n = n\Delta t, n = 1, 2, \ldots, N, \Delta t = T/N$, and N is a positive integer and where we have denoted by q_n and p_n the approximations of $q(t_n)$ and $p(t_n)$, respectively.

For example, in [8, 9], the authors proved that (1.6) holds true for the midpoint stochastic Runge–Kutta method for quadratic Hamiltonian functions. In [11], the authors provided an implicit drift-preserving numerical scheme capable of reproducing the behavior described by (1.6) for any smooth Hamiltonian function.

1.2. Stochastic Hamiltonian systems of Stratonovich type. In the existing literature, many authors considered an alternative form of stochastic Hamiltonian problems to get a conservative structure similarly to the deterministic setting. Then, we consider the following Hamiltonian system [25, 27, 28, 29, 30]:

$$\begin{cases} \mathrm{d}q(t) = \nabla_p H(q(t), p(t)) \left(\mathrm{d}t + \widetilde{\Sigma}^{\mathsf{T}} \circ \mathrm{d}W(t)\right), \\ \mathrm{d}p(t) = -\nabla_q H(q(t), p(t)) \left(\mathrm{d}t + \widetilde{\Sigma}^{\mathsf{T}} \circ \mathrm{d}W(t)\right), \end{cases} \tag{1.7}$$

with $\widetilde{\Sigma} \in \mathbb{R}^d$ and where we have denoted by $\circ$ the stochastic integral in the Stratonovich sense [20, 23]. For the specific case of separable Hamiltonian functions of type (1.3), problem (1.7) assumes the form

$$\begin{cases} \mathrm{d}q(t) = p(t) \left(\mathrm{d}t + \widetilde{\Sigma}^{\mathsf{T}} \circ \mathrm{d}W(t)\right), \\ \mathrm{d}p(t) = -\nabla_q V(q(t)) \left(\mathrm{d}t + \widetilde{\Sigma}^{\mathsf{T}} \circ \mathrm{d}W(t)\right). \end{cases} \tag{1.8}$$

Using the chain rule for SDEs of Stratonovich type [4], one can prove that the Hamiltonian is conserved along exact flow of (1.7). In fact,

$$\mathrm{d}H(q(t), p(t)) = \partial_q H(q(t), p(t))\mathrm{d}q(t) + \partial_p H(q(t), p(t))\mathrm{d}p(t) = 0.$$

Several papers (see, for instance, [3, 17, 21, 22, 25, 27, 28, 29, 30] and references threin) are focused on providing numerical numerical methods preserving the Hamiltonian along numerical paths, i.e., they constructed numerical methods satisfiying

$$H(q_{n+1}, p_{n+1}) = H(q_n, p_n), \quad n = 0, 1, \ldots. \tag{1.9}$$

For example, symplectic stochastic Runge–Kutta methods are provided in [25, 27, 28], while in [29], the author gives a conservative numerical scheme arising from the stochastic version of Greenspan's scheme that preserves the Hamiltonian of deterministic Hamiltonian problems.

1.3. Motivation, purposes, and plan of this paper. In this work, we focus our attention on providing a rigorous long-term analysis of numerical methods for stochastic Hamiltonian systems (1.4) and (1.7), in terms of drift-preservation for systems (1.4) and Hamiltonian conservation for (1.7). We aim to investigate the long-term behavior of methods analyzed in [25, 27, 28, 29, 30] and of other methods arising in the deterministic scenario (such as the energy preserving numerical schemes [10, 18]) properly adapted to the stochastic case.

Our analysis is focused on understanding the validity of (1.6)–(1.9) for large time windows and for large values of the entries of Σ, in the direction of providing a stochastic counterpart of the well-known Benettin–Giorgilli theorem (see [18, Chapter IX, Theorem 8.1]) explaining the long-term behavior of symplectic schemes for the deterministic Hamiltonian problems, in the spirit of a backward error analysis (see, for instance, [2, 15, 16, 18, 31, 33] and references therein).

The key ingredient for a weak backward error analysis is given by modified differential equations developed, in the stochastic case, in [1, 2, 16, 31, 33] and references therein. To the best of our knowledge, the use of such modified differential equations in the direction of providing long-term estimates of the Hamiltonian deviation over numerical solutions has not yet been addressed in the stochastic case. We also observe that other approaches are possible in order to compute modified differential equations in the stochastic case, for instance, by looking at Kolmogorov equations associated to an SDE, as in [16, 33]. However, such an approach is not considered in this paper, as we mostly move in the direction of [31] for the computation of modified SDEs given in terms of power series of the stepsize.

This paper is organized as follows: in section 2, we prove that time discretizations to (1.8) suffer from the existence of a *secular term* that corrupts the long-time conservation of the Hamiltonian function; in sections 3 and 4, we construct modified SDEs in both Itô and Stratonovich cases, useful to provide the long-term analysis presented in sections 5 and 6. Both sections are also equipped with selected numerical experiments confirming the effectiveness of the given analysis. Some conclusions are addressed in section 7. Finally, an example of extension to the above arguments in the multidimensional case is provided in Appendix A, and further computations on nonseparable Hamiltonians are provided in Appendix B.

2. σ-expansion for Stratonovich systems. In this section, we aim to show how a general discretization of solution to Stratonovich Hamiltonian systems (1.8) may fail in preserving the expectation of the Hamiltonian function along the corresponding numerical dynamics, due to the presence of a *secular term* destroying the overall accuracy. The following analysis is inspired by the idea of σ-expansions [19], extended in [14] to the case of Itô Hamiltonian problems. The analysis has been performed with respect to the linear test problem, i.e., (1.8) with quadratic Hamiltonian. This allows us to also gain insights on the more complex general system (1.7). In correspondence to the potential function $V(q) = q^2/2$, we consider the following linear scalar test problem of Stratonovich Hamiltonian type (1.8):

$$dX(t) = JX(t)\mathrm{d}t + \sigma JX(t) \circ \mathrm{d}W(t), \quad t \geq 0, \tag{2.1}$$

where

$$X(t) = \begin{bmatrix} q(t) \\ p(t) \end{bmatrix}, \quad J = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix},$$

equipped with the deterministic initial conditions $X(0) = [q_0, p_0]^{\mathsf{T}}$. Let us assume, as crucial ansatz, that the solution $X(t)$ to (2.1) can be written as power series of the diffusion parameter σ, i.e.,

$$X(t) = \sum_{i \geq 0} X_i(t)\sigma^i. \tag{2.2}$$

Replacing (2.2) in (2.1) yields

$$\sum_{i \geq 0} \mathrm{d}X_i(t)\sigma^i = \sum_{i \geq 0} JX_i(t)\sigma^i \mathrm{d}t + \sum_{i \geq 0} JX_i(t)\sigma^{i+1} \circ \mathrm{d}W(t). \tag{2.3}$$

For $i = 0$, we have

$$\mathrm{d}X_0(t) = JX_0(t)\mathrm{d}t, \quad X_0(0) = X(0), \tag{2.4}$$

whose solution is given by

$$X_0(t) = \exp(Jt)X(0). \tag{2.5}$$

For $i = 1$, we get

$$\mathrm{d}X_1(t) = JX_1(t)\mathrm{d}t + JX_0(t) \circ \mathrm{d}W(t), \quad X_1(0) = 0. \tag{2.6}$$

As visible in (2.5), the term $X_0(t)$ does not depend on $X_1(t)$ and, as a consequence, the Stratonovich equation (2.6) coincides with the Itô equation

$$\mathrm{d}X_1(t) = JX_1(t)\mathrm{d}t + JX_0(t)\mathrm{d}W(t), \quad X_1(0) = 0, \tag{2.7}$$

whose solution is given by [23]

$$X_1(t) = \int_0^t \exp\left(J(t-s)\right) JX_0(s)\,\mathrm{d}W(s).$$

Denoting

$$\overline{X}(t) := \begin{bmatrix} \overline{q}(t) \\ \overline{p}(t) \end{bmatrix} = X_0(t) + \sigma X_1(t),$$

we obtain the following first order σ-expansion of the solution to (2.1):

$$\overline{X}(t) = \exp(Jt)X(0) + \sigma \int_0^t \exp(J(t-s))JX_0(s)\mathrm{d}W(s). \tag{2.8}$$

Equation (2.8) is useful in finding an amenable expression for the expected Hamiltonian function $H(\overline{q}(t), \overline{p}(t))$ as follows. Denoting by $\|\cdot\|$ the vector 2-norm, we obtain from (2.8) the following form for the mean-square of $\overline{X}(t)$:

$$\begin{aligned}
\mathbb{E}\left[\left\|\overline{X}(t)\right\|^2\right] &= \mathbb{E}\left[\|\exp(Jt)X(0)\|^2\right] + \sigma^2 \mathbb{E}\left[\left\|\int_0^t \exp(J(t-s))JX_0(s)\,\mathrm{d}W(s)\right\|^2\right] \\
&= \mathbb{E}\left[\|\exp(Jt)X(0)\|^2\right] + \sigma^2 \int_0^t \|\exp(J(t-s))JX_0(s)\|^2\,\mathrm{d}s \\
&= \mathbb{E}\left[\|\exp(Jt)X(0)\|^2\right] + \sigma^2 \int_0^t \|\exp(J(t-s))J\exp(Jt)X(0)\|^2\,\mathrm{d}s.
\end{aligned}$$

Since the matrices $\exp(Jt)$ and J are orthogonal, assuming $X(0)$ deterministic, we have

$$\mathbb{E}\left[\left\|\overline{X}(t)\right\|^2\right] = \|X(0)\|^2 + \sigma^2 \int_0^t \|X(0)\|^2\,\mathrm{d}s = \|X(0)\|^2 + \sigma^2 \|X(0)\|^2 t.$$

Finally,

$$\mathbb{E}\left[H\left(\overline{q}(t), \overline{p}(t)\right)\right] = \frac{1}{2}\mathbb{E}\left[\left\|\overline{X}(t)\right\|^2\right]$$

yields

$$\mathbb{E}\left[H\left(\overline{q}(t), \overline{p}(t)\right)\right] = H(q_0, p_0)\left(1 + \sigma^2 t\right). \tag{2.9}$$

Equation (2.9) reveals the presence of a linear growth in time of the averaged Hamiltonian, also influenced by the diffusion parameter σ. The term $\sigma^2 t$, denoted as secular term, gives us an alert on the potential inefficacy of numerical methods in the long-term conservation of the expected Hamiltonian. The presence of a secular term is also visible in the case of Itô Hamiltonian problems, as observed in [14]. A rigorous investigation, based on weak backward error analysis arguments, is then necessary in order to understand the long-term behavior of stochastic numerical methods when applied to stochastic Hamiltonian problems.

3. Construction of modified equations for Itô Hamiltonian systems. In this section we aim to derive modified equations for stochastic Hamiltonian systems (1.4), making use of the so-called Itô–Taylor expansions [20, 23, 31]. We observe that an alternative procedure is also possible, based on Kolmogorov equations, as described in [33].

In what follows, given a stochastic numerical method for (1.4), we assume that the following equality holds true:

$$\mathbb{E}\left[H(q_n,p_n)\right] = \mathbb{E}\left[H(q(t_n),p(t_n))\right] + \mathcal{O}\left(\Delta t^r\right), \tag{3.1}$$

where r is a positive number, (q_n, p_n) approximates the exact solution $[q(t), p(t)]^{\mathsf{T}}$ to (1.4), and $t_n = n\Delta t$. This assumption certainly covers both the case of methods tailored to numerically recover the trace equality (1.5) (in this case, the value of r is large and, as a direct consequence, the remainder in (3.1) is negligible) and the general case of any existing numerical method, not specifically designed to exhibit (1.5) over the numerical dynamics (in this case, a smaller value of r, eventually equal to the weak order of the methods, is expected, at least for smooth enough Hamiltonian functions).

For Itô Hamiltonian systems (1.4), taking into account the trace equation (1.5), condition (3.1) is equivalent to requiring that r has to be the integer such that

$$\mathbb{E}\left[H(q_n,p_n)\right] = H\left(q_0,p_0\right) + \frac{1}{2}\mathrm{Tr}\left(\Sigma^{\mathsf{T}}\Sigma\right) t_n + \mathcal{O}\left(\Delta t^r\right). \tag{3.2}$$

It is convenient to look at the expectation computed after one single time step and, hence, the expression (3.2) reveals that r satisfies the following condition [23, 26]:

$$\mathbb{E}\left[H(q_1,p_1)\right] = H\left(q_0,p_0\right) + \frac{1}{2}\mathrm{Tr}\left(\Sigma^{\mathsf{T}}\Sigma\right)\Delta t + \mathcal{O}\left(\Delta t^{r+1}\right). \tag{3.3}$$

We now aim to find other two processes $\widetilde{q}(t)$ and $\widetilde{p}(t)$ such that

$$\mathbb{E}\left[H(q_n,p_n)\right] = \mathbb{E}\left[H(\widetilde{q}(t_n),\widetilde{p}(t_n))\right] + \mathcal{O}\left(\Delta t^{r+1}\right); \tag{3.4}$$

that is, we require

$$\mathbb{E}\left[H(q_1,p_1)\right] = \mathbb{E}\left[H(\widetilde{q}(\Delta t),\widetilde{p}(\Delta t))\right] + \mathcal{O}\left(\Delta t^{r+2}\right). \tag{3.5}$$

In other terms, we look for $\widetilde{q}(t)$ and $\widetilde{p}(t)$ such that the expected Hamiltonian in these values coincides with that in the numerical solution, up to order $\mathcal{O}(\Delta t^{r+1})$.

