SIAM J. NUMER. ANAL.
Vol. 63, No. 2, pp. 1000–1024

A NEW CLASS OF SPLITTING METHODS THAT PRESERVE ERGODICITY AND EXPONENTIAL INTEGRABILITY FOR THE STOCHASTIC LANGEVIN EQUATION*

CHUCHU CHEN†, TONGHE DANG‡, JIALIN HONG†, AND FENGSHAN ZHANG§

Abstract. In this paper, we propose a new class of splitting methods to solve the stochastic Langevin equation, which can simultaneously preserve the ergodicity and exponential integrability of the original equation. The central idea is to extract a stochastic subsystem that possesses the strict dissipation from the original equation, which is inspired by the inheritance of the Lyapunov structure for obtaining the ergodicity. We prove that the exponential moment of the numerical solution is bounded, thus validating the exponential integrability of the proposed methods. Further, we show that under moderate verifiable conditions, the methods have the first-order convergence in both strong and weak senses, and we present several concrete splitting schemes based on the methods. The splitting strategy of methods can be readily extended to construct conformal symplectic methods and high-order methods that preserve both the ergodicity and the exponential integrability, as demonstrated in numerical experiments. Our numerical experiments also show that the proposed methods have good performance in the long-time simulation.

Key words. stochastic Langevin equation, splitting method, ergodicity, exponential integrability, convergence

MSC codes. 60H35, 65C30, 37M25

DOI. 10.1137/24M1687686

1. Introduction.

In this paper, we study the construction and numerical analysis of splitting methods that preserve intrinsic properties of the following stochastic Langevin equation:

$$\begin{cases} dP(t) = -\upsilon P(t)dt - \nabla U(Q(t))dt + \sigma dW_t, \\ dQ(t) = P(t)dt, \end{cases} \tag{1.1}$$

where the initial value $(P(0), Q(0)) \in \mathbb{R}^2$ is deterministic, $\upsilon > 0$ is the friction coefficient, $\sigma > 0$ is the diffusion coefficient, $U > 0$ is the potential function which may exhibit superquadratic growth, and W_t is a one-dimensional standard Wiener process on a filtered complete probability space $(\Omega, \mathcal{F}, \{\mathcal{F}_t\}_{t\geq 0}, \mathbb{P})$. For simplicity, we consider the $\mathbb{R}^2$-valued solution of (1.1), and, in fact, our results hold for the general

*Received by the editors August 26, 2024; accepted for publication (in revised form) February 11, 2025; published electronically April 28, 2025.
https://doi.org/10.1137/24M1687686
Funding: This work was funded by the National Key R&D Program of China (grants 2024YFA1015900 and 2020YFA0713701), the National Natural Science Foundation of China (grants 12031020, 12461160278, and 12471386), and the Youth Innovation Promotion Association CAS.
†LSEC, ICMSEC, Academy of Mathematics and Systems Science, Chinese Academy of Sciences, Beijing 100190, People's Republic of China, and School of Mathematical Sciences, University of Chinese Academy of Sciences, Beijing 100049, People's Republic of China (chenchuchu@lsec.cc.ac.cn, hjl@lsec.cc.ac.cn).
‡Academy of Mathematics and Systems Science, Chinese Academy of Sciences, Beijing 100190, People's Republic of China, and Department of Applied Mathematics, The Hong Kong Polytechnic University, Hung Hom, Kowloon, Hong Kong, People's Republic of China (tonghe.dang@polyu.edu.hk).
§Corresponding author. LSEC, ICMSEC, Academy of Mathematics and Systems Science, Chinese Academy of Sciences, Beijing 100190, People's Republic of China (zhangfs23@lsec.cc.ac.cn).

$\mathbb{R}^{2d}$ case. The dynamical variables $Q(t)$ and $P(t)$ denote the position and momentum of a Hamiltonian system with the energy function

$$H_0(p,q)=\frac{p^2}{2}+U(q). \tag{1.2}$$

The stochastic Langevin equation has wide applications in many fields, such as chemical interactions, molecular simulations, and quantum systems; see, e.g., [7, 11]. For instance, it is a fundamental model for describing the behavior of microscopic particles in statistical physics systems, capturing the dynamic characteristics of particles under the influence of random collisions from surrounding molecules.

1.1. Ergodicity and exponential integrability. It is known that the dynamical system generated by (1.1) is ergodic; i.e., for all smooth test functions g,

$$\lim_{T\to\infty}\frac{1}{T}\int_0^T \mathbb{E}[g(P(t),Q(t))]dt=\int_{\mathbb{R}^2} g(p,q)\pi(dp,dq) \text{ in } L^2(\mathbb{R}^2;\pi),$$

which is proved by the uniform moment boundedness and the Hörmander condition for the solution. Here, π is the unique invariant measure, which is characterized by the Gibbs density function, $\pi(dp,dq)=\frac{1}{Z}e^{-\frac{2v}{\sigma^2}H_0(p,q)}dpdq$, where Z is a normalization constant to ensure that $\int_{\mathbb{R}^2}\pi(dp,dq)=1$; see, e.g., [19]. Ergodicity describes the unity between state space and time, implying that the long-time behavior of the stochastic process can be effectively captured by the invariant measure. The integral $\int_{\mathbb{R}^2} g(p,q)\pi(dp,dq)=:\pi(g)$, often referred to as the ergodic limit, is closely related to some important macroscopic physical quantities in practical applications. Thus, approximating the ergodic limit becomes crucial for predicting these physical quantities. A fundamental approach to approximating the ergodic limit is by constructing numerical methods that preserve the ergodicity of (1.1), which ensures that the true statistical properties of the solution process can be accurately reflected by numerical solutions.

Exponential integrability is an important property that helps in establishing theoretical analysis of systems across various fields, including stability analysis and large deviation theory; see, e.g., [8] and the references therein. When the potential U is a polynomial of even order, (1.1) is proved to admit the exponential integrability, i.e.,

$$\sup_{t\in[0,T]}\mathbb{E}\left[\exp\left\{\frac{C_1H_0(P(t),Q(t))}{e^{\sigma^2 t}}\right\}\right]\le e^{C_2(T+1)+H_0(P_0,Q_0)}, \tag{1.3}$$

where $C_1,C_2>0$ are some generic constants. We give the detailed proof in Appendix A. For SDEs with the nonmonotone-type condition, for example, (1.1) with U being of superquadratic growth, it is important to ensure the preservation of exponential integrability for numerical methods. This enables establishing a positive strong convergence order for the numerical solution; see, e.g., [10, 15].

Therefore, for (1.1) with the superquadratically growing U, the study on numerical methods that preserve both the ergodicity and the exponential integrability is of great importance, as it provides an effective way to accurately capture the essential dynamics of the original system in both theoretical and practical contexts.