Taking into account (3.3), let us assume that

$$\mathbb{E}\left[H(q_1,p_1)\right] = H(q_0,p_0) + \frac{1}{2}\mathrm{Tr}\left(\Sigma^{\mathsf{T}}\Sigma\right)\Delta t + \beta_1\Delta t^{r+1} + \mathcal{O}\left(\Delta t^{r+2}\right), \tag{3.6}$$

with $\beta_1 \in \mathbb{R}$. Moreover, we also assume that

$$\mathbb{E}\left[H(\widetilde{q}(\Delta t),\widetilde{p}(\Delta t))\right] = H(q_0,p_0) + \frac{1}{2}\mathrm{Tr}\left(\Sigma^{\mathsf{T}}\Sigma\right)\Delta t + \alpha_1 \Delta t^{r+1} + \mathcal{O}\left(\Delta t^{r+2}\right), \tag{3.7}$$

with $\alpha_1 \in \mathbb{R}$. Hence, condition (3.5) is satisfied by imposing the condition

$$\alpha_1 = \beta_1. \tag{3.8}$$

3.1. Expansions. We now aim to focus on the expression (3.7) for the modified stochastic Itô Hamiltonian systems (1.4), i.e., our goal is to give a form of the coefficient α_1 when $\widetilde{q}(t)$ and $\widetilde{p}(t)$ are solution to the modified Itô Hamiltonian system (1.4) assuming the following formulation:

$$\begin{cases} d\widetilde{q} = (\widetilde{p} + \Delta t^r f_q(\widetilde{q},\widetilde{p}))\,\mathrm{d}t, \\ d\widetilde{p} = (-\nabla_q V(\widetilde{q}) + \Delta t^r f_p(\widetilde{q},\widetilde{p}))\,\mathrm{d}t + \Sigma\,\mathrm{d}W(t), \end{cases} \tag{3.9}$$

where $f_q, f_p \in \mathbb{R}^m$ are denoted as *modified terms* and r is the number satisfying (3.6). By denoting

$$F = \begin{bmatrix} \widetilde{p} + \Delta t^r f_q(\widetilde{q},\widetilde{p}) \\ -\nabla_q V(\widetilde{q}) + \Delta t^r f_p(\widetilde{q},\widetilde{p}) \end{bmatrix}, \qquad G = \begin{bmatrix} 0_{m\times d} & 0_{m\times d} \\ 0_{m\times d} & \Sigma \end{bmatrix},$$

the stochastic Itô–Taylor expansion applied to the Hamiltonian function $H(\widetilde{q},\widetilde{p})$ yields

$$dH(\widetilde{q}(t),\widetilde{p}(t)) = \mathcal{L}_0 H(\widetilde{q}(t),\widetilde{p}(t))\mathrm{d}t + M_g, \tag{3.10}$$

where M_g is a martingale and

$$\mathcal{L}_0 H = F\cdot H_x + \frac{1}{2}\mathrm{Tr}\left(GG^{\mathsf{T}} H_{xx}\right),$$

where H_x denotes the gradient of the Hamiltonian function H and H_{xx} the Hessian matrix of H. Passing to the expectation in (3.10), we get

$$\mathbb{E}\left[H(\widetilde{q}(\Delta t),\widetilde{p}(\Delta t))\right] = H(q_0,p_0) + \int_0^{\Delta t} \mathbb{E}\left[\mathcal{L}_0 H(\widetilde{q}(t),\widetilde{p}(t))\right]\mathrm{d}t. \tag{3.11}$$

By applying the same procedure to the last integrand, we have

$$\mathbb{E}\left[\mathcal{L}_0 H(\widetilde{q}(t),\widetilde{p}(t))\right] = \mathcal{L}_0 H(q_0,p_0) + \int_0^{t} \mathbb{E}\left[\mathcal{L}_0^2 H(\widetilde{q}(s),\widetilde{p}(s))\right]\mathrm{d}s,$$

hence

$$\mathbb{E}\left[H(\widetilde{q}(\Delta t),\widetilde{p}(\Delta t))\right] = H(q_0,p_0) + \Delta t\mathcal{L}_0 H(q_0,p_0) + \int_0^{\Delta t}\int_0^{t} \mathbb{E}\left[\mathcal{L}_0^2 H(\widetilde{q}(s),\widetilde{p}(s))\right]\mathrm{d}s\,\mathrm{d}t.$$

Then, we have obtained the expansion

$$\mathbb{E}\left[H(\widetilde{q}(\Delta t),\widetilde{p}(\Delta t))\right] = H(q_0,p_0) + \sum_{k=1}^{r+1}\frac{1}{k!}\mathcal{L}_0^k H(q_0,p_0)\Delta t^k + \mathcal{O}(\Delta t^{r+2}). \tag{3.12}$$

Note that the expression in (3.12) coincides with that in [33] derived via Kolmogorov equations.

We now aim to specialize the expansion (3.12) to the case of Hamiltonian functions (1.3). For $H(q,p)$ in (1.3), we have

$$H_x = \begin{bmatrix} \nabla_q V(q) \\ p \end{bmatrix}, \quad H_{xx} = \begin{bmatrix} \nabla_{qq} V(q) & O_{m\times m} \\ O_{m\times m} & \mathcal{I}_{m\times m} \end{bmatrix},$$

with $O_{m\times m}$ and $\mathcal{I}_{m\times m}$ equal to the zero and the identity m-dimensional matrices, respectively. We now look at the first term of the summation in (3.12). Taking into account the modified equations (3.9), we have

$$\mathcal{L}_0 H = F \cdot H_x + \frac{1}{2}\mathrm{Tr}\left(GG^{\mathsf{T}} H_{xx}\right) = \Delta t^r \left(f_q \cdot \nabla_q V + f_p \cdot p\right) + \frac{1}{2}\mathrm{Tr}\left(GG^{\mathsf{T}} H_{xx}\right),$$

where

$$GG^{\mathsf{T}} H_{xx} = \begin{bmatrix} O_{m\times m} & O_{m\times m} \\ O_{m\times m} & \Sigma\Sigma^{\mathsf{T}} \end{bmatrix}.$$

Hence

$$\mathcal{L}_0 H = \Delta t^r \left(f_q \cdot \nabla_q V + f_p \cdot p\right) + \frac{1}{2}\mathrm{Tr}\left(\Sigma^{\mathsf{T}}\Sigma\right). \tag{3.13}$$

Substituting (3.13) into (3.12), we get

$$\begin{aligned} \mathbb{E}\left[H(\widetilde{q}(\Delta t), \widetilde{p}(\Delta t))\right] &= H(q_0,p_0) + \frac{1}{2}\mathrm{Tr}\left(\Sigma^{\mathsf{T}}\Sigma\right)\Delta t \\ &\quad + \Delta t^{r+1}\left[f_q(q_0,p_0)\cdot \nabla_q V(q_0) + f_p(q_0,p_0)\cdot p_0\right] + \mathcal{O}(\Delta t^{r+2}). \end{aligned} \tag{3.14}$$

Comparing the expression (3.14) with the general expansion (3.7), we find that

$$\alpha_1 = f_q(q_0,p_0)\cdot \nabla_q V(q_0) + f_p(q_0,p_0)\cdot p_0. \tag{3.15}$$

Let us observe that, for scalar Itô Hamiltonian systems (1.4), equation (3.14) reads

$$\begin{aligned} \mathbb{E}\left[H(\widetilde{q}(\Delta t), \widetilde{p}(\Delta t))\right] &= H(q_0,p_0) + \frac{1}{2}\sigma^2 \Delta t + \mathcal{O}(\Delta t^{r+2}) \\ &\quad + \Delta t^{r+1}\left[f_q(q_0,p_0)\cdot V'(q_0) + f_p(q_0,p_0)\cdot p_0\right]. \end{aligned} \tag{3.16}$$

3.2. Euler–Maruyama. We now compute the modified terms for the Euler–Maruyama method applied to (1.4) in the scalar case. Let us consider a single step of the method, i.e.,

$$q_1 = q_0 + \Delta t p_0, \qquad p_1 = p_0 - \Delta t V'(q_0) + \sigma \Delta W_0,$$

where ΔW_0 is distributed as normal random variable of 0 mean and variance Δt. We aim to expand $\mathbb{E}[q_1,p_1]$ in powers of Δt and to compare this expansion with (3.16). By Taylor series arguments, we have

$$\begin{aligned} H(q_1,p_1) &= H(q_0,p_0) + \Delta t V'(q_0) p_0 - p_0(\Delta t V'(q_0) - \sigma\Delta W_0) \\ &\quad + \frac{1}{2}\Delta t^2 p_0^2 V''(q_0) - \frac{1}{2}(\Delta t V'(q_0) - \sigma \Delta W_0)^2 + \mathcal{O}(\Delta t^3). \end{aligned}$$

Hence, passing to the expectation yields

$$\mathbb{E}\left[H(q_1,p_1)\right] = H(q_0,p_0) + \frac{1}{2}\sigma^2\Delta t + \frac{1}{2}\left(p_0^2 V''(q_0) + V'(q_0)^2\right)\Delta t^2 + \mathcal{O}(\Delta t^3). \tag{3.17}$$

Comparing the expansion (3.17) with (3.6) reveals that, for the Euler–Maruyama method, we have $r=1$. This is not surprising since it is well known that the Euler–Maruyama method has weak error equal to 1 [20]. Moreover, for such method,

$$\beta_1 = \frac{1}{2}\left(p_0^2 V''(q_0) + V'(q_0)^2\right).$$

Hence, due to (3.15), the choice

$$f_q(q,p) = \frac{1}{2}V'(q), \quad f_p(q,p) = \frac{1}{2}pV''(q) \tag{3.18}$$

results in

$$\mathbb{E}\left[H(\widetilde{q}(\Delta t),\widetilde{p}(\Delta t))\right] - \mathbb{E}\left[H(q_1,p_1)\right] = \mathcal{O}(\Delta t^3),$$

as required.

The choice (3.18) leads to the following modified system:

$$\begin{cases} \mathrm{d}\widetilde{q} = \left(\widetilde{p} + \dfrac{\Delta t}{2}V'(\widetilde{q})\right)\mathrm{d}t, \\ \mathrm{d}\widetilde{p} = -\left(V'(\widetilde{q}) - \dfrac{\Delta t}{2}\widetilde{p}\, V''(\widetilde{q})\right)\mathrm{d}t + \sigma \mathrm{d}W(t). \end{cases} \tag{3.19}$$

It can be verified that the modified system (3.19) does not admit any Hamiltonian function.

3.3. Symplectic Euler. A single step of the symplectic Euler method applied to the scalar version of problem (1.4) reads

$$q_1 = q_0 + \Delta t p_1, \qquad p_1 = p_0 - \Delta t V'(q_0) + \sigma \Delta W_0,$$

that is,

$$q_1 = q_0 + \Delta t p_0 - \Delta t^2 V'(q_0) + \sigma \Delta t \Delta W_0, \qquad p_1 = p_0 - \Delta t V'(q_0) + \sigma \Delta W_0. \tag{3.20}$$

Hence, by using Taylor expansion, we have

$$\begin{aligned} \mathbb{E}\left[H(q_1,p_1)\right] = H(q_0,p_0) &+ V'(q_0)\mathbb{E}\left[\Delta t p_0 - \Delta t^2 V'(q_0)\right] - p_0 V'(q_0)\Delta t \\ &+ \frac{1}{2}V''(q_0)\mathbb{E}\left[\left|\Delta t p_0 - \Delta t^2 V'(q_0) + \sigma \Delta t \Delta W_0\right|^2\right] \\ &+ \frac{1}{2}\mathbb{E}\left[\sigma^2 \Delta W_0^2 + \Delta t^2 V'(q_0)^2\right] + \mathcal{O}(\Delta t^3), \end{aligned}$$

that is,

$$\mathbb{E}\left[H(q_1,p_1)\right] = H(q_0,p_0) + \frac{1}{2}\sigma^2\Delta t + \frac{1}{2}\left(V''(q_0)p_0^2 - V'(q_0)^2\right)\Delta t^2 + \mathcal{O}(\Delta t^3).$$

Hence, for the symplectic Euler method, we have $r=1$ and

$$\beta_1 = \frac{1}{2}\left(V''(q_0)p_0^2 - V'(q_0)^2\right).$$

Therefore, with

$$f_q(q,p) = -\frac{1}{2}V'(q), \quad f_p(q,p) = \frac{1}{2}V''(q)p, \tag{3.21}$$

the equality

$$\mathbb{E}\left[H(q_1,p_1)\right] = \mathbb{E}\left[H(\widetilde{q}(\Delta t),\widetilde{p}(\Delta t))\right] + \mathcal{O}\left(\Delta t^3\right)$$

is achieved.

Finally, the following modified system is obtained:

$$\begin{cases} d\widetilde{q} = \left(\widetilde{p} - \dfrac{\Delta t}{2}V'(\widetilde{q})\right)\mathrm{d}t, \\ d\widetilde{p} = \left(-V'(\widetilde{q}) + \dfrac{\Delta t}{2}\widetilde{p}V''(\widetilde{q})\right)\mathrm{d}t + \sigma \mathrm{d}W(t), \end{cases} \tag{3.22}$$

that is, an Itô Hamiltonian system (1.4) with modified Hamiltonian

$$\widetilde{H}(q,p) = \frac{1}{2}p^2 + V(q) - \frac{\Delta t}{2}V'(q)p = H(q,p) + \mathcal{O}\left(\Delta t\right).$$

It is worth noting that the modified terms in (3.21) coincide with those computed, for example, in [18] for the deterministic symplectic Euler method.