1.2. Existing works, motivation, and plan. For the stochastic Langevin equation with the quadratically growing U, there have been many works on the construction and convergence analysis for ergodicity-preserving numerical methods (see, e.g., [1, 2, 12, 13, 16, 17, 18] and the references therein), while for the superquadratic case, the analysis is more technical, and there are only a few works. A pioneering work is [21], where the ergodicity and first-order weak convergence of the implicit Euler scheme are established. For strong convergence analysis, as previously mentioned, exponential integrability of the numerical solution becomes crucial for deriving the convergence order. For example, the authors of [9] prove the exponential integrability of the splitting averaged vector field scheme for (1.1) and establish its strong convergence order. See also [10, 15] for the study of exponential integrability and strong convergence order of a class of stopped increment-tamed Euler approximations for SDEs.

We aim to construct new class of numerical methods of (1.1) that preserve both the ergodicity and the exponential integrability, based on the splitting technique. Splitting techniques are widely recognized as useful tools not only for constructing numerical methods that preserve the properties of the original equation but also for obtaining high-order numerical schemes; see, e.g., [2, 16] and the references therein. In order to describe splitting methods in a convenient way, it is useful to introduce the generators $\mathcal{L}_1 := -\nabla U(q)\nabla_p$, $\mathcal{L}_2 := p\nabla_q$, $\mathcal{L}_3 := -\upsilon p\nabla_p$, and $\mathcal{L}_4 := \frac{1}{2}\sigma^2\Delta_p$. Then the generator of (1.1) is $\mathcal{L} = \mathcal{L}_1 + \mathcal{L}_2 + \mathcal{L}_3 + \mathcal{L}_4$. We use $e^{\tau\mathcal{L}_i}$ to denote the one-step evolution operator of the dynamics generated by $\mathcal{L}_i$ with step size τ.

As for (1.1), one usually splits the original equation into an integrable deterministic Hamiltonian subsystem and a solvable stochastic subsystem. For example, a commonly used splitting of (1.1) has the evolution operator $\mathcal{P}_\tau^{\mathcal{L}_1+\mathcal{L}_2,\mathcal{L}_3+\mathcal{L}_4} := e^{\tau(\mathcal{L}_1+\mathcal{L}_2)}e^{\tau(\mathcal{L}_3+\mathcal{L}_4)}$, which determines the splitting solution $\{(P_\tau(t_n), Q_\tau(t_n))^\top\}_{n\in\mathbb{N}}$ with $t_n := n\tau$. Here, $e^{\tau(\mathcal{L}_1+\mathcal{L}_2)}$ is the one-step evolution operator of the deterministic Hamiltonian subsystem

$$d\begin{pmatrix}\bar{P}(t)\\ \bar{Q}(t)\end{pmatrix} = \begin{pmatrix}-\nabla U(\bar{Q}(t))dt\\ \bar{P}(t)dt\end{pmatrix}, \quad \begin{pmatrix}\bar{P}(t_n)\\ \bar{Q}(t_n)\end{pmatrix} = \begin{pmatrix}P_\tau(t_n)\\ Q_\tau(t_n)\end{pmatrix},$$

whose solution satisfies $H_0(\bar{P}(t_{n+1}), \bar{Q}(t_{n+1})) = H_0(\bar{P}(t_n), \bar{Q}(t_n))$ and where $e^{\tau(\mathcal{L}_3+\mathcal{L}_4)}$ represents that of the stochastic subsystem

$$d\begin{pmatrix}\tilde{P}(t)\\ \tilde{Q}(t)\end{pmatrix} = \begin{pmatrix}-\upsilon\tilde{P}(t)dt + \sigma dW_t\\ 0\end{pmatrix}, \quad \begin{pmatrix}\tilde{P}(t_n)\\ \tilde{Q}(t_n)\end{pmatrix} = \begin{pmatrix}\bar{P}(t_{n+1})\\ \bar{Q}(t_{n+1})\end{pmatrix}, \tag{1.4}$$

whose solution $(\tilde{P}(t_{n+1}), \tilde{Q}(t_{n+1}))^\top = (P_\tau(t_{n+1}), Q_\tau(t_{n+1}))^\top$ satisfies that $\mathbb{E}[\tilde{P}(t_{n+1})^2] = e^{-\upsilon\tau}\mathbb{E}[\tilde{P}(t_n)^2] + \frac{\sigma^2}{2\upsilon}(1-e^{-2\upsilon\tau})$ and $\mathbb{E}[U(\tilde{Q}(t_{n+1}))] = \mathbb{E}[U(\tilde{Q}(t_n))]$. It is known that this splitting admits the exponential integrability (see, e.g., [9]).

The well-known Lyapunov structure for obtaining the ergodicity has the form of

$$\mathbb{E}[\mathcal{V}(P_\tau(t_{n+1}), Q_\tau(t_{n+1}))|\mathcal{F}_{t_n}] \le \alpha\mathcal{V}(P_\tau(t_n), Q_\tau(t_n)) + \beta \tag{1.5}$$

with $\alpha \in (0,1)$ and $\beta > 0$, where $\mathcal{V} > 0$ is the Lyapunov functional. Since the deterministic Hamiltonian subsystem is energy-preserving, a natural choice for the Lyapunov functional is $\mathcal{V} = H_0$. Then it is critical to possess the strict dissipation for the stochastic subsystem to obtain the ergodicity, while for (1.4), it holds that

$$\mathbb{E}[H_0(P_\tau(t_{n+1}), Q_\tau(t_{n+1}))|\mathcal{F}_{t_n}] = \frac{e^{-\upsilon\tau}}{2}\bar{P}(t_{n+1})^2 + U(\bar{Q}(t_{n+1})) + \frac{\sigma^2}{4\upsilon}(1-e^{-2\upsilon\tau}).$$

Thus, there are no parameters $\alpha \in (0,1), \beta > 0$ such that (1.5) holds with the Lyapunov functional H_0, which can also be illustrated by the red line in Figure 1.

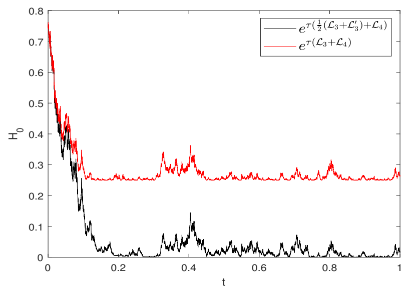


FIG. 1. *Evolution of* $H_0(\tilde{P}(t), \tilde{Q}(t))$.