3.4. Stochastic midpoint Runge–Kutta methods. Let us now focus on the stochastic midpoint Runge–Kutta method [8, 9] applied to the scalar version of (1.4) that, over a single step, reads as follows:

$$\begin{aligned} q &= q_0 + \frac{\Delta t}{2}p, \qquad p = p_0 - \frac{\Delta t}{2}V'(q) + \frac{1}{\sqrt{2}}\Delta W_1 \sigma, \\ q_1 &= q_0 + \Delta t p, \qquad p_1 = p_0 - \Delta t V'(q) + \frac{1}{\sqrt{2}}\left(\Delta W_1 + \Delta W_2\right)\sigma, \end{aligned} \tag{3.23}$$

where ΔW_1 and ΔW_2 are normal independent random variables of 0 mean and variance Δt. Then, we have

$$\begin{aligned} \mathbb{E}\left[H(q_1,p_1)\right] &= H(q_0,p_0) + V'(q_0)\Delta t \mathbb{E}\left[p_0 - \frac{\Delta t}{2}V'(q)\right] - \Delta t p_0 \mathbb{E}\left[V'(q)\right] \\ &\quad + \frac{1}{2}V''(q_0)\Delta t^2 \mathbb{E}\left[\left|p_0 - \frac{\Delta t}{2}V'(q) + \frac{1}{\sqrt{2}}\Delta W_1 \sigma\right|^2\right] \\ &\quad + \frac{1}{2}\mathbb{E}\left[\left|-\Delta t V'(q) + \frac{1}{\sqrt{2}}\left(\Delta W_1 + \Delta W_2\right)\sigma\right|^2\right] \\ &\quad + \frac{1}{6}V'''(q_0)\Delta t^3 p_0^3 + \mathcal{O}(\Delta t^4). \end{aligned} \tag{3.24}$$

Since

$$\begin{aligned} \mathbb{E}\left[V'(q)\right] = V'(q_0) &+ \frac{1}{2}\Delta t V''(q_0)p_0 \\ &+ \frac{1}{4}\Delta t^2\left(\frac{1}{2}V'''(q_0)p_0^2 - V''(q_0)V'(q_0)\right) + \mathcal{O}\left(\Delta t^3\right), \end{aligned}$$

$$\mathbb{E}\left[\left|p_0-\frac{\Delta t}{2}V'(q)+\frac{1}{\sqrt{2}}\Delta W_1\sigma\right|^2\right]=p_0^2+\frac{1}{2}\Delta t\sigma^2-p_0\Delta tV'(q_0)+\mathcal{O}(\Delta t^2)$$

and

$$\mathbb{E}\left[\left|-\Delta tV'(q)+\frac{1}{\sqrt{2}}\left(\Delta W_1+\Delta W_2\right)\sigma\right|^2\right]=\Delta t\sigma^2+\Delta t^2V'(q_0)+\mathcal{O}\left(\Delta t^4\right)$$
$$+\Delta t^3\left(V'(q_0)V''(q_0)p_0-\frac{1}{2}\sigma^2V''(q_0)\right).$$

Equation (3.24) reduces to

$$\mathbb{E}\left[H(q_1,p_1)\right]=H(q_0,p_0)+\frac{\Delta t}{2}\sigma^2 + \frac{\Delta t^3}{4}\left(\frac{1}{6}p_0^3\;V'''(q_0)+\left(V''(q_0)-1\right)\sigma^2\right)+\mathcal{O}\left(\Delta t^4\right). \tag{3.25}$$

We observe that (3.25) leads to

$$f_q(q,p)=\frac{1}{4V'(q)}\left(V''(q)-1\right)\sigma^2,\quad f_p(q,p)=\frac{1}{24}p^2\;V'''(q),$$

and $r=2$. Finally, the modified stochastic system is then given by

$$\begin{cases} d\widetilde{q}=\left(\widetilde{p}+\dfrac{\Delta t^2}{4V'(\widetilde{q})}\left(V''(\widetilde{q})-1\right)\sigma^2\right)\mathrm{d}t,\\ d\widetilde{p}=\left(-V'(\widetilde{q})+\dfrac{\Delta t^2}{24}\widetilde{p}^2\;V'''(\widetilde{q})\right)\mathrm{d}t+\sigma\mathrm{d}W(t).\end{cases} \tag{3.26}$$

We also observe that, for quadratic potentials $V(q)=\frac{1}{2}q^{\mathsf{T}}q$, the coefficient of the cubic term in Δt appearing in (3.25) vanishes. High order terms also annihilate (since they depend on high order derivatives), and, as a consequence, the method exactly preserves the trace equality when the potential is quadratic, coherently with the analysis provided in [8, 9] for the stochastic midpoint Runge–Kutta method (3.23).

4. Modified equations for Stratonovich Hamiltonian systems. Let us now focus our attention on the computation of modified terms for Stratonovich Hamiltonian systems (1.7). To this purpose, we recast a Stratonovich Hamiltonian system (1.7) in its equivalent Itô form [20, 23], i.e.,

$$\begin{cases} \mathrm{d}q=\left[\nabla_pH(q,p)+\dfrac{\widetilde{\sigma}}{2}\Big(\nabla_{qp}H(q,p)\nabla_pH(q,p)-\nabla_{pp}H(q,p)\nabla_qH(q,p)\Big)\right]\mathrm{d}t\\ \qquad\qquad+\nabla_pH(q,p)\widetilde{\Sigma}^{\mathsf{T}}\mathrm{d}W(t),\\ \mathrm{d}p=-\left[\nabla_qH(q,p)-\dfrac{\widetilde{\sigma}}{2}\Big(\nabla_{pq}H(q,p)\nabla_qH(q,p)-\nabla_{qq}H(q,p)\nabla_pH(q,p)\Big)\right]\mathrm{d}t\\ \qquad\qquad-\nabla_qH(q,p)\widetilde{\Sigma}^{\mathsf{T}}\mathrm{d}W(t),\end{cases} \tag{4.1}$$

where $\widetilde{\sigma}=\widetilde{\Sigma}^{\mathsf{T}}\widetilde{\Sigma}$. Also in the Stratonovich case, given a stochastic numerical method for (4.1), in what follows we assume that

$$\mathbb{E}\left[H(q_n,p_n)\right]=H(q_0,p_0)+\mathcal{O}\left(\Delta t^r\right) \tag{4.2}$$

for positive r and, focusing on a single step, condition (4.2) requires

$$\mathbb{E}\left[H(q_1,p_1)\right] = H(q_0,p_0) + \gamma_1 \Delta t^{r+1} + \mathcal{O}\left(\Delta t^{r+2}\right). \tag{4.3}$$

Our attention is now addressed to providing a modified system for (4.1); i.e., we look for $\widetilde{q}(t)$ and $\widetilde{p}(t)$ solutions to

$$\begin{cases} \mathrm{d}\widetilde{q} = \Big[\nabla_p H(\widetilde{q},\widetilde{p}) + \Delta t^r f_q(\widetilde{q},\widetilde{p}) \\ \qquad\qquad + \dfrac{\widetilde{\sigma}}{2}\Big(\nabla_{qp} H(\widetilde{q},\widetilde{p})\nabla_p H(\widetilde{q},\widetilde{p}) - \nabla_{pp} H(\widetilde{q},\widetilde{p})\nabla_q H(\widetilde{q},\widetilde{p})\Big)\Big]\mathrm{d}t \\ \qquad\qquad + \nabla_p H(\widetilde{q},\widetilde{p})\widetilde{\Sigma}^{\mathsf{T}}\mathrm{d}W(t), \\ \mathrm{d}\widetilde{p} = \Big[\Delta t^r f_p(\widetilde{q},\widetilde{p}) - \nabla_q H(\widetilde{q},\widetilde{p}) \\ \qquad\qquad + \dfrac{\widetilde{\sigma}}{2}\Big(\nabla_{pq} H(\widetilde{q},\widetilde{p})\nabla_q H(\widetilde{q},\widetilde{p}) - \nabla_{qq} H(\widetilde{q},\widetilde{p})\nabla_p H(\widetilde{q},\widetilde{p})\Big)\Big]\mathrm{d}t \\ \qquad\qquad - \nabla_q H(\widetilde{q},\widetilde{p})\widetilde{\Sigma}^{\mathsf{T}}\mathrm{d}W(t), \end{cases} \tag{4.4}$$

such that

$$\mathbb{E}\left[H(\widetilde{q}(\Delta t),\widetilde{q}(\Delta t))\right] = H(q_0,p_0) + \delta_1 \Delta t^{r+1} + \mathcal{O}(\Delta t^{r+2}). \tag{4.5}$$

Comparing (4.3) and (4.5), condition

$$\gamma_1 = \delta_1 \tag{4.6}$$

provides

$$\mathbb{E}\left[H(q_n,p_n)\right] - \mathbb{E}\left[H(\widetilde{q}(t_n),\widetilde{p}(t_n))\right] = \mathcal{O}(\Delta t^{r+1}), \tag{4.7}$$

where (q_n,p_n) is the numerical solution at the time $t_n, n = 1,2,\dots N$. Applying to (4.4) similar arguments as those given for Itô problems in the previous section yields

$$\delta_1 = f_q(q_0,p_0)^{\mathsf{T}}\nabla_q H(q_0,p_0) + f_p(q_0,p_0)^{\mathsf{T}}\nabla_p H(q_0,p_0). \tag{4.8}$$

A proof of (4.8) is provided in Appendix B.

It is worth specializing the analysis to the case of Hamiltonian functions of type (1.3). For this choice of H, problem (4.1) reads

$$\begin{cases} \mathrm{d}q = \left(p - \dfrac{\widetilde{\sigma}}{2}\nabla_q V(q)\right)\mathrm{d}t + p\widetilde{\Sigma}^{\mathsf{T}}\mathrm{d}W(t), \\ \mathrm{d}p = -\left(\nabla_q V(q) + \dfrac{\widetilde{\sigma}}{2}\nabla_{qq} V(q)p\right)\mathrm{d}t - \nabla_q V(q)\widetilde{\Sigma}^{\mathsf{T}}\mathrm{d}W(t), \end{cases} \tag{4.9}$$

and its modified counterpart assumes the form

$$\begin{cases} \mathrm{d}\widetilde{q} = \left(\widetilde{p} - \dfrac{\widetilde{\sigma}}{2}\nabla_q V(\widetilde{q}) + \Delta t^r f_q(\widetilde{q},\widetilde{p})\right)\mathrm{d}t + \widetilde{p}\widetilde{\Sigma}^{\mathsf{T}}\mathrm{d}W(t), \\ d\widetilde{p} = -\left(\nabla_q V(\widetilde{q}) + \dfrac{\widetilde{\sigma}}{2}\nabla_{qq} V(\widetilde{q})\widetilde{p} - \Delta t^r f_p(\widetilde{q},\widetilde{p})\right)\mathrm{d}t - \nabla_q V(\widetilde{q})\,\widetilde{\Sigma}^{\mathsf{T}}\mathrm{d}W(t). \end{cases} \tag{4.10}$$

Correspondingly, for system (4.10), we have

$$\delta_1 = \alpha_1 = f_q(q_0,p_0)^{\mathsf{T}}\nabla_q V(q_0) + f_p(q_0,p_0)^{\mathsf{T}}p_0. \tag{4.11}$$

4.1. Examples. We now provide selected examples of computation of modified differential equations for Stratonovich Hamiltonian systems. It is worth noting here that, in the scalar case and with Hamiltonian function given by (1.3), the knowledge of the modified terms $f_q(q,p)$ and $f_p(q,p)$ allows us to recover the Stratonovich formulation

$$\begin{cases} d\widetilde{q} = \widetilde{p}\big(\mathrm{d}t + \sigma \circ \mathrm{d}W(t)\big) + \Delta t^r \; f_q(\widetilde{q},\widetilde{p})\mathrm{d}t, \\ d\widetilde{p} = -V'(\widetilde{q})\big(\mathrm{d}t + \sigma \circ \mathrm{d}W(t)\big) + \Delta t^r \; f_p\left(\widetilde{q},\widetilde{p}\right)\big)\,\mathrm{d}t \end{cases} \tag{4.12}$$

equivalent to the modified system (4.10).