In order to make the stochastic subsystem strictly dissipative such that the resulting splitting system can inherit the Lyapunov structure, we introduce a new operator $\mathcal{L}_3' := -\upsilon q \nabla_q$. Then we propose a novel splitting strategy as

$$\mathcal{P}_\tau^{\mathcal{L}_1+\mathcal{L}_2+\frac{1}{2}(\mathcal{L}_3-\mathcal{L}_3'),\frac{1}{2}(\mathcal{L}_3+\mathcal{L}_3')+\mathcal{L}_4} := e^{\tau(\mathcal{L}_1+\mathcal{L}_2+\frac{1}{2}(\mathcal{L}_3-\mathcal{L}_3'))}e^{\tau(\frac{1}{2}(\mathcal{L}_3+\mathcal{L}_3')+\mathcal{L}_4)}. \tag{1.6}$$

Precisely, we have

$$d\begin{pmatrix} P(t) \\ Q(t) \end{pmatrix} = \underbrace{\begin{pmatrix} -\frac{\upsilon}{2}P(t) - \nabla U(Q(t)) \\ P(t) + \frac{\upsilon}{2}Q(t) \end{pmatrix} dt}_{\Psi^D} + \underbrace{\begin{pmatrix} -\frac{\upsilon}{2}P(t)dt + \sigma dW_t \\ -\frac{\upsilon}{2}Q(t)dt \end{pmatrix}}_{\Psi^S}, \tag{1.7}$$

where Ψ^D and Ψ^S are flows for the deterministic subsystem and stochastic subsystem, respectively. This new splitting strategy has several advantages:

(i) The deterministic subsystem Ψ^D is still a Hamiltonian system with the new Hamiltonian

$$H(p, q) := H_0(p, q) + \frac{\upsilon}{2}pq. \tag{1.8}$$

Moreover, the new Hamiltonian H is equivalent to the original energy function H_0 in a certain sense; i.e., there exists $C_0 > 0$ such that $C_1 H_0 \le H + C_0 \le C_2(H_0 + 1)$ with some positive constants $C_1 \le C_2$.

(ii) The stochastic subsystem Ψ^S is strictly dissipative (see also the black line in Figure 1) such that the splitting system admits the Lyapunov structure (1.5) with the Hamiltonian H, $\alpha = e^{-\upsilon\tau}$ and some $\beta > 0$. Therefore, the splitting system is uniquely ergodic; see Proposition 2.4.

Based on the proposed splitting strategy (1.7), we construct a new class of splitting methods that can simultaneously preserve the ergodicity and the exponential integrability of (1.1). To be specific, these splitting methods are obtained by applying general conservative methods to the deterministic part and solving the stochastic part exactly. A key ingredient for the ergodicity of the methods is the uniform moment boundedness of numerical solutions over long times. This is achieved by the good balance between the preservation of the Hamiltonian for the deterministic subsystem and the dissipative property for the stochastic subsystem. In addition, this balance brings the exponential integrability of the methods as well, controlling the exponential moment of the numerical solution from explosion over finite time. Combining the stochastic Grönwall inequality, we show that the proposed methods have the first-order strong convergence under some moderate verifiable conditions on the one-step approximation. Moreover, leveraging the Kolmogorov equation and the uniform moment boundedness, we prove the first-order convergence for the ergodic limit of the proposed methods.

Several concrete splitting schemes based on our methods are presented by incorporating the developed conservative methods for deterministic Hamiltonian systems. Then we perform numerical experiments to verify our theoretical results on strong and weak convergence in section 4.1. In addition, as shown by numerical experiments, the proposed splitting methods have the good ability to simulate the ergodic limit of the exact solution. As part of our investigation, based on our splitting strategy, we construct the second-order methods that preserve both the ergodicity and the exponential integrability by employing the Strang splitting technique and also present the conformal symplectic methods by applying the symplectic methods for the deterministic Hamiltonian system, which are demonstrated by numerical experiments in sections 4.2 and 4.3.

The rest of the paper is organized as follows. In section 2, we introduce the new class of splitting methods and show the inheritance of the ergodicity and the exponential integrability. In section 3, by using the moment properties of the numerical solution, we prove that the strong and weak convergence orders are both 1. In section 4, we present numerical experiments to verify our theoretical results. Appendix A is devoted to some auxiliary proofs.

Throughout this article, we use C to denote a positive constant which may not be the same in each occurrence. More specific constants which depend on certain parameters $a, b, \ldots,$ are numbered as $C(a, b, \ldots)$.

2. A new class of splitting methods.

In this section, we aim to introduce a new class of splitting methods that preserve both the ergodicity and the exponential integrability of (1.1). We take the potential $U(q) := \frac{1}{4}q^4$ in this paper as an example to illustrate the main idea, and we remark that the approach can be extended to the case of general polynomials of even order: $U(q) = \sum_{j=1}^{m} \frac{1}{2j} q^{2j}$ with some integer $m \geq 2$. Some concrete numerical schemes based on our methods are also given. In addition, we present the uniform moment boundedness, ergodicity, and exponential integrability of numerical solutions for proposed methods.

2.1. Construction.

Let $\tau \in (0, 1)$ be the uniform time step-size, and let $t_n := n\tau$, $n \in \mathbb{N}$. Recalling (1.6),

$$\mathcal{P}_\tau^{\mathcal{L}_1+\mathcal{L}_2+\frac{1}{2}(\mathcal{L}_3-\mathcal{L}_3'),\frac{1}{2}(\mathcal{L}_3+\mathcal{L}_3')+\mathcal{L}_4} = e^{\tau(\mathcal{L}_1+\mathcal{L}_2+\frac{1}{2}(\mathcal{L}_3-\mathcal{L}_3'))} e^{\tau(\frac{1}{2}(\mathcal{L}_3+\mathcal{L}_3')+\mathcal{L}_4)},$$

we split (1.1) in the time interval $T_n := [t_n, t_{n+1})$ into a deterministic Hamiltonian system with one-step evolution operator $e^{\tau(\mathcal{L}_1+\mathcal{L}_2+\frac{1}{2}(\mathcal{L}_3-\mathcal{L}_3'))}$ and a linear SDE with one-step evolution operator $e^{\tau(\frac{1}{2}(\mathcal{L}_3+\mathcal{L}_3')+\mathcal{L}_4)}$. The solution of the splitting system is written as

$$X_\tau(t_{n+1}) = \Phi_{T_n}^S \Phi_{T_n}^D (X_\tau(t_n)), \quad n \in \mathbb{N}, \tag{2.1}$$

where $\{\Phi_{T_n}^D(t)\}_{t \in T_n}$ is the flow of the nonlinear Hamiltonian system with random initial datum

$$\begin{cases} d\bar{P}_{T_n}(t) = -\frac{v}{2}\bar{P}_{T_n}(t)dt - \bar{Q}_{T_n}^3(t)dt, & \bar{P}_{T_n}(t_n) = P_\tau(t_n), \\ d\bar{Q}_{T_n}(t) = \bar{P}_{T_n}(t)dt + \frac{v}{2}\bar{Q}_{T_n}(t)dt, & \bar{Q}_{T_n}(t_n) = Q_\tau(t_n), \end{cases} \tag{2.2}$$