4.1.1. Euler–Maruyama. The application of a single step of the Euler–Maruyama method to the system (4.9) reads as follows:

$$q_1 = q_0 + \Delta t\left[p_0 - \frac{1}{2}\sigma^2 V'(q_0)\right] + \sigma p_0 \Delta W_0,$$

$$p_1 = p_0 + \Delta t\left[-V'(q_0) - \frac{1}{2}\sigma^2 V''(q_0)p_0\right] - \sigma V'(q_0)\Delta W_0.$$

Then, by Taylor series arguments, we have

$$\begin{aligned} H(q_1,p_1) = {} & H(q_0,p_0) + V'(q_0)\left[\Delta t\left(p_0 - \frac{1}{2}\sigma^2 V'(q_0)\right) + \sigma p_0 \Delta W_0\right] \\ & + p_0\left[\Delta t\left(-V'(q_0) - \frac{1}{2}\sigma^2 V''(q_0)p_0\right) - \sigma V'(q_0)\Delta W_0\right] \\ & + \frac{1}{2}V''(q_0)\left|\Delta t\left(p_0 - \frac{1}{2}\sigma^2 V'(q_0)\right) + \sigma p_0 \Delta W_0\right|^2 \\ & + \frac{1}{2}\left|\Delta t\left(V'(q_0) + \frac{1}{2}\sigma^2 V''(q_0)p_0\right) + \sigma V'(q_0)\Delta W_0\right|^2 \\ & + \frac{1}{6}V'''(q_0)\left[\Delta t\left(p_0 - \frac{1}{2}\sigma^2 V'(q_0)\right) + \sigma p_0 \Delta W_0\right]^3 \\ & + \frac{1}{24}V^{(4)}(q_0)\left|\Delta t\left(p_0 - \frac{1}{2}\sigma^2 V'(q_0)\right) + \sigma p_0 \Delta W_0\right|^4 + \mathcal{O}\left(\Delta t^3\right). \end{aligned}$$

Taking the expectation, we get

$$\begin{aligned} \mathbb{E}\left[H(q_1,p_1)\right] = {} & H(q_0,p_0) + \frac{\Delta t^2}{2}\left[V''(q_0)\left(p_0 - \frac{1}{2}\sigma^2 V'(q_0)\right)^2 \right. \\ & \left. + \left(V'(q_0) + \frac{1}{2}\sigma^2 V''(q_0)p_0\right)^2\right] \\ & + \frac{1}{6}V'''(q_0)\mathbb{E}\left[\left(\Delta t\left(p_0 - \frac{1}{2}\sigma^2 V'(q_0)\right) + \sigma p_0 \Delta W_0\right)^3\right] \\ & + \frac{1}{24}V^{(4)}(q_0)\mathbb{E}\left[\left|\Delta t\left(p_0 - \frac{1}{2}\sigma^2 V'(q_0)\right) + \sigma p_0 \Delta W_0\right|^4\right] + \mathcal{O}(\Delta t^3). \end{aligned}$$

Since

$$\mathbb{E}\left[\left(\Delta t\left(p_0-\frac{1}{2}\sigma^2V'(q_0)\right)+\sigma p_0\Delta W_0\right)^3\right]=3\sigma^2p_0^2\left(p_0-\frac{1}{2}\sigma^2V'(q_0)\right)\Delta t^2+\mathcal{O}(\Delta t^3)$$

and

$$\mathbb{E}\left[\left|\Delta t\left(p_0-\frac{1}{2}\sigma^2V'(q_0)\right)+\sigma p_0\Delta W_0\right|^4\right]=3\sigma^4p_0^4\Delta t^2+\mathcal{O}(\Delta t^3), \tag{4.13}$$

we end up with

$$\mathbb{E}\left[H(q_1,p_1)\right]=H(q_0,p_0)+\gamma_1\Delta t^2+\mathcal{O}(\Delta t^3), \tag{4.14}$$

where

$$\begin{aligned}\gamma_1=\frac{1}{2}\Bigg[&V''(q_0)\left(p_0-\frac{1}{2}\sigma^2V'(q_0)\right)^2+\left(V'(q_0)+\frac{1}{2}\sigma^2V''(q_0)p_0\right)^2\\&+V'''(q_0)\left(p_0-\frac{1}{2}\sigma^2V'(q_0)\right)\sigma^2p_0^2\Bigg]+\frac{1}{8}V^{(4)}(q_0)\sigma^4p_0^4.\end{aligned}$$

From (4.14), we recognize $r=1$, and if

$$f_q(q,p)=\frac{1}{2}V'(q)+\frac{1}{8}\sigma^4V'(q)V''(q)-\frac{1}{2}p\sigma^2V''(q)+\frac{1}{2}\sigma^2V''(q)p-\frac{1}{4}\sigma^4V'''(q)p^2,$$

$$f_p(q,p)=\frac{1}{2}V''(q)p+\frac{1}{8}\sigma^4V''(q)p+\frac{1}{2}\sigma^2V'''(q)p^2+\frac{1}{8}V^{(4)}\sigma^4p^3,$$

then condition (4.6) is fulfilled.

4.1.2. A symplectic Runge–Kutta method. Let us consider the stochastic symplectic Runge–Kutta method introduced in [25], applied to (1.8) in the scalar case, obtaining

$$q_1=q_0+\xi_0\ p,\qquad p_1=p_0-\xi_0\ V'(q), \tag{4.15}$$

where $\xi_0=\Delta t+\sigma\Delta W_0$ and

$$q=q_0+\frac{1}{2}\xi_0\ p,\qquad p=p_0-\frac{1}{2}\xi_0\ V'(q). \tag{4.16}$$

Let us first compute expansions for q and p, leading to

$$\begin{aligned}q&=q_0+\frac{1}{2}\xi_0\ p\\&=q_0+\frac{1}{2}\xi_0\left(p_0-\frac{1}{2}\xi_0\ V'(q)\right)\\&=q_0+\frac{1}{2}\xi_0\ p_0-\frac{1}{4}\xi_0^2V'(q_0)-\frac{1}{8}V''(q_0)\xi_0^3\ p-\frac{1}{32}V'''(q_0)\xi_0^4\ p^2+\mathcal{O}(\xi_0^5).\end{aligned}$$

Replacing the expression for p gives the following expansion of q in terms of powers of ξ_0:

$$\begin{aligned}q=q_0+\frac{1}{2}p_0\xi_0-\frac{1}{4}V'(q_0)\xi_0^2-\frac{1}{8}V''(q_0)\xi_0^3p_0&\\+\frac{1}{16}\left(V''(q_0)V'(q_0)-\frac{1}{2}V'''(q_0)p_0\right)\xi_0^4+\mathcal{O}(\xi_0^5).&\end{aligned} \tag{4.17}$$

Proceeding in a similar way for the expansion of p yields

$$p = p_0 - \frac{1}{2}V'(q_0)\xi_0 - \frac{1}{4}V''(q_0)p_0\xi_0^2 + \frac{1}{8}\left(V''(q_0)V'(q_0) - \frac{1}{2}V'''(q_0)p_0^2\right)\xi_0^3 + \frac{1}{16}\left(V''(q_0)^2p_0 - V'''(q_0)V'(q_0)p_0 - \frac{1}{6}V^{(4)}(q_0)p_0\right)\xi_0^4 + \mathcal{O}(\xi_0^5). \tag{4.18}$$

Therefore, using (4.17) and (4.18), we can compute an expansion for $H(q_1,p_1)$, as follows:

$$\begin{aligned} H(q_1,p_1) &= H(q_0+\xi_0 p, p_0 - \xi_0 V'(q)) \\ &= H(q_0,p_0) + \frac{1}{4}\left[V'(q_0)p_0 - V''(q_0)p_0V'(q_0) + \frac{1}{6}V'''(q_0)p_0^3\right]\xi_0^3 \\ &\quad + \frac{1}{4}\Big[V''(q_0)V'(q_0)^2 - V'''(q_0)V'(q_0)p_0^2 + \frac{1}{2}V''(q_0)p_0^2 \\ &\quad + \frac{1}{12}V^{(4)}(q_0)p_0^4 - V'(q_0)^2 - \frac{1}{2}V''(q_0)^2p_0^2\Big]\xi_0^4 + \mathcal{O}(\xi_0^5). \end{aligned}$$

Since

$$\mathbb{E}\left[\xi_0^3\right] = 3\sigma^2\Delta t^2 + \mathcal{O}(\Delta t^3), \quad \mathbb{E}\left[\xi_0^4\right] = 3\sigma^4\Delta t^2 + \mathcal{O}(\Delta t^3), \quad \mathbb{E}\left[\xi_0^5\right] = \mathcal{O}(\Delta t^3),$$

we can argue that

$$\mathbb{E}\left[H(q_1,p_1)\right] = H(q_0,p_0) + \gamma_1\Delta t^2 + \mathcal{O}(\Delta t^3), \tag{4.19}$$

where

$$\begin{aligned} \gamma_1 = \frac{3}{4}\sigma^2 &\left[V'(q_0)p_0 - V''(q_0)p_0V'(q_0) + \frac{1}{6}V'''(q_0)p_0^3\right] \\ &+ \frac{3}{4}\sigma^4\Big[V''(q_0)V'(q_0)^2 - V'''(q_0)V'(q_0)p_0^2 + \frac{1}{2}V''(q_0)p_0^2 \\ &+ \frac{1}{12}V^{(4)}(q_0)p_0^4 - V'(q_0)^2 - \frac{1}{2}V''(q_0)^2p_0^2\Big]. \end{aligned}$$

Here, as in the previous example, $r=1$. Finally, in order to achieve (4.6), it is enough to take

$$f_q(q,p) = \frac{3}{4}\sigma^2\left(p - V''(q)p + \sigma^2V''(q)V'(q) - \sigma^2V'''(q)p^2\right) \tag{4.20}$$

and

$$f_p(q,p) = \frac{1}{8}\sigma^2V'''(q)p^2 - \frac{3}{8}\sigma^4\left(V''(q)^2p - \frac{1}{6}V^{(4)}(q)p^3 - V''(q)p\right). \tag{4.21}$$

We also observe that, for quadratic potentials $V(q) = \frac{1}{2}q^{\mathsf{T}}q$, the value of γ_1 is zero and the remainder term in (4.19) vanishes. Then, the method exactly preserves the Hamiltonian when the potential is quadratic, coherently with the analysis provided in [25] for (4.15).

4.1.3. Perturbation of a deterministic energy-preserving method. Let us now consider the stochastic perturbation of a well-known deterministic energy-preserving numerical scheme, introduced and analyzed in [10]. Over a single step, it reads as

$$\begin{aligned} q_1 &= q_0 + \frac{\xi_0}{3}\left[\frac{1}{2}p_0 + (p_0+p_1) + \frac{1}{2}p_1\right] = q_0 + \frac{\xi_0}{2}\,(p_0+p_1)\,, \\ p_1 &= p_0 - \frac{\xi_0}{3}\left[\frac{1}{2}V'(q_0) + 2V'\left(\frac{q_0+q_1}{2}\right) + \frac{1}{2}V'(q_1)\right], \end{aligned} \tag{4.22}$$

where $\xi_0 = \Delta t + \sigma\Delta W_0$. As shown in the aforementioned paper, the deterministic version of method (4.22) (i.e., (4.22) with $\sigma = 0$) is capable of conserving quartic Hamiltonian functions.

Since

$$V'\left(\frac{q_0+q_1}{2}\right) = V'(q_0) + \frac{1}{2}V''(q_0)\,(q_1-q_0) + \frac{1}{8}V'''(q_0)\,|q_1-q_0|^2 + \mathcal{O}(\xi_0^3),$$

expanding q_1 and p_1 in power series of ξ_0 and iteratively applying (4.22) yields

$$\begin{aligned} q_1 = q_0 + \xi_0 p_0 - \frac{\xi_0^2}{2}V'(q_0) - \frac{\xi_0^3}{4}V''(q_0)p_0 \\ + \frac{\xi_0^4}{4}\left[\frac{1}{2}V''(q_0)V'(q_0) - \frac{1}{3}V'''(q_0)p_0^2\right] + \mathcal{O}(\xi_0^5). \end{aligned}$$

Replacing the last equation into the expression for p_1 leads to

$$\begin{aligned} p_1 = p_0 - \xi_0 V'(q_0) - \frac{\xi_0^2}{2}p_0V''(q_0) + \frac{\xi_0^3}{2}\left[\frac{1}{2}V''(q_0)V'(q_0) - \frac{1}{3}V'''(q_0)p_0^2\right] \\ + \frac{\xi_0^4}{2}\left[\frac{1}{4}V''(q_0)^2p_0 + \frac{1}{3}V'''(q_0)V'(q_0)p_0 - \frac{1}{12}V^4(q_0)p_0^3\right] + \mathcal{O}(\xi_0^5). \end{aligned}$$

Then, previous relations lead to the following expansion of $H(q_1,p_1)$:

$$\begin{aligned} H(q_1,p_1) = H(q_0,p_0) + \frac{\xi_0^4}{4}\Bigg[\frac{1}{2}V''(q_0)^2p_0^3 - \frac{1}{2}V''(q_0)^2p_0^2 \\ - V''(q_0)V'(q_0)^2 - \frac{1}{3}V'''(q_0)V'(q_0)p_0^2\Bigg] + \mathcal{O}(\xi_0^5), \end{aligned}$$

and passing to side-by-side expectation gives

$$\begin{aligned} \mathbb{E}\left[H(q_1,p_1)\right] = H(q_0,p_0) + \frac{3}{4}\sigma^4\Delta t^2\Bigg[\frac{1}{2}V''(q_0)^2p_0^3 - \frac{1}{2}V''(q_0)^2p_0^2 \\ - V''(q_0)V'(q_0)^2 - \frac{1}{3}V'''(q_0)V'(q_0)p_0^2\Bigg] + \mathcal{O}(\Delta t^3), \end{aligned}$$

where we recognize $r=1$ and, with reference to (4.2),

$$\gamma_1 = \frac{3}{4}\sigma^4\left[\frac{1}{2}V''(q_0)^2p_0^3 - \frac{1}{2}V''(q_0)^2p_0^2 - V''(q_0)V'(q_0)^2 - \frac{1}{3}V'''(q_0)V'(q_0)p_0^2\right].$$

Hence, assuming

$$f_q(q,p) = -\frac{1}{4}\sigma^4\left(3V''(q)V'(q) + V'''(q)p^2\right) \tag{4.23}$$

and

$$f_p(q,p) = -\frac{3}{8}\sigma^4 V''(q)^2 p\,(p-1) \tag{4.24}$$

specializes (4.6) to the setting described for (4.22), leading to

$$\mathbb{E}\left[H(\widetilde{q}(\Delta t), \widetilde{p}(\Delta t))\right] - \mathbb{E}\left[H(q_1,p_1)\right] = \mathcal{O}(\Delta t^3),$$

as required.

4.1.4. A stochastic energy-preserving scheme. Let us consider the following stochastic energy-preserving scheme introduced in [29, 30]:

$$\begin{aligned} q_1 &= q_0 + \frac{\xi_0}{2(p_1-p_0)}\left[H(q_1,p_1) + H(q_0,p_1) - H(q_1,p_0) - H(q_0,p_0)\right], \\ p_1 &= p_0 - \frac{\xi_0}{2(q_1-q_0)}\left[H(q_1,p_1) + H(q_1,p_0) - H(q_0,p_1) - H(q_0,p_0)\right]. \end{aligned} \tag{4.25}$$

By means of Taylor series arguments, we get

$$\begin{aligned} q_1 = q_0 + \frac{\xi_0}{2(p_1-p_0)}\Bigg[&H(q_0,p_0) + p_0(p_1-p_0) + \frac{1}{2}(p_1-p_0)^2 \\ &+ \sum_{k=1}^{\infty}\frac{V^{(k)}(q_0)}{k!}(q_1-q_0)^k + H(q_0,p_0) + p_0(p_1-p_0) \\ &+ \frac{1}{2}(p_1-p_0)^2 - H(q_0,p_0) - \sum_{k=1}^{\infty}\frac{V^{(k)}(q_0)}{k!}(q_1-q_0)^k - H(q_0,p_0)\Bigg], \end{aligned}$$

i.e.,

$$q_1 = q_0 + \xi_0 p_0 + \frac{\xi_0}{2}(p_1-p_0). \tag{4.26}$$

Since

$$p_1 = p_0 - \xi_0\sum_{k=1}^{\infty}\frac{V^{(k)}(q_0)}{k!}(q_1-q_0)^{k-1}, \tag{4.27}$$

we obtain

$$q_1 = q_0 + \xi_0 p_0 - \frac{\xi_0^2}{2}\sum_{k=1}^{\infty}\frac{V^{(k)}(q_0)}{k!}(q_1-q_0)^{k-1}. \tag{4.28}$$

Applying again Taylor series arguments yields

$$H(q_1,p_1) - H(q_0,p_0) = p_0(p_1-p_0) + \frac{1}{2}(p_1-p_0)^2 + \sum_{i=1}^{\infty}\frac{V^{(k)}(q_0)}{k!}(q_1-q_0)^k,$$

which, under (4.27), reads

$$\begin{aligned} H(q_1,p_1) &= H(q_0,p_0) - \xi_0 p_0 \sum_{i=1}^{\infty} \frac{V^{(k)}(q_0)}{k!}(q_1-q_0)^{k-1} \\ &\qquad + \frac{\xi_0^2}{2}\left(\sum_{i=1}^{\infty} \frac{V^{(k)}(q_0)}{k!}(q_1-q_0)^{k-1}\right)^2 + \sum_{i=1}^{\infty} \frac{V^{(k)}(q_0)}{k!}(q_1-q_0)^{k} \\ &= H(q_0,p_0) + \sum_{i=1}^{\infty} \frac{V^{(k)}(q_0)}{k!}(q_1-q_0)^{k-1}(q_1-q_0-\xi_0 p_0) \\ &\qquad + \frac{\xi_0^2}{2}\left(\sum_{i=1}^{\infty} \frac{V^{(k)}(q_0)}{k!}(q_1-q_0)^{k-1}\right)^2 . \end{aligned}$$

By replacing (4.28), the last equation reduces to $H(q_1,p_1)=H(q_0,p_0)$. In summary, method (4.25) satisfies $\mathbb{E}[H(q_1,p_1)] = H(q_0,p_0)$, i.e., (4.25) provides a method preserving the expected Hamiltonian, as highlighted in [29, 30].

4.2. Extension to higher dimensions. In this section, we discuss the construction of modified equations for Stratonovich system (1.8) in the multidimensional case. Let us consider a single step of the following numerical method for (4.9):

$$q^1 = q^0 + \Delta q, \quad p^1 = p^0 + \Delta p, \tag{4.29}$$

with $q^1,p^1,\Delta q,\Delta p \in \mathbb{R}^m$ and $q^0=q_0, p^0=p_0$. Then, some computations yield

$$\begin{aligned} H(q^1,p^1) &= H(q^0,p^0) + {p^0}^{\mathsf{T}}\Delta p + \nabla_q V(q^0)^{\mathsf{T}}\Delta q + \frac{1}{2}\Delta p^{\mathsf{T}}\Delta p \\ &\qquad + \frac{1}{2}\Delta q^{\mathsf{T}}\nabla_{qq}V(q^0)\Delta q + D_3(q^0) + D_4(q^0) + Z(q^0), \end{aligned} \tag{4.30}$$

where $D_3(q^0)$ and $D_4(q^0)$ contain all the terms arising from the computation of the third and fourth derivatives of the potential, respectively, and $Z(q^0)$ contains higher weak order terms (i.e., $\mathbb{E}[Z(q^0)] = \mathcal{O}(\Delta t^{r+2})$). Passing to side-by-side expectation in (4.30), after some computations, we achieve

$$\mathbb{E}\left[H(q^1,p^1)\right] = H(q_0,p_0) + \gamma_1 \Delta t^{r+1} + \mathcal{O}(\Delta t^{r+2}), \tag{4.31}$$

with γ_1 depending on the method. As an example, in Appendix A we discuss the case of the Euler–Maruyama method applied to (4.9) with $m=2$.

5. Long-term analysis in the Itô Hamiltonian case. In this section, we make use of modified Itô equations (3.9) to provide long-term estimates of time discretizations to Itô Hamiltonian systems (1.4), revealing the attitude of such schemes in reproducing the trace equation (1.5) along the numerical dynamics. We give the following theorem.

THEOREM 5.1. *Let us consider the stochastic Hamiltonian system of Itô type* (1.4)*, where the Hamiltonian function $H(q(t),p(t))$ is defined as in* (1.3)*, and let $(q_n,p_n), n=1,2,\dots,N$, be any suitable numerical solution to system* (1.4) *with fixed stepsize $\Delta t = T/N$, such that* (3.1) *holds. Then, by denoting*

$$e(t_n) = \mathbb{E}\left[H(q_n,p_n)\right] - \mathbb{E}\left[H(q(t_n),p(t_n))\right], \quad n=1,2,\dots,N, \tag{5.1}$$

if there exists a positive integer $2 \leq k < \infty$ *such that* $\mathbb{E}[\mathcal{L}_0^k H(\widetilde{q},\widetilde{p})]$ *is uniformly bounded, then the following estimate holds true:*

$$e(t_n) = \alpha_1 \Delta t^r \ t_n + \mathcal{O}(\Delta t^r t_n^k), \tag{5.2}$$

where α_1 *is defined in* (3.15). *Otherwise, if such an index* k *does not exist and we have* $\alpha_1 = H(\widetilde{q},\widetilde{p})$, *then the error* $e(t_n)$ *admits the following exponential growth:*

$$e(t_n) = \mathcal{O}(e^{\Delta t^r t_n}). \tag{5.3}$$

Proof. First, we recall that the key point is given by looking at the modified system (3.9), whose solution $(\widetilde{q}(t),\widetilde{p}(t))$ satisfies

$$\mathbb{E}\left[H(q_n,p_n)\right] = \mathbb{E}\left[H(\widetilde{q}(t_n),\widetilde{p}(t_n))\right] + \mathcal{O}(\Delta t^{r+1}). \tag{5.4}$$

As a consequence, (5.4) allows us to achieve an estimate for $\mathbb{E}[H(q_n,p_n)]$ by analyzing $\mathbb{E}[H(\widetilde{q}(t),\widetilde{p}(t))]$.

The proof is given proceeding as follows. The iterated application of the stochastic Itô–Taylor expansion, applied to $\mathbb{E}[H(\widetilde{q}(t),\widetilde{p}(t))]$ and passing to expectation, yields

$$\begin{aligned}
\mathbb{E}\left[H(\widetilde{q}(t),\widetilde{p}(t))\right] &= H(q_0,p_0) + \int_0^t \mathbb{E}\left[\mathcal{L}_0 H(\widetilde{q}(s),\widetilde{p}(s))\right] \mathrm{d}s \\
&= H(q_0,p_0) + \int_0^t \left[\mathcal{L}_0 H(q_0,p_0) + \int_0^s \mathbb{E}\left[\mathcal{L}_0^2 H(\widetilde{q}(u),\widetilde{p}(u))\right] \mathrm{d}u\right] \mathrm{d}s \\
&= H(q_0,p_0) + \mathcal{L}_0 H(q_0,p_0) t + \int_0^t \int_0^s \mathbb{E}\left[\mathcal{L}_0^2 H(\widetilde{q}(u),\widetilde{p}(u))\right] \mathrm{d}u\, \mathrm{d}s \\
&= H(q_0,p_0) + \sum_{j=1}^{k-1} \mathcal{L}_0^j H(q_0,p_0) \frac{t^j}{j!} \\
&\qquad + \int_0^t \int_0^{s_1} \dots \int_0^{s_{k-1}} \mathbb{E}\left[\mathcal{L}_0^k H(\widetilde{q}(u),\widetilde{p}(u))\right] \mathrm{d}u \dots \mathrm{d}s_1.
\end{aligned} \tag{5.5}$$

Since

$$\mathcal{L}_0 H = \frac{1}{2} \mathrm{Tr}\left(\Sigma^{\mathsf{T}} \Sigma\right) + \alpha_1 \Delta t^r,$$

by evaluating (5.5) for $t = t_n$, $n = 1,2,\dots,N$, and under the assumption on the boundedness of $\mathbb{E}[\mathcal{L}_0 H]$, we get

$$\begin{aligned}
\mathbb{E}\left[H(\widetilde{q}(t_n),\widetilde{p}(t_n))\right] &= H(q_0,p_0) + \frac{1}{2} \mathrm{Tr}\left(\Sigma^{\mathsf{T}} \Sigma\right) t_n + \alpha_1 \Delta t^r \ t_n \\
&\qquad + \sum_{j=2}^{k-1} \mathcal{L}_0^j H(q_0,p_0) \frac{t_n^j}{j!} + \frac{C}{k!} t_n^k.
\end{aligned} \tag{5.6}$$

Equation (5.2) holds true since

$$\mathbb{E}\left[H(q(t_n),p(t_n))\right] = H(q_0,p_0) + \frac{1}{2} \mathrm{Tr}\left(\Sigma^{\mathsf{T}} \Sigma\right) t_n.$$

Finally, let us assume that such an index k does not exist and that $\alpha_1 = H(\widetilde{q},\widetilde{p})$. Then, we have

$$\mathbb{E}\left[H(\widetilde{q}(t_n),\widetilde{p}(t_n))\right] = \mathbb{E}\left[H(q(t_n),p(t_n))\right] + \Delta t^r \int_0^t \mathbb{E}\left[H(\widetilde{q}(s),\widetilde{p}(s))\right] \mathrm{d}s. \tag{5.7}$$

The estimate in (5.3) holds true under the application of standard Grönwall arguments for (5.7). ◻

Remark 1. It is worth remarking that in case of nonexistence of an index k such that $\mathbb{E}[\mathcal{L}_0^k H(\widetilde{q},\widetilde{p})]$ remains bounded, Theorem 5.1 covers the case $\alpha_1 = H(\widetilde{q},\widetilde{p})$. Similar arguments can be applied to the case $\alpha_1 \neq H(\widetilde{q},\widetilde{p})$, by writing the Hamiltonian deviation $\mathbb{E}[H(\widetilde{q}(t_n),\widetilde{p}(t_n))] - H(q_0,p_0)$ as in (5.5) and, supposing that there exists an index s such that $\mathcal{L}_0^s H(\widetilde{q},\widetilde{p}) = H(\widetilde{q},\widetilde{p})$, the thesis holds true by applying the Grönwall lemma for multiple integrals. Finally, if such an index s does not exist, repeatedly applying Itô–Taylor expansions in (5.5) for arbitrarily large values of the summation index leads to an exponential growth for the Hamiltonian deviation.

Remark 2. The estimate given in (5.2) does not take into account the term $\mathcal{O}(\Delta t^{r+1})$ arising from (5.4), since usual local error arguments show that it behaves as $\mathcal{O}(t_n \Delta t^{r+1})$ and, hence, it is negligible in estimating $e(t_n)$ in (5.2).

Remark 3. It is worth mentioning that, for a drift-preserving method solving (1.4), we have $\alpha_1 = 0$ and, hence, $\mathcal{L}^1 H = \mathrm{Tr}(\Sigma^{\mathsf{T}}\Sigma)/2$ and $\mathcal{L}_0^p H = 0,\ p \geq 2$. This also holds true in the case of symplectic methods applied to quadratic Hamiltonians. Moreover, from Theorem 5.1, we realize that in the absence of a drift-preserving character in the numerical solution of (1.4), at best, such a method is able to exhibit a linear growth of the averaged Hamiltonian but with a coefficient that appears to be $\mathcal{O}(\Delta t^r)$ far from the exact one, i.e., $\mathrm{Tr}(\Sigma^{\mathsf{T}}\Sigma)/2$. This is the case of a method such that $\alpha_1 \neq 0$ and $\mathbb{E}[\mathcal{L}_0^2 H] = 0$.

In order to confirm this result, let us consider the following numerical experiment arising from the application of the symplectic Euler method (3.20) to the scalar linear Itô Hamiltonian problem (1.4), thus corresponding to the potential $V(q) = q^2/2$. Then, the method reads as follows:

$$q_{n+1} = q_n + \Delta t p_{n+1}, \qquad p_{n+1} = p_n - \Delta t q_n + \sigma \Delta W_n, \tag{5.8}$$

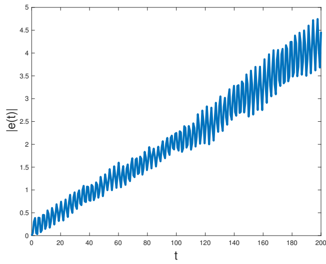
and according to the computations provided in section 3.3, its modified terms are given by (3.21), i.e.,

$$f_q(q,p) = -\frac{1}{2}q, \qquad f_p(q,p) = \frac{1}{2}p.$$

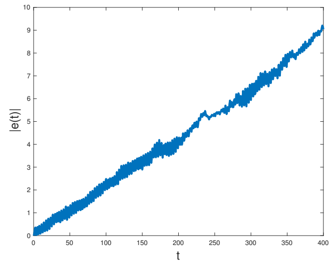
Hence, the corresponding value of α_1 in (3.15) is given by

$$\alpha_1 = -\frac{1}{2}\left(q_0^2 - p_0^2\right).$$

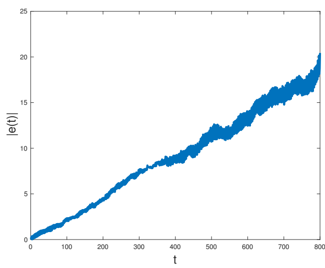
Figure 1 displays and confirms the error growth provided in (5.2) for increasing values of T. Clearly, this growth is more visible as the length of the time windows is increased. In addition, Figure 2 compares the patterns of exact and numerical Hamiltonians, when the stochastic midpoint method (3.23) is applied to the Hamiltonian system (1.4) with quartic potential $V(q) = q^4/4 - q^2/2$ for selected values of the stepsizes. We can observe that for $\Delta t \approx 0.3$, the size of the time window in which the numerical Hamiltonian remains close to the exact one is larger than that obtained for $\Delta t \approx 0.6$.