and $\{\Phi^S_{T_n}(t)\}_{t\in T_n}$ is the flow of the linear SDE

$$\begin{cases} d\tilde{P}_{T_n}(t) = -\frac{\upsilon}{2}\tilde{P}_{T_n}(t)dt + \sigma dW_t, \quad \tilde{P}_{T_n}(t_n) = \bar{P}_{T_n}(t_{n+1}), \\ d\tilde{Q}_{T_n}(t) = -\frac{\upsilon}{2}\tilde{Q}_{T_n}(t)dt, \quad \tilde{Q}_{T_n}(t_n) = \bar{Q}_{T_n}(t_{n+1}), \end{cases} \tag{2.3}$$

and $X_\tau(t_{n+1}) = (P_\tau(t_{n+1}), Q_\tau(t_{n+1}))^\top = (\tilde{P}_{T_n}(t_{n+1}), \tilde{Q}_{T_n}(t_{n+1}))^\top$. Especially for $t \in T_0$, the initial datum for (2.2) is $(\bar{P}_{T_0}(0), \bar{Q}_{T_0}(0)) = (P(0), Q(0))$. It is observed that for any constant C, $H + C$ is the Hamiltonian of (2.2).

We apply the one-step approximation to (2.2) which preserves the Hamiltonian and solves the linear subsystem (2.3) exactly to obtain a new class of splitting methods. The numerical solution $X_n := (P_n, Q_n)^\top$ is defined recurrently by $(P_0, Q_0) := (P(0), Q(0))$ and

$$X_{n+1} = \Phi^S_{T_n, t_{n+1}} \Upsilon^D_\tau(X_n), \quad n \in \mathbb{N}, \tag{2.4}$$

where Υ^D_τ represents the one-step mapping defined by

$$\begin{cases} \bar{P}_{T_n, t_{n+1}} = P_n + \mathcal{A}^n_\tau, \\ \bar{Q}_{T_n, t_{n+1}} = Q_n + \mathcal{B}^n_\tau \end{cases} \tag{2.5}$$

and $\Phi^S_{T_n,t} := (\tilde{P}_{T_n,t}, \tilde{Q}_{T_n,t})^\top$ denotes the solution of (2.3) at time $t \in T_n$ with initial datum $(\tilde{P}_{T_n,t_n}, \tilde{Q}_{T_n,t_n}) = (\bar{P}_{T_n,t_{n+1}}, \bar{Q}_{T_n,t_{n+1}})$. Here, $\mathcal{A}^n_\tau$ and $\mathcal{B}^n_\tau$ are measurable maps defined, respectively, as $\mathcal{A}^n_\tau := \mathcal{A}_\tau(P_n, Q_n, \bar{P}_{T_n,t_{n+1}}, \bar{Q}_{T_n,t_{n+1}})$ and $\mathcal{B}^n_\tau := \mathcal{B}_\tau(P_n, Q_n, \bar{P}_{T_n,t_{n+1}}, \bar{Q}_{T_n,t_{n+1}})$. In addition, without loss of generality, the conservative method (2.5) is required to be solvable; namely, there exist measurable maps $\psi_\tau, \phi_\tau : \mathbb{R}^2 \to \mathbb{R}$ such that $\bar{P}_{T_n,t_{n+1}} = \psi_\tau(P_n, Q_n)$ and $\bar{Q}_{T_n,t_{n+1}} = \phi_\tau(P_n, Q_n)$.

For the Hamiltonian system, there have been some conservative methods in the literature, such as the average vector field (AVF) method, the discrete-gradient (DG) method, and the partitioned AVF (PAVF) method; see, e.g., [3, 4, 6, 20, 22, 23] and the references therein. Hence, one can obtain a class of splitting schemes via (2.4). This approach to construct numerical schemes has distinct advantages, especially in the intrinsic property-preserving aspect. We will show this in the next subsection.

We give some concrete examples of the splitting method (2.4) based on the conservative methods for the Hamiltonian system:

(i) When the one-step mapping Υ^D_τ in (2.5) is defined by the AVF scheme, which reads as

$$\bar{P}_{T_n,t_{n+1}} = P_n - \frac{\tau\upsilon}{4}(\bar{P}_{T_n,t_{n+1}} + P_n) - \tau\int_0^1 (Q_n + \lambda(\bar{Q}_{T_n,t_{n+1}} - Q_n))^3 d\lambda,$$
$$\bar{Q}_{T_n,t_{n+1}} = Q_n + \frac{\tau}{2}(\bar{P}_{T_n,t_{n+1}} + P_n) + \frac{\tau\upsilon}{4}(\bar{Q}_{T_n,t_{n+1}} + Q_n),$$

the corresponding splitting scheme (2.4) is called the splitting AVF (SAVF) scheme below.

(ii) When the one-step mapping Υ^D_τ in (2.5) is defined by the DG scheme

$$\bar{P}_{T_n,t_{n+1}} = P_n - \tau\bar{\nabla}_q H(\bar{P}_{T_n,t_{n+1}}, \bar{Q}_{T_n,t_{n+1}}; P_n, Q_n),$$
$$\bar{Q}_{T_n,t_{n+1}} = Q_n + \tau\bar{\nabla}_p H(\bar{P}_{T_n,t_{n+1}}, \bar{Q}_{T_n,t_{n+1}}; P_n, Q_n),$$

the corresponding splitting scheme (2.4) is called the splitting DG (SDG) scheme below. Here, $\bar{\nabla} H(\hat{p}, \hat{q}; p, q) := (\bar{\nabla}_p H(\hat{p}, \hat{q}; p, q); \bar{\nabla}_q H(\hat{p}, \hat{q}; p, q))$ is defined as $\bar{\nabla} H(\hat{p}, \hat{q}; p, q) = \nabla H(\bar{p}, \bar{q}) + \frac{H(\hat{p},\hat{q}) - H(p,q) - \nabla H(\bar{p},\bar{q})^T\delta}{\|\delta\|^2}\delta$, where $\delta = (\hat{p} - p; \hat{q} - q)$, $\quad (\bar{p}; \bar{q}) = (\frac{\hat{p}+p}{2}; \frac{\hat{q}+q}{2})$.

(iii) When the one-step mapping Υ_τ^D in (2.5) is defined by the PAVF scheme

$$\bar{P}_{T_n,t_{n+1}} = P_n - \frac{\tau\upsilon}{2}\bar{P}_{T_n,t_{n+1}} - \tau\int_0^1 (Q_n + \lambda(\bar{Q}_{T_n,t_{n+1}} - Q_n))^3 d\lambda,$$
$$\bar{Q}_{T_n,t_{n+1}} = Q_n + \frac{\tau}{2}(\bar{P}_{T_n,t_{n+1}} + P_n) + \frac{\tau\upsilon}{2}Q_n,$$

the corresponding splitting scheme (2.4) is called the splitting PAVF (SPAVF) scheme below.