(a) $T = 200$

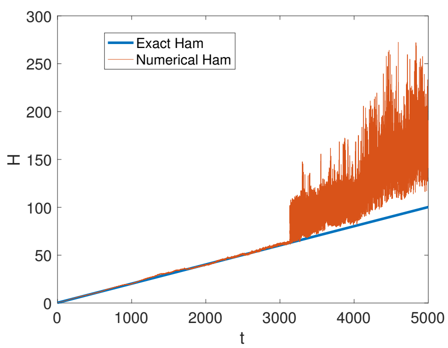


(b) $T = 400$

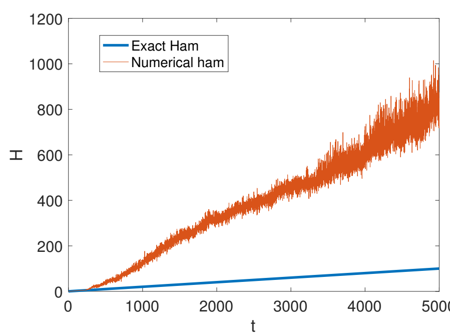


(c) $T = 800$

FIG. 1. *Linear error growth of the error* (5.2) *for the symplectic Euler method* (5.8) *applied to* (1.4) *with potential* $V = q^2/2$ *averaging on* $M = 5000$ *paths for selected values of* T. *The simulation has been performed in a fixed stepsize environment with* $\Delta t = 0.7812$.



(a) $\Delta t = 0.3$



(b) $\Delta t = 0.6$

FIG. 2. *Comparison between exact and numerical Hamiltonian averaged paths for the stochastic midpoint Runge–Kutta method* (3.23) *applied to* (1.4) *with quartic potential* $V = q^4/4 - q^2/2$ *for* $T = 5000$. *The simulation has been performed with selected stepsizes.*

6. Long-term analysis for Stratonovich Hamiltonian systems. We now aim to perform an analogous long-term analysis of time discretizations to Stratonovich Hamiltonian systems (1.7). Let us also recall that, in what follows, we assume

$$\mathbb{E}\left[H(q_n, p_n)\right] = H(q_0, p_0) + \mathcal{O}\left(\Delta t^r\right). \tag{6.1}$$

In order to analyze the long-term behavior of $\mathbb{E}[H(q_n, p_n)]$, let us consider the modified Stratonovich system

$$\begin{cases} \mathrm{d}\widetilde{q} = \nabla_p H(\widetilde{q},\widetilde{p}) \left(\mathrm{d}t + \widetilde{\Sigma}^{\mathsf{T}} \circ \mathrm{d}W(t)\right) + \Delta t^r f_q(\widetilde{q},\widetilde{p})\mathrm{d}t, \\ \mathrm{d}\widetilde{p} = -\nabla_q H(\widetilde{q},\widetilde{p}) \left(\mathrm{d}t + \widetilde{\Sigma}^{\mathsf{T}} \circ \mathrm{d}W(t)\right) + \Delta t^r f_p(\widetilde{q},\widetilde{p})\mathrm{d}t, \end{cases} \tag{6.2}$$

where the functions $f_q(q,p)$ and $f_p(q,p)$ are the modified terms depending on the specific employed numerical method, satisfying

$$\mathbb{E}\left[H(\widetilde{q}(t_n),\widetilde{p}(t_n))\right] = \mathbb{E}\left[H(q_n,p_n)\right] + \mathcal{O}\left(\Delta t^{r+1}\right). \tag{6.3}$$

We are now ready to state the following theorem, representing the main novelty of this paper.

THEOREM 6.1. *Let us consider the stochastic Stratonovich Hamiltonian system* (1.8)*, and let* (q_n,p_n)*,* $n = 1,2,\ldots,N$*, be any numerical approximation to* (1.7)*, computed with the fixed stepsize* $\Delta t = T/N$*, such that* (6.1) *holds true. Then, for any* $n = 1,2,\ldots,N$*, the expected numerical Hamiltonian* $\mathbb{E}[H(q_n,p_n)]$ *satisfies the following estimate:*

$$\begin{aligned} \mathbb{E}\left[H(q_n,p_n)\right] &= H(q_0,p_0) + \mathcal{O}\left(\Delta t^r \mathrm{e}^{C(\sigma)\Delta t^r t_n}\right) + \mathcal{O}\left(\Delta t^{r+1}\right) + \mathcal{O}\left(C(\sigma) t_n \Delta t^r\right) \\ &\quad + \mathcal{O}\left(\Delta t^r t_n\, \mathrm{e}^{C(\sigma)\Delta t^r t_n}\right) + \mathcal{O}\left(C(\sigma)\left(\Delta t^r t_n\right)^2 \mathrm{e}^{C(\sigma)\Delta t^r t_n}\right). \end{aligned} \tag{6.4}$$

Furthermore, the exponential term in (6.4) *remains bounded on intervals of length* $\mathcal{O}(\Delta t^{-r})$*.*

Proof. As previously observed for the Itô case, (6.3) suggests working directly on the continuous object $\mathbb{E}[H(\widetilde{q}(t_n),\widetilde{p}(t_n))]$. To this purpose and according to (6.2), the application of the stochastic chain rule for Stratonovich systems (see, for instance, [20, 23]), leads to

$$\mathrm{d}H(\widetilde{q}(t),\widetilde{p}(t)) = \eta(\widetilde{q}(t),\widetilde{p}(t))\Delta t^r \mathrm{d}t, \tag{6.5}$$

where $\eta(\widetilde{q}(t),\widetilde{p}(t))$ is such that $\eta(q_0,p_0) = \delta_1$, with δ_1 defined in (4.8).

We now assume that there exist a σ-dependent constant $C(\sigma) > 0$ and a function $\ell(q,p)$, both depending on the chosen numerical method, such that the function $\eta(q(t),p(t))$ can be written in the following form (this is, in general, possible after computations):

$$\eta(\widetilde{q}(t),\widetilde{p}(t)) = C(\sigma)H(\widetilde{q}(t),\widetilde{p}(t)) + \ell(\widetilde{q}(t),\widetilde{p}(t)). \tag{6.6}$$

Taking the integral form of (6.5), under (6.6), and passing to side-by-side expectation, we achieve the result

$$\begin{aligned} \mathbb{E}\left[H(\widetilde{q}(t),\widetilde{p}(t))\right] &= H(q_0,p_0) + \Delta t^r \\ &\quad \cdot \left(C(\sigma)\int_0^t \mathbb{E}\left[H(\widetilde{q}(s),\widetilde{p}(s))\right]\mathrm{d}s + \int_0^t \mathbb{E}\left[\ell(\widetilde{q}(s),\widetilde{p}(s))\right]\mathrm{d}s\right). \end{aligned} \tag{6.7}$$

Let us first estimate the term $\mathbb{E}[\ell(\widetilde{q}(t),\widetilde{p}(t))]$. From (6.3) and (6.6), we get

$$\begin{aligned} \mathbb{E}\left[\ell(\widetilde{q}(t),\widetilde{p}(t))\right] &= \mathbb{E}\left[\eta(\widetilde{q}(t),\widetilde{p}(t))\right] - C(\sigma)\mathbb{E}\left[H(\widetilde{q}(t),\widetilde{p}(t))\right] \\ &= \mathbb{E}\left[\eta(\widetilde{q}(t),\widetilde{p}(t))\right] - C(\sigma)\left(\mathbb{E}\left[H(q_n,p_n)\right] + \mathcal{O}\left(\Delta t^{r+1}\right)\right). \end{aligned} \tag{6.8}$$

Moreover, according to (6.1), we obtain

$$\mathbb{E}\left[\ell(\widetilde{q}(t),\widetilde{p}(t))\right] = \mathbb{E}\left[\eta(\widetilde{q}(t),\widetilde{p}(t))\right] - C(\sigma)\left(H(q_0,p_0) + \mathcal{O}\left(\Delta t^r\right)\right). \tag{6.9}$$

Since the left-hand side of (6.5) is $\mathcal{O}(\Delta t^r)$, we can argue from (6.9) that

$$\mathbb{E}\left[\ell(\widetilde{q}(t),\widetilde{p}(t))\right] = \mathcal{O}\left(1\right) + \mathcal{O}\left(\Delta t^r\right). \tag{6.10}$$

As a consequence, (6.7) leads to

$$\mathbb{E}\left[H(\widetilde{q}(t),\widetilde{p}(t))\right] \le H(q_0,p_0) + C(\sigma)\Delta t^r \int_0^t \mathbb{E}\left[H(\widetilde{q}(s),\widetilde{p}(s))\right] \mathrm{d}s + \mathcal{O}\left(t\Delta t^r\right). \tag{6.11}$$

The application of the Grönwall lemma to inequality (6.11) yields

$$\begin{aligned}\mathbb{E}\left[H(\widetilde{q}(t),\widetilde{p}(t))\right] &\le H(q_0,p_0) + \mathcal{O}\left(t\Delta t^r\right)\\ &\quad + C(\sigma)\Delta t^r \mathrm{e}^{C(\sigma)\Delta t^r t}\int_0^t \Big(H(q_0,p_0)+\mathcal{O}\left(s\Delta t^r\right)\Big)\mathrm{e}^{-C(\sigma)\Delta t^r s}\,\mathrm{d}s,\end{aligned}$$

and integrating by parts, we obtain

$$\begin{aligned}\mathbb{E}\left[H(\widetilde{q}(t),\widetilde{p}(t))\right] &\le H(q_0,p_0) + \mathcal{O}\left(t\Delta t^r\right)\\ &\quad + \mathrm{e}^{C(\sigma)\Delta t^r t}\Big[H(q_0,p_0) - \mathrm{e}^{-C(\sigma)\Delta t^r t}\big(H(q_0,p_0)+\mathcal{O}\left(t\Delta t^r\right)\big)\\ &\quad + \mathcal{O}\left(\Delta t^r\right)\int_0^t \mathrm{e}^{-C(\sigma)\Delta t^r s}\,ds\Big]\\ &= H(q_0,p_0)\mathrm{e}^{C(\sigma)\Delta t^r t} + \mathcal{O}\left(t\Delta t^r\right)\\ &\quad + \mathcal{O}\left(\Delta t^r\right)\mathrm{e}^{C(\sigma)\Delta t^r t}\int_0^t \mathrm{e}^{-C(\sigma)\Delta t^r s}\,ds.\end{aligned}$$

Computing the last integral in the above inequality, we can write the last term in the form

$$\mathcal{O}\left(\frac{1}{C(\sigma)}\right)\left[1-\mathrm{e}^{-C(\sigma)\Delta t^r t}\right]\mathrm{e}^{C(\sigma)\Delta t^r t},$$

which, using Taylor series arguments, reads

$$\mathcal{O}\left(\frac{1}{C(\sigma)}\right)\left[C(\sigma)\Delta t^r t + \mathcal{O}\Big(\big(C(\sigma)\Delta t^r t\big)^2\Big)\right]\mathrm{e}^{C(\sigma)\Delta t^r t},$$

that is,

$$\mathcal{O}\left(\Delta t^r t\ \mathrm{e}^{C(\sigma)\Delta t^r t}\right) + \mathcal{O}\left(C(\sigma)\big(\Delta t^r t\big)^2\mathrm{e}^{C(\sigma)\Delta t^r t}\right).$$

Then, we finally obtain

$$\begin{aligned}\mathbb{E}\left[H(\widetilde{q}(t),\widetilde{p}(t))\right] &\le H(q_0,p_0) + H(q_0,p_0)\left(\mathrm{e}^{C(\sigma)\Delta t^r t}-1\right) + \mathcal{O}\left(t\Delta t^r\right)\\ &\quad + \mathcal{O}\left(\Delta t^r t\ \mathrm{e}^{C(\sigma)\Delta t^r t}\right) + \mathcal{O}\left(C(\sigma)\big(\Delta t^r t\big)^2\mathrm{e}^{C(\sigma)\Delta t^r t}\right).\end{aligned}$$

Since $\mathrm{e}^{C(\sigma)\Delta t^r t}-1 = \mathcal{O}(C(\sigma)\Delta t^r t) + \mathcal{O}(\Delta t^r \mathrm{e}^{C(\sigma)\Delta t^r t})$, we end up with

$$\begin{aligned}\mathbb{E}\left[H(\widetilde{q}(t),\widetilde{p}(t))\right] &\le H(q_0,p_0) + \mathcal{O}\left(\Delta t^r \mathrm{e}^{C(\sigma)\Delta t^r t}\right) + \mathcal{O}\big(C(\sigma)\Delta t^r t\big)\\ &\quad + \mathcal{O}\left(\Delta t^r t\ \mathrm{e}^{C(\sigma)\Delta t^r t}\right) + \mathcal{O}\left(C(\sigma)\big(\Delta t^r t\big)^2\mathrm{e}^{C(\sigma)\Delta t^r t}\right).\end{aligned} \tag{6.12}$$

Equation (6.4) arises from the evaluation of (6.12) in t_n and taking into account (6.3). The boundedness of the exponential term in (6.4) on intervals of length $\mathcal{O}(\Delta t^{-r})$ straightforwardly derives from (6.4) itself, taking into account that $C(\sigma)$ is independent of Δt. ∎

It is worth observing that, for several numerical methods, it is always possible to compute (6.6) in terms of algebraic computations, as discussed in an example reported in the conclusion of this paper. Moreover, although we may not have unicity in the determination of the σ-dependent coefficient C and, hence, in the definition of the function ℓ, its choice does not affect the qualitative trend of the numerical discretization.