2.2. Ergodicity and exponential integrability. In this subsection, we first give the uniform moment boundedness of the numerical solution for the proposed splitting method (2.4). Then we prove that the numerical solution is uniquely ergodic and admits the exponential integrability. These properties play an important role in obtaining the strong and weak convergence orders of the proposed methods. Denote $n_s := \max\{n \in \mathbb{N} : t_n \leq s\}$ for $s \geq 0$.

LEMMA 2.1. *For any $\mathfrak{p} \geq 1$ and $T > 0$, there exists a constant $C := C(\mathfrak{p}, T) > 0$ such that*

$$\mathbb{E}\left[\sup_{t\in[0,T]}(|\tilde{P}_{T_{n_t},t}|^{2\mathfrak{p}} + |\tilde{Q}_{T_{n_t},t}|^{4\mathfrak{p}})\right] \leq C(1 + |H(P_0,Q_0)|^{\mathfrak{p}}). \tag{2.6}$$

In addition, there exists a constant $C := C(\mathfrak{p}) > 0$ such that

$$\sup_{n\in\mathbb{N}}\mathbb{E}[|P_n|^{2\mathfrak{p}} + |Q_n|^{4\mathfrak{p}}] \leq C(1 + |H(P_0,Q_0)|^{\mathfrak{p}}). \tag{2.7}$$

The proof of Lemma 2.1 is postponed to Appendix A. The uniform moment boundedness of a numerical solution implies the existence of the numerical invariant measure. Furthermore, we can show that the numerical invariant measure is uniquely ergodic. Before that, it is observed that by the Young inequality, there exists a constant $C_H > 0$ such that $H + C_H \geq 1$. For instance, one can take $C_H = \frac{\upsilon^4}{64} + 1$. Then using the Young inequality twice gives

$$\begin{aligned} H(p,q) + C_H &\geq \frac{p^2}{2} + \frac{q^4}{4} - \frac{\upsilon}{4}\left(\frac{2p^2}{\upsilon} + \frac{\upsilon q^2}{2}\right) + C_H \\ &\geq \frac{q^4}{4} - \frac{\upsilon^2}{16}\left(\frac{4}{\upsilon^2}q^4 + \frac{\upsilon^2}{4}\right) + C_H \geq 1. \end{aligned} \tag{2.8}$$

In addition, there exist constants $C, C_e > 0$ such that

$$C_e(p^2 + q^4) \leq H(p,q) + C \leq C(p^2 + q^4 + 1). \tag{2.9}$$

In fact, this can be obtained by applying the Young inequality as follows:

$$\begin{aligned} H(p,q) &\geq \frac{p^2}{2} + \frac{q^4}{4} - \frac{\upsilon}{4}\left(\frac{p^2}{\upsilon} + \upsilon q^2\right) \geq \frac{p^2}{4} + \frac{1}{4}q^4 - \frac{\upsilon^2}{4}\left(\frac{1}{2\upsilon^2}q^4 + \frac{\upsilon^2}{2}\right) \\ &\geq \frac{1}{8}(p^2 + q^4) - \frac{\upsilon^4}{8}, \\ H(p,q) &\leq \frac{p^2}{2} + \frac{q^4}{4} + \frac{\upsilon}{4}\left(p^2 + \frac{q^4}{2} + \frac{1}{2}\right) \leq \left(\frac{1}{2} + \frac{\upsilon}{4}\right)(p^2 + q^4 + 1). \end{aligned}$$

PROPOSITION 2.2. *For each $\tau \in (0,1)$, the numerical solution $\{(P_n,Q_n)\}_{n\in\mathbb{N}}$ admits a unique invariant measure π_τ. Furthermore, for $\mathfrak{p}\geq 1$, there exist constants $\kappa := \kappa(\mathfrak{p}) \in (0,1)$ and $C := C(\mathfrak{p}) > 0$ such that for any measurable functions g satisfying $|g| \leq (H + C_H)^{\mathfrak{p}}$, it holds that*

$$|\mathbb{E}[g(P_n,Q_n)] - \pi_\tau(g)| \leq C\kappa^n(1 + |H(P_0,Q_0)|^{\mathfrak{p}}).$$

Proof. We first show the ergodicity for the sequence $\{(P_{2n},Q_{2n})\}_{n\in\mathbb{N}}$. By [17, Theorem 2.5], the proof is split into the following two steps, which are related to the Lyapunov condition and the minorization condition, respectively.

Step 1. We show that there exist constants $\alpha \in (0,1)$ and $\beta \in (0,\infty)$ such that

$$\mathbb{E}[H(P_{n+1},Q_{n+1}) + C_H|\mathcal{F}_n] \leq \alpha(H(P_n,Q_n) + C_H) + \beta.$$

In fact, it follows from (2.4) that

$$\begin{aligned}
&H(P_{n+1},Q_{n+1})\\
&\quad = \frac{|P_{n+1}|^2}{2} + \frac{|Q_{n+1}|^4}{4} + \frac{\upsilon}{2}P_{n+1}Q_{n+1}\\
&\quad = e^{-\upsilon\tau}\Bigg(\frac{1}{2}|\bar{P}_{T_n,t_{n+1}}|^2 + \frac{1}{4}e^{-\upsilon\tau}|\bar{Q}_{T_n,t_{n+1}}|^4 + \frac{\upsilon}{2}\bar{P}_{T_n,t_{n+1}}\bar{Q}_{T_n,t_{n+1}}\\
&\qquad + \frac{1}{2}\left|\int_{t_n}^{t_{n+1}} e^{-\frac{\upsilon}{2}(t_{n+1}-t)}\sigma dW_t\right|^2 e^{\upsilon\tau} + e^{\frac{\upsilon\tau}{2}}\bar{P}_{T_n,t_{n+1}}\int_{t_n}^{t_{n+1}} e^{-\frac{\upsilon}{2}(t_{n+1}-t)}\sigma dW_t\\
&\qquad + \frac{\upsilon}{2}e^{\frac{\upsilon\tau}{2}}\bar{Q}_{T_n,t_{n+1}}\int_{t_n}^{t_{n+1}} e^{-\frac{\upsilon}{2}(t_{n+1}-t)}\sigma dW_t\Bigg).
\end{aligned}$$

Noting that $(\bar{P}_{T_n,t_{n+1}},\bar{Q}_{T_n,t_{n+1}})^\top$ is $\mathcal{F}_{t_n}$-measurable, which is independent of the increment $\int_{t_n}^{t_{n+1}} e^{-\frac{\upsilon}{2}(t_{n+1}-t)}\sigma dW_t$, we obtain

$$\begin{aligned}
\mathbb{E}[H(P_{n+1},Q_{n+1})|\mathcal{F}_{t_n}] &\leq e^{-\upsilon\tau}H(\bar{P}_{T_n,t_{n+1}},\bar{Q}_{T_n,t_{n+1}}) + \frac{\sigma^2(1-e^{-\upsilon\tau})}{2\upsilon}\\
&= e^{-\upsilon\tau}H(P_n,Q_n) + \frac{\sigma^2(1-e^{-\upsilon\tau})}{2\upsilon},
\end{aligned}$$

where in the last step we use that the subsystem (2.5) preserves the Hamiltonian H.

Step 2. For any given $y,y^* \in \mathbb{R}^2$, we show that ΔW_0 and ΔW_1 can be determined to ensure that $(P_2,Q_2)^\top = y^* = (y_1^*,y_2^*)^\top$ for any initial value $(P_0,Q_0)^\top = y$. In fact, the solvability of (2.5) gives that $\bar{P}_{T_0,t_1} = \psi_\tau(y)$ and $\bar{Q}_{T_0,t_1} = \phi_\tau(y)$, which, together with (2.3), leads to

$$\begin{aligned}
&P_1 = e^{-\frac{\upsilon\tau}{2}}\psi_\tau(y) + \int_{t_0}^{t_1} e^{-\frac{\upsilon}{2}(t_1-t)}\sigma dW_t \overset{d}{=} e^{-\frac{\upsilon\tau}{2}}\psi_\tau(y) + \sigma\sqrt{\frac{1-e^{-\upsilon\tau}}{\upsilon\tau}}\Delta W_0,\\
&Q_1 = e^{-\frac{\upsilon\tau}{2}}\phi_\tau(y),
\end{aligned}$$

where $X \overset{d}{=} Y$ means that random variables X,Y are equal in distribution. Using again the solvability of $\bar{Q}_{T_1,t_2}$, we have $\bar{Q}_{T_1,t_2} = \phi_\tau(P_1,Q_1) = e^{\frac{\upsilon\tau}{2}}Q_2 = e^{\frac{\upsilon\tau}{2}}y_2^*$, which determines P_1 and hence gives ΔW_0. Then utilizing $y_1^* = P_2 \overset{d}{=} e^{-\frac{\upsilon\tau}{2}}\psi_\tau(P_1,Q_1) + \sigma\sqrt{\frac{1-e^{-\upsilon\tau}}{\upsilon\tau}}\Delta W_1$ determines ΔW_1. In addition, the above procedure implies that the transition kernel $\mathbb{P}_{2n}(x, A)$, $x \in \mathbb{R}^2, A \in \mathcal{B}(\mathbb{R}^2)$ admits a continuous density function $p_{2n}(x, y)$ satisfying $\mathbb{P}_{2n}(x, A) = \int_A p_{2n}(x, y)dy$.

Combining Steps 1 and 2 gives that $|\mathbb{E}[g(P_{2n}, Q_{2n})] - \pi_\tau(g)| \leq C\kappa^n(1 + |H(P_0, Q_0)|^{\mathfrak{p}})$. Then similar to the proof of [17, Theorem 7.3] and by virtue of Lemma 2.1, one can obtain the desired result for the sequence $\{(P_n, Q_n)\}_{n\in\mathbb{N}}$. The proof is finished. ☐

The following proposition shows the exponential integrability of the numerical solution of (2.4), which indicates the boundedness of exponential moment of the numerical solution.

PROPOSITION 2.3. *There exists a constant $C > 0$ such that*

$$\sup_{t_n\in[0,T]} \mathbb{E}\left[\exp\left\{\frac{C_e(|P_n|^2 + |Q_n|^4)}{e^{\sigma^2 t_n}}\right\}\right] \leq e^{C(T+1)+H(P_0,Q_0)},$$

where C_e is given in (2.9).

Proof. Denote $\tilde{\mu}(p, q) := -\frac{\upsilon}{2}(p, q)^\top$ and $\tilde{\sigma} := (\sigma, 0)^\top$. Then we have

$$\mathcal{D}H(p, q)\tilde{\mu}(p, q) = -\frac{\upsilon}{2}p^2 - \frac{\upsilon}{2}q^4 - \frac{\upsilon^2}{2}pq,$$
$$tr(\mathcal{D}^2 H(p, q)\tilde{\sigma}\tilde{\sigma}^T) = \sigma^2, \quad |\tilde{\sigma}^T\mathcal{D}H(p, q)|^2 = \left|\sigma\left(p + \frac{\upsilon}{2}q\right)\right|^2.$$

This implies that

$$\begin{aligned}\tilde{\mathcal{E}} :=& \mathcal{D}H(\tilde{P}_{T_n,t}, \tilde{Q}_{T_n,t})\tilde{\mu}(\tilde{P}_{T_n,t}, \tilde{Q}_{T_n,t}) + \frac{tr(\mathcal{D}^2H(\tilde{P}_{T_n,t}, \tilde{Q}_{T_n,t})\tilde{\sigma}\tilde{\sigma}^T)}{2} \\ &+ \frac{|\tilde{\sigma}^T\mathcal{D}H(\tilde{P}_{T_n,t}, \tilde{Q}_{T_n,t})|^2}{2e^{\beta t}} \\ =& -\frac{\upsilon}{2}\big(|\tilde{P}_{T_n,t}|^2 + \upsilon\tilde{P}_{T_n,t}\tilde{Q}_{T_n,t} + |\tilde{Q}_{T_n,t}|^4\big) \\ &+ \frac{\sigma^2}{2e^{\beta t}}\left(|\tilde{P}_{T_n,t}|^2 + \upsilon\tilde{P}_{T_n,t}\tilde{Q}_{T_n,t} + \frac{\upsilon^2}{4}|\tilde{Q}_{T_n,t}|^2\right) \\ &+ \frac{\sigma^2}{2} \leq -\upsilon H(\tilde{P}_{T_n,t}, \tilde{Q}_{T_n,t}) + \sigma^2 H(\tilde{P}_{T_n,t}, \tilde{Q}_{T_n,t}) + \frac{\sigma^2\upsilon^4}{64} + \frac{\sigma^2}{2}.\end{aligned}$$

By [5, Lemma 2.5], we obtain

$$\begin{aligned}&\mathbb{E}\left[\exp\left\{\frac{H(\tilde{P}_{T_n,t}, \tilde{Q}_{T_n,t})}{e^{\sigma^2(t-t_n)}} + \int_{t_n}^t \frac{\upsilon H(\tilde{P}_{T_n,r}, \tilde{Q}_{T_n,r}) - \frac{\sigma^2}{2} - \frac{\sigma^2\upsilon^4}{64}}{e^{\sigma^2(r-t_n)}}dr\right\}\right] \\ &\leq \mathbb{E}\big[\exp\big\{H(\tilde{P}_{T_n,t_n}, \tilde{Q}_{T_n,t_n})\big\}\big] = \mathbb{E}\big[\exp\big\{H(P_n, Q_n)\big\}\big],\end{aligned}$$

where in the last equality, we use the preservation of the Hamiltonian for (2.5). By considering $e^{-\sigma^2 t_n}H$ instead of H and using (2.8), we arrive at

$$\begin{aligned}&\mathbb{E}\left[\exp\left\{\frac{H(\tilde{P}_{T_n,t}, \tilde{Q}_{T_n,t})}{e^{\sigma^2 t}}\right\}\right] \\ &\quad \leq \exp\left\{\left(\upsilon C_H + \frac{\sigma^2}{2} + \frac{\sigma^2\upsilon^4}{64}\right)(t - t_n)\right\}\mathbb{E}\left[\exp\left\{\frac{H(P_n, Q_n)}{e^{\sigma^2 t_n}}\right\}\right].\end{aligned}$$

By iteration and combining (2.9), we complete the proof. ☐

Similarly, one can also prove the uniform moment boundedness, the ergodicity, and the exponential integrability of the solution for the splitting system (2.1). For our convenience, we list these properties in the following proposition and omit the proof.