Theorem 6.1 gives information on the long-term behavior of a given numerical solution (q_n, p_n) to Stratonovich Hamiltonian systems (1.8) and, to some extent, this result can be seen as a stochastic analogue of the well-known Benettin–Giorgilli theorem for deterministic Hamiltonians (see [18], section IX, Theorem 8.1). Equation (6.4) reveals the presence of an exponential growth in the numerical Hamiltonian, whose exponent depends on the values of r and $C(\sigma) > 0$. Moreover, it is worth observing that the length of the interval where such an exponential term remains bounded also depends on the parameter σ dictating the amplitude of the stochastic term in (1.8).

6.1. Numerical experiments. In order to confirm the results arising from the previous section, let us provide the numerical evidence arising from the application of selected numerical methods to the double-well potential Stratonovich problem [8, 9, 11], i.e., (1.8) with quartic potential given by

$$V(q,p) = \frac{1}{4}q^4 - \frac{1}{2}q^2, \tag{6.13}$$

leading to the Hamiltonian function (1.3)

$$H(q,p) = \frac{1}{2}p^2 + V(q) = \frac{1}{2}p^2 + \frac{1}{4}q^4 - \frac{1}{2}q^2 \tag{6.14}$$

and the corresponding Stratonovich Hamiltonian system (1.8)

$$\begin{cases} dq = p\,(\mathrm{d}t + \sigma \circ \mathrm{d}W(t)), \\ dp = -(q^3 - q)\,(\mathrm{d}t + \sigma \circ \mathrm{d}W(t)). \end{cases} \tag{6.15}$$

6.1.1. Energy-preserving method. We first consider the stochastic energy-preserving method (4.22), recalling that, for $\sigma = 0$, it is capable of preserving the quartic Hamiltonian function (6.14) (see [10]). The modified terms, given by (4.23)–(4.24), are

$$f_q(q,p) = -\frac{1}{4}\sigma^4\left(3(3q^2-1)(q^3-q) + 6qp^2\right), \quad f_p(q,p) = -\frac{3}{8}\sigma^4(3q^2-1)^2 p(p-1).$$

We now specialize (6.6) to this case. By definition, we have

$$\begin{aligned} \eta(q,p) &= f_q(q,p)V'(q) + f_p(q,p)p = f_q(q,p)(q^3-q) + f_p(q,p)p \\ &= -\frac{1}{4}\sigma^4(q^3-q)\left[3(3q^2-1)(q^3-q) + 6qp^2\right] - \frac{3}{8}\sigma^4(p^3-p^2)(3q^2-1)^2 \\ &= A(q,p) + \frac{3}{8}\sigma^4 p^2 - \frac{3}{4}\sigma^4 q(q^3-q), \end{aligned}$$

where

$$A(q,p) = -\frac{3}{8}\sigma^4\left[p^3(3q^2-1)^2 - p^2q^2(5q^2-2) + 2q^4(q^2-1)(3q^2-4)\right].$$

Moreover, we have

$$\frac{3}{8}\sigma^4 p^2 - \frac{3}{4}\sigma^4 q(q^3 - q) = \frac{3}{4}\sigma^4 H(q,p) + \frac{3}{8}\sigma^4 q^2\left(3 - \frac{5}{2}q^2\right).$$

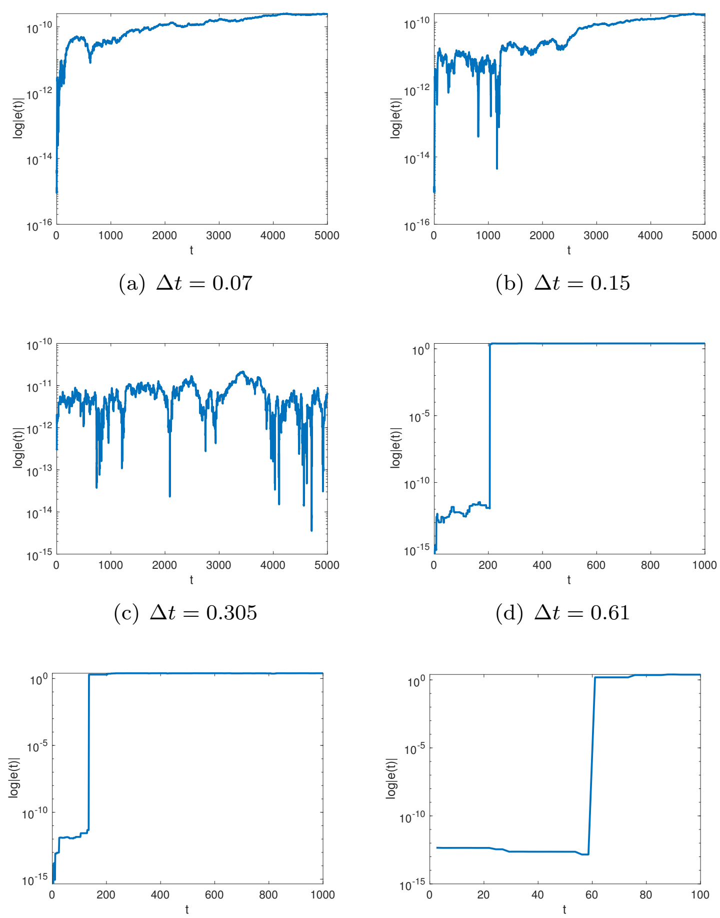
Thus, we end up with

$$\eta(q,p) = \frac{3}{4}\sigma^4 H(q,p) + A(q,p) + \frac{3}{8}\sigma^4 q^2\left(3 - \frac{5}{2}q^2\right).$$

Therefore, method (4.22) applied to the Stratonovich system (6.15) satisfies (6.6) with

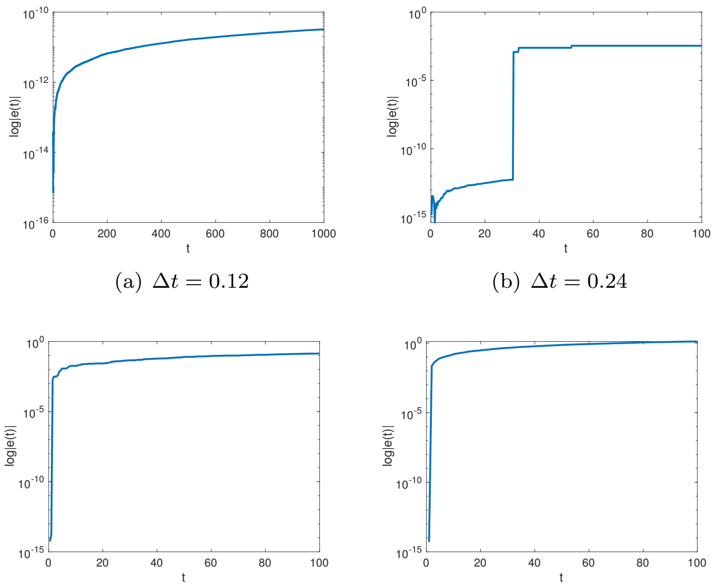
$$C(\sigma) = \frac{3}{4}\sigma^4, \qquad \ell(q,p) = A(q,p) + \frac{3}{8}\sigma^4 q^2\left(3 - \frac{5}{2}q^2\right). \tag{6.16}$$

The pattern depicted in Figure 3 shows the time evolution of the absolute value of the Hamiltonian error given by $e(t_n) = H(q_n,p_n) - H(q_0,p_0)$ for selected values



(a) $\Delta t = 0.07$ (b) $\Delta t = 0.15$ (c) $\Delta t = 0.305$ (d) $\Delta t = 0.61$ (e) $\Delta t = 1.22$ (f) $\Delta t = 2.44$

Fig. 3. *Time evolution of the Hamiltonian deviation* $|e(t)|$ *associated to* (4.22) *applied to the double-well potential problem* (6.15) *for selected values of the stepsize* Δt*. Here,* $\sigma = 1, q_0 = 2$*, and* $p_0 = 1$*. The y-axes are displayed in logarithmic scale.*



(a) $\Delta t = 0.12$ (b) $\Delta t = 0.24$

(c) $\Delta t = 0.48$ (d) $\Delta t = 0.96$

FIG. 4. *Expected error* $|\mathbb{E}[H(q_n, p_n)] - H(q_0, p_0)|$ *associated to* (4.22)*, applied to the double-well potential problem* (6.15) *for selected values of* Δt*. Here,* $\sigma = 1, q_0 = 2$*, and* $p_0 = 1$*. The y-axes are displayed in logarithmic scale. The average has been computed over* $M = 1000$ *paths.*

of Δt, confirming the exponential error growth provided in Theorem 6.1 and the boundedness over intervals of length $\mathcal{O}(\Delta t^{-1})$. Indeed, halving the stepsize makes the interval where the error bounded twice as big. Similarly, Figure 4 shows the growth of the expected error in time for selected values of the stepsize.

6.1.2. Symplectic Runge–Kutta method. Regarding the symplectic Runge–Kutta method (4.15)–(4.16) applied to (6.15), the modified terms (4.20)–(4.21) are given by

$$f_q(q,p) = \frac{3}{4}\sigma^2 \left[p - (3q^2-1)p + \sigma^2(3q^2-1)(q^3-q) - 6\sigma^2 q p^2\right]$$

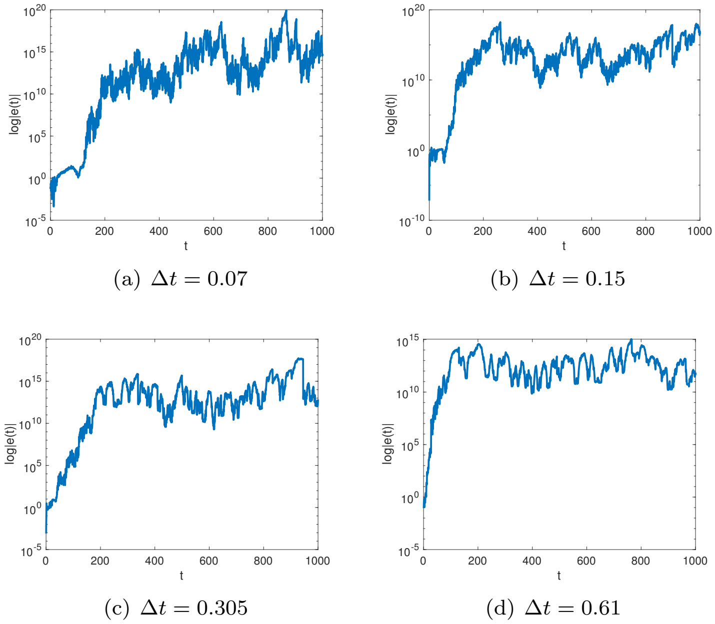
and

$$f_p(q,p) = \frac{3}{4}\sigma^2 q\ p^2 - \frac{3}{8}\sigma^4 \left[(3q^2-1)^2 p - p^3 - (3q^2-1)p\right].$$

Furthermore,

$$C(\sigma) = 6\sigma^4. \tag{6.17}$$

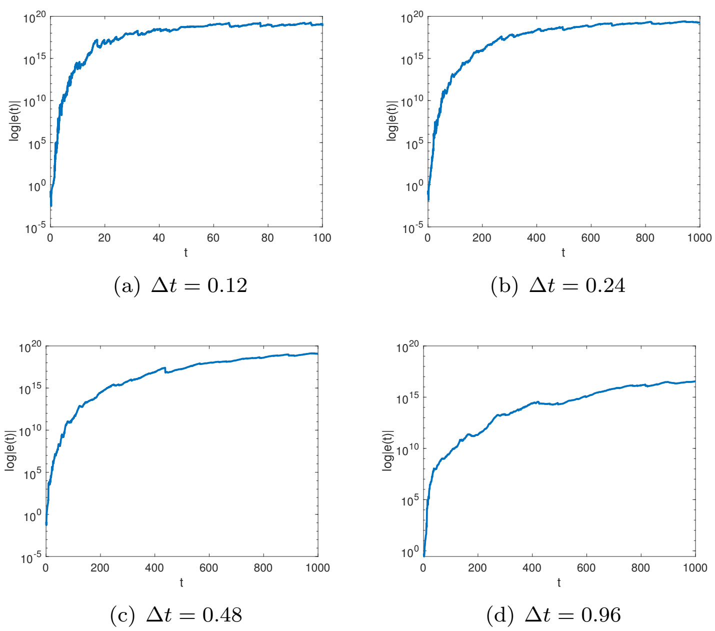
The numerical evidence is shown in Figures 5–6. Specifically, in Figure 5, a single realization has been provided, while in Figure 6 the average over $M = 1000$ paths has been displayed. Figure 5 confirms the analysis provided in Theorem 6.1 and the sharpness of the $\mathcal{O}(\Delta t^{-1})$ estimate. Moreover, the factor $C(\sigma)$ in (6.17) is larger than that defined in (6.16) and, as a consequence, the growth of the Hamiltonian error for the symplectic Runge–Kutta method (4.15)–(4.16) is faster than that for (4.22).