PROPOSITION 2.4. *The following hold:*

(i) *For any $\mathfrak{p}\geq 1$, there exists a constant $C:=C(\mathfrak{p})>0$ such that*

$$\sup_{n\in\mathbb{N}}\sup_{t\in T_n}\mathbb{E}[(\bar{P}_{T_n}(t))^{2\mathfrak{p}}+(\bar{Q}_{T_n}(t))^{4\mathfrak{p}}+(\tilde{P}_{T_n}(t))^{2\mathfrak{p}}+(\tilde{Q}_{T_n}(t))^{4\mathfrak{p}}]\\ \leq C(1+|H(P_0,Q_0)|^{\mathfrak{p}}).$$

In addition, the solution of the splitting system (2.1) *is uniquely ergodic.*

(ii) *There exists a constant $C>0$ such that*

$$\mathbb{E}\left[\exp\left\{\frac{H(P_\tau(t_n),Q_\tau(t_n))}{e^{\sigma^2 t_n}}\right\}\right]\leq \exp(H(P_0,Q_0)+Ct_n).$$

3. Strong and weak convergence orders. In this section, we first present that under moderate verifiable conditions on the one-step approximation (2.5), the splitting method (2.4) converges to the exact solution with the strong convergence order of 1. The proof is also given based on the decomposition of the error and the utilization of the exponential integrability and the stochastic Grönwall inequality. Then based on the Kolmogorov equation and the uniform moment boundedness, we prove the first-order weak convergence for approximating the ergodic limit via the numerical ergodic limit. The main result on the strong convergence order is stated as follows.

THEOREM 3.1. *Suppose that the one-step approximation* (2.5) *satisfies*

$$\left|\frac{\upsilon}{2}P_m+Q_m^3+\tau^{-1}\mathcal{A}_\tau^m\right|\leq C(|\bar{P}_{T_m,t_{m+1}}-P_m|^a+|\bar{Q}_{T_m,t_{m+1}}-Q_m|^b)\Theta_1^m, \tag{3.1}$$

$$\left|P_m+\frac{\upsilon}{2}Q_m-\tau^{-1}\mathcal{B}_\tau^m\right|\leq C(|\bar{P}_{T_m,t_{m+1}}-P_m|^a+|\bar{Q}_{T_m,t_{m+1}}-Q_m|^b)\Theta_2^m \tag{3.2}$$

for constants $C>0, a\wedge b\geq 1$, where maps $\Theta_1^m:=\Theta_1(P_m,Q_m,\bar{P}_{T_m,t_{m+1}},\bar{Q}_{T_m,t_{m+1}})$ and $\Theta_2^m:=\Theta_2(P_m,Q_m,\bar{P}_{T_m,t_{m+1}},\bar{Q}_{T_m,t_{m+1}})$ are of polynomial growth. In addition, let

$$\sup_{t_n\in[0,T]}(\|\tau^{-1}\mathcal{A}_\tau^n\|_{L^{6\mathfrak{p}a}(\Omega)}+\|\tau^{-1}\mathcal{B}_\tau^n\|_{L^{6\mathfrak{p}b}(\Omega)})\leq C \tag{3.3}$$

for $\mathfrak{p}>0$. Then for $T>0$, there exist $\tilde{\tau}_0:=\tilde{\tau}_0(T)\in(0,1)$ and $C:=C(T)>0$ such that for $\tau\in(0,\tilde{\tau}_0)$ and $\mathfrak{p}>0$,

$$\sup_{t_m\in[0,T]}\|(P(t_m),Q(t_m))^\top-(P_m,Q_m)^\top\|_{L^{2\mathfrak{p}}(\Omega)}\leq C\tau.$$

Below we present the convergence order between numerical and exact ergodic limits.

THEOREM 3.2. *Under conditions in Theorem* 3.1, *for measurable functions $g\in\mathcal{G}_l=\{g:|g(x)-g(y)|\leq C(1+|x|^{2l-1}+|y|^{2l-1})|x-y|,|g(x)|\leq(H(x)+C_H)^l\}$, we have $|\pi(g)-\pi_\tau(g)|\leq C\tau$, where $C>0$ is time-independent.*

Proof. Introduce the function $u(t,p,q):=\mathbb{E}_{(p,q)}[g(P(t),Q(t))]-\pi(g)$, which is the solution of the Kolmogorov equation $\frac{\partial u(t,p,q)}{\partial t}=\mathcal{L}u(t,p,q)$. Here, $\mathcal{L}$ is the infinitesimal generator of (1.1), and $\mathbb{E}_{(p,q)}$ is the conditional expectation with respect to the initial (p,q). We let $b_2(p,q)=(-\frac{\upsilon}{2}p,-\frac{\upsilon}{2}q)^\top$. It follows from (2.4) and (2.5) that

$$X_{n+1}=X_n+(\mathcal{A}_\tau^n,\mathcal{B}_\tau^n)^\top+\int_{t_n}^{t_{n+1}}b_2(\tilde{P}_{T_n,r},\tilde{Q}_{T_n,r})dr+(\sigma\Delta W_n,0)^\top.$$

Then by the Taylor expansion, (2.5), and (3.1)–(3.2), one can derive that for $j \geq 0, n \geq 0$,

$$\mathbb{E}[u(j\tau, X_{n+1})] \leq \mathbb{E}[u(j\tau, X_n)] + \mathbb{E}[\mathcal{L}u(j\tau, X_n)]\tau + \mathcal{C}_{j,n+1}\tau + r_{j,n+1}\tau^2. \tag{3.4}$$

Here, the function $\mathcal{C}_{j,n+1}$ is the term of type $\mathbb{E}[\|Du(j\tau, X_n)\|(\tau\mathbb{J}^n_{1,1} + \int_{t_n}^{t_{n+1}} \mathbb{J}^n_{1,2}(r)dr) + \tau(\|D^2u(j\tau, X_n)\| + \|D^3u(j\tau, X_n + \theta(X_{n+1} - X_n))\|)\mathbb{J}^n_{1,3}]$, where D^iu is the standard ith derivative of u, $\theta \in (0,1)$, $\mathbb{J}^n_{1,1} := \mathbb{J}_{1,1}(X_n, \bar{P}_{T_n,t_{n+1}}, \bar{Q}_{T_n,t_{n+1}}, \tau^{-1}\mathcal{A}^n_\tau, \tau^{-1}\mathcal{B}^n_\tau)$, $\mathbb{J}^n_{1,2}(r) := \mathbb{J}_{1,2}(X_n, \tilde{P}_{T_n,r}, \tilde{Q}_{T_n,r})$, and $\mathbb{J}^n_{1,3} := \mathbb{J}_{1,3}(X_n)$ are functions with polynomial growth at infinity. The remainder term $r_{j,n+1}$ is the term of type $\mathbb{E}[(\|D^2u(j\tau, X_n)\| + \|D^3u(j\tau, X_n + \theta(X_{n+1} - X_n))\|)(\tau\mathbb{J}^n_{2,1} + \int_{t_n}^{t_{n+1}} \mathbb{J}^n_{2,2}(r)dr)]$, where functions $\mathbb{J}^n_{2,1} := \mathbb{J}_{2,1}(X_n, \bar{P}_{T_n,t_{n+1}}, \bar{Q}_{T_n,t_{n+1}}, \tau^{-1}\mathcal{A}^n_\tau, \tau^{-1}\mathcal{B}^n_\tau)$ and $\mathbb{J}^n_{2,2}(r) := \mathbb{J}_{2,2}(X_n, \tilde{P}_{T_n,r}, \tilde{Q}_{T_n,r})$ are of polynomial growth at infinity. According to [21, Theorem 3.1], Lemma 2.1, and (3.3), we obtain that for some $\mathfrak{q}_i > 0, i = 0,1,2$, and $C > 0$,

$$\begin{aligned}&\sup_{n\geq 0}\sum_{j=0}^{\infty}|r_{j,n+1}| \\ &\quad\leq C\big(1 + \sup_{n\in\mathbb{N}}(\|X_n\|^{\mathfrak{q}_1}_{L^{\mathfrak{q}_0}(\Omega)} + \|\mathbb{J}^n_{1,1}\|_{L^{\mathfrak{q}_2}(\Omega)} + \sup_{r\in T_n}\|\mathbb{J}^n_{1,2}(r)\|_{L^{\mathfrak{q}_2}(\Omega)})\big)\tau\sum_{j=0}^{\infty}e^{-Cj\tau} \leq C.\end{aligned}$$

It is observed that the Taylor expansion gives

$$\mathbb{E}[u((j+1)\tau, X_n)] = \mathbb{E}[u(j\tau, X_n)] + \mathbb{E}[\mathcal{L}u(j\tau, X_n)]\tau + \tfrac{1}{2}\mathbb{E}[\mathcal{L}^2u(j\tau, X_n)]\tau^2 + \tilde{r}_{j+1,n}. \tag{3.5}$$

Here, the term $\mathcal{L}^2u(j\tau, X_n)$ is a summation of terms of type $\partial^i u(j\tau, X_n)\tilde{\mathbb{J}}_1(X_n), i = 1,2,3,4$, where ∂^i is the ith partial derivatives with respect to (p,q) and $\tilde{\mathbb{J}}_1$ is a polynomial. The remainder $\tilde{r}_{j+1,n}$ is a summation of terms of type $\int_{j\tau}^{(j+1)\tau}\int_0^1 \partial^i u(j\tau + \tilde{\theta}(t - j\tau), X_n)\tilde{\mathbb{J}}_2(X_n)(t - j\tau)^2 d\tilde{\theta}dt, i = 1,\ldots,6$, where $\tilde{\mathbb{J}}_2$ is a polynomial.

Combining (3.4) and (3.5) leads to

$$\mathbb{E}[u(j\tau, X_{n+1})] \leq \mathbb{E}[u((j+1)\tau, X_n)] + \tilde{\mathcal{C}}_{j,n+1}\tau + R_{j+1,n+1},$$

where $\tilde{\mathcal{C}}_{j,n+1}$ is the summation of terms $\mathcal{C}_{j,n+1}$ and $\mathbb{E}[\tau\|D^iu(j\tau, X_n)\| \cdot |\tilde{\mathbb{J}}_1(X_n)|], i = 1,\ldots,4$, and $R_{j+1,n+1}$ is a summation of terms $r_{j,n+1}\tau^2$ and $\int_{j\tau}^{(j+1)\tau}\int_0^1 \mathbb{E}[|\tilde{\mathbb{J}}_2(X_n)| \cdot \|D^iu(j\tau + \tilde{\theta}(t - j\tau))\|](t - j\tau)^2 d\tilde{\theta}dt, i = 1,\ldots,6$. Therefore, we arrive at

$$\begin{aligned}\frac{1}{N}\sum_{n=1}^{N}\mathbb{E}[g(X_n) - \pi(g)] &= \frac{1}{N}\sum_{n=1}^{N}\mathbb{E}[u(0, X_n)] \\ &\leq \frac{1}{N}\sum_{n=1}^{N}\mathbb{E}\left[u(n\tau, X_0) + \sum_{j=0}^{n-1}\tilde{\mathcal{C}}_{j,n-j}\tau + \sum_{j=0}^{n-1}R_{j+1,n-j}\right].\end{aligned}$$

The ergodicity of the exact solution implies that $\frac{1}{N}\sum_{n=1}^{N}\mathbb{E}[u(n\tau, X_0)] \to 0$ as $N \to \infty$. From [21, Theorem 3.1], Lemma 2.1, and (3.3), we obtain $\sup_{N\geq 1}\frac{1}{N}\sum_{n=1}^{N}\sum_{j=0}^{n-1}\tilde{\mathcal{C}}_{j,n-j} \leq C\sum_{j=0}^{\infty}e^{-Cj\tau}\tau \leq C$ and $\sup_{N\geq 1}\frac{1}{N}\sum_{n=1}^{N}\sum_{j=0}^{n-1}R_{j+1,n-j} \leq C\tau^3\sum_{j=0}^{\infty}e^{-Cj\tau} \leq C\tau^2$. Hence, by virtue of the ergodicity of the numerical solution, we derive that $|\pi(g) - \pi_\tau(g)| \leq C\tau$. The proof is finished. $\square$

Proof of Theorem 3.1. The proof is divided into two steps based on the decomposition of the error.

Step 1. Show that for $T>0$, there exist $\tilde{\tau}_0 := \tilde{\tau}_0(T) \in (0,1)$ and $C := C(T) > 0$ such that for any $\tau \in (0, \tilde{\tau}_0)$ and $\mathfrak{p} > 