(a) $\Delta t = 0.07$ (b) $\Delta t = 0.15$

(c) $\Delta t = 0.305$ (d) $\Delta t = 0.61$

FIG. 5. *Time evolution of the Hamiltonian deviation* $|e(t)| = |H(q_n, p_n) - H(q_0, p_0)|$ *associated to the symplectic Runge–Kutta method* (4.15)–(4.16) *applied to the double-well potential problem* (6.15) *for selected values of the stepsize. Here,* $\sigma = 1$, $q_0 = 2$, *and* $p_0 = 1$. *The y-axes are shown in logarithmic scale.*



(a) $\Delta t = 0.12$ (b) $\Delta t = 0.24$

(c) $\Delta t = 0.48$ (d) $\Delta t = 0.96$

FIG. 6. *Expected error* $|e(t)| = |\mathbb{E}[H(q_n, p_n)] - H(q_0, p_0)|$ *associated to the symplectic Runge–Kutta method* (4.15)–(4.16) *applied to the double-well potential problem* (6.15). *Here,* $\sigma = 1, q_0 = 2$, *and* $p_0 = 1$. *The y-axes are displayed in logarithmic scale. The average has been computed over* $M = 1000$ *paths.*

7. Conclusions. In this work, we provided long-term estimates characterizing the numerical preservation of the Hamiltionian function for both Itô (1.4) and Stratonovich Hamiltonian systems (1.7). In particular, in the case of Itô Hamiltonian systems, the analysis has been performed with reference to the preservation of invariance trace law (1.5) while, for Stratonovich Hamiltonian problems, the long-term numerical conservation of the Hamiltonian function (1.3) is analyzed. A key ingredient in our analysis is given by the computation of the modified terms in both scenarios and for several selected numerical schemes. Subsequently, the analysis has led to long-term estimates for the error growth in time: for Itô Hamiltonian problems, (5.2) shows a linear error growth in time; in the Stratonovich case, (6.4) reveals the presence of an exponential term that remains bounded only on intervals of length $\mathcal{O}(\Delta t^{-r})$. Finally, selected numerical experiments confirm the effectiveness of our analysis.

Appendix A. Modified differential equations for the Euler–Maruyama method in the two-dimensional case. As an example arising from the arguments contained in section 4.2, we compute the coefficient $\widetilde{\alpha}_1$ in the case of the Euler–Maruyama method applied to (4.9) with $m=2$. The method reads as follows:

$$
\begin{aligned}
q^1 &= q^0 + \Delta t\left[p^0 - \frac{\widetilde{\sigma}}{2}\nabla_q V(q^0)\right] + p^0\widetilde{\Sigma}^{\mathsf{T}}\Delta W_0,\\
p^1 &= p^0 - \Delta t\left[\nabla_q V(q^0) + \frac{\widetilde{\sigma}}{2}\nabla_{qq}V(q^0)p^0\right] - \nabla_q V(q^0)\widetilde{\Sigma}^{\mathsf{T}}\Delta W_0.
\end{aligned}
\tag{A.1}
$$

It is possible to show that the Euler–Maruyama method (A.1) satisfies (4.30) with

$$
\begin{aligned}
\gamma_1 &= \frac{1}{2}\left[{p^0}^{\mathsf{T}}\nabla_{qq}V(q^0) + \frac{\widetilde{\sigma}^2}{4}{p^0}^{\mathsf{T}}\left(\nabla_{qq}V(q^0)\right)^2\right]p^0\\
&+ \frac{1}{2}\left[\frac{\widetilde{\sigma}^2}{4}\nabla_q V(q^0)^{\mathsf{T}}\nabla_{qq}V(q^0) + \nabla_q V(q^0)^{\mathsf{T}}\right]\nabla_q V(q^0)\\
&+ \frac{\widetilde{\sigma}}{2}p_i^0\sum_{i=1}^{2}\frac{\partial^3 V(q^0)}{\partial q_i^3}\tau_i p_i^0 + \frac{\alpha(\widetilde{\Sigma})}{12}\frac{\partial^4 V(q^0)}{\partial q_i^4}\left(p_i^0\right)^3 + \frac{\widetilde{\sigma}}{2}\frac{\partial^3 V(q^0)}{\partial q_i^2\partial q_j}\left(p_i^0\tau_j + 2p_j^0\tau_i\right)\\
&+ \alpha(\widetilde{\Sigma})\left[\frac{1}{3}\frac{\partial^4 V(q^0)}{\partial q_i^3\partial q_j}\left(p_i^0\right)^3 p_j^0 + \frac{1}{2}\frac{\partial^4 V(q^0)}{\partial q_i^2\partial q_j^2}p_i^0\left(p_j^0\right)^2\right], \quad j = i + (-1)^{i+1},
\end{aligned}
$$

where

$$
\tau_k = p_k^0 - \frac{\widetilde{\sigma}}{2}\frac{\partial V(q^0)}{\partial q_k}, \quad \alpha(\widetilde{\Sigma}) = 3\sum_{j=1}^{d}\sigma_j^4 + \sum_{\substack{j,k=1\\ j\neq k}}^{d}\sigma_j^2\sigma_k^2.
$$

In case of quadratic potential, i.e., if $V(q,p) = q^{\mathsf{T}}q/2$, then γ_1 reduces to

$$
\gamma_1 = \frac{1}{2}\left(1 + \frac{1}{4}\widetilde{\sigma}^2\right)\left[{p^0}^{\mathsf{T}}p^0 + {q^0}^{\mathsf{T}}q^0\right] = \left(1 + \frac{1}{4}\widetilde{\sigma}^2\right)H(q^0,p^0).
\tag{A.2}
$$

Comparing the expression in (A.2) with (4.11), we get the modified terms for the Euler–Maruyama method (A.1), in case of quadratic Hamiltonians, given by $f_q(q,p) = \lambda q,\ f_p(q,p) = \lambda p$, where $\lambda = \frac{1}{2}\left[\frac{1}{4}\widetilde{\sigma}^2 + 1\right]$. For general separable Hamiltonians (1.3), the following choice fulfills (4.7):

$$f_q(q,p) = \frac{1}{2}\left(\frac{1}{4}\widetilde{\sigma}^2 \nabla_{qq} V(q) + \mathcal{I}\right)\nabla_q V(q),$$

$$\begin{aligned} f_{p_k}(q,p) = \frac{1}{2}\Bigg[\sum_{i=1}^{2} p_i^0 \left(\frac{\partial^2 V(q^0)}{\partial q_i \partial q_k} + \frac{1}{4}\widetilde{\sigma}^2 \sum_{j=1}^{2} \frac{\partial^2 V(q^0)}{\partial q_i \partial q_j}\frac{\partial^2 V(q^0)}{\partial q_j \partial q_k}\right)\Bigg] \\ + \frac{1}{2}\widetilde{\sigma}\frac{\partial^3 V(q^0)}{\partial q_k^3}\tau_k p_k^0 + \frac{\alpha(\widetilde{\Sigma})}{24}\frac{\partial^4 V(q^0)}{\partial q_k^4}\left(p_k^0\right)^3 + \frac{1}{2}\widetilde{\sigma}\frac{\partial^3 V(q^0)}{\partial q_k^2 \partial q_l}\left[p_k^0 \tau_l + 2p_l^0 \tau_k\right] \\ + \frac{1}{2}\alpha(\widetilde{\Sigma})\left[\frac{1}{3}\frac{\partial^4 V(q^0)}{\partial q_k^3 \partial q_l}\left(p_k^0\right)^2 p_l^0 + \frac{1}{2}\frac{\partial^4 V(q^0)}{\partial q_k^2 \partial q_l^2}\left(p_l^0\right)^2 p_k^0\right], \end{aligned}$$

where $k = 1, 2$ and $l = k + (-1)^{k+1}$.

Appendix B. Proof of (4.8). Let us write the modified system (4.4) as

$$\mathrm{d}\widetilde{X}(t) = F(\widetilde{X}(t))\mathrm{d}t + G(\widetilde{X}(t)) \circ \mathrm{d}W(t),$$

where $\widetilde{X}(t) = \begin{bmatrix}\widetilde{q} \\ \widetilde{p}\end{bmatrix} \in \mathbb{R}^{2m}$, while F and G are given by

$$F = \begin{bmatrix} \nabla_p H + \frac{\widetilde{\sigma}}{2}\left[\nabla_{qp} H \nabla_p H - \nabla_{pp} H \nabla_q H\right] \\ -\nabla_q H + \frac{\widetilde{\sigma}}{2}\left[\nabla_{pq} H \nabla_q H - \nabla_{qq} \nabla_p H\right] \end{bmatrix} + \Delta t^r \begin{bmatrix} f_q \\ f_p \end{bmatrix} \in \mathbb{R}^{2m} \tag{B.1}$$

and

$$G = \begin{bmatrix} \nabla_p H\ \widetilde{\Sigma}^{\mathsf{T}} \\ -\nabla_q H\ \widetilde{\Sigma}^{\mathsf{T}} \end{bmatrix} \in \mathbb{R}^{2m \times d}, \tag{B.2}$$

all evaluated at $\widetilde{X}$. Then, we have

$$\begin{aligned} F^{\mathsf{T}} \nabla H = \frac{1}{2}\widetilde{\sigma}\Big[\left(\nabla_{qp} H \nabla_q H\right)^{\mathsf{T}} \nabla_q H - \left(\nabla_{pp} H \nabla_q H\right)^{\mathsf{T}} \nabla_q H \\ + \left(\nabla_{qp} H \nabla_p H\right)^{\mathsf{T}} \nabla_p H - \left(\nabla_{qq} H \nabla_p H\right)^{\mathsf{T}} \nabla_p H\Big] \\ + \Delta t^r \left(f_q^{\mathsf{T}} \nabla_q H + f_p^{\mathsf{T}} \nabla_p H\right) \end{aligned} \tag{B.3}$$

and

$$GG^{\mathsf{T}} = \widetilde{\sigma}\begin{bmatrix} \nabla_p H \nabla_p H^{\mathsf{T}} & -\nabla_p H \nabla_q H^{\mathsf{T}} \\ -\nabla_q H \nabla_p H^{\mathsf{T}} & \nabla_q H \nabla_q H^{\mathsf{T}} \end{bmatrix}, \quad \nabla^2 H = \begin{bmatrix} \nabla_{qq} H & \nabla_{qp} H \\ \nabla_{qp} H & \nabla_{pp} H \end{bmatrix}.$$

Moreover,

$$\begin{aligned} \mathrm{Tr}\left(GG^{\mathsf{T}} \nabla^2 H\right) = \widetilde{\sigma}\big[\mathrm{Tr}\left(\nabla_p H \nabla_p H^{\mathsf{T}} \nabla_{qq} H - \nabla_p H \nabla_q H^{\mathsf{T}} \nabla_{qp} H\right) \\ + \mathrm{Tr}\left(\nabla_q H \nabla_p H^{\mathsf{T}} \nabla_{qp} H - \nabla_q H \nabla_q^{\mathsf{T}} \nabla_{pp} H\right)\big]. \end{aligned} \tag{B.4}$$

Taking into account (B.3) and (B.4), we need to show that

$$F^{\mathsf{T}}\nabla H+\frac{1}{2}\mathrm{Tr}\left(GG^{\mathsf{T}}\nabla^2 H\right)=\Delta t^r\left[f_q^{\mathsf{T}}\nabla_q H+f_p^{\mathsf{T}}\nabla_p H\right]. \tag{B.5}$$

We have

$$\begin{aligned}\mathrm{Tr}\left(\nabla_p H\nabla_p H^{\mathsf{T}}\nabla_{qq}H\right)&=\sum_{i=1}^m\left(\nabla_p H\nabla_p H^{\mathsf{T}}\nabla_{qq}H\right)_{ii}\\&=\sum_{i=1}^m\sum_{k=1}^m\left(\nabla_p H\nabla_p H^{\mathsf{T}}\right)_{ik}\nabla_{qq}H_{ki}\\&=\sum_{i,k=1}^m\frac{\partial H}{\partial p_i}\frac{\partial H}{\partial p_k}\frac{\partial^2 H}{\partial q_i\partial q_k}\end{aligned} \tag{B.6}$$

and

$$\begin{aligned}\left(\nabla_{qq}H\nabla_p H\right)^{\mathsf{T}}\nabla_p H&=\sum_{i=1}^m\left(\nabla_{qq}H\nabla_p H\right)_i\left(\nabla_p H\right)_i\\&=\sum_{i=1}^m\sum_{k=1}^m\nabla_{qq}H_{ik}\nabla_p H_k\nabla_P H_i\\&=\sum_{i,k=1}^m\frac{\partial^2 H}{\partial q_i\partial q_k}\frac{\partial H}{\partial p_i}\frac{\partial H}{\partial p_k}.\end{aligned} \tag{B.7}$$

Then, by (B.6) and (B.7), we have

$$\mathrm{Tr}\left(\nabla_p H\nabla_p H^{\mathsf{T}}\nabla_{qq}H\right)=\left(\nabla_{qq}H\nabla_p H\right)^{\mathsf{T}}\nabla_p H. \tag{B.8}$$

In a similar manner,

$$\begin{aligned}\mathrm{Tr}\left(\nabla_p H\nabla_q H^{\mathsf{T}}\nabla_{qp}H\right)&=\sum_{i=1}^m\left(\nabla_p H\nabla_q H^{\mathsf{T}}\nabla_{qp}H\right)_{ii}\\&=\sum_{i=1}^m\sum_{k=1}^m\left(\nabla_p H\nabla_q H^{\mathsf{T}}\right)_{ik}\nabla_{qp}H_{ki}\\&=\sum_{i,k=1}^m\frac{\partial H}{\partial p_i}\frac{\partial H}{\partial q_k}\frac{\partial^2 H}{\partial q_k\partial p_i}=\left(\nabla_{qp}H\nabla_q H\right)^{\mathsf{T}}\nabla_p H.\end{aligned} \tag{B.9}$$

Then, (B.5) holds true thanks to (B.8)–(B.9) and applying similar computations to all terms in (B.5), taking (B.3) and (B.4) into account.

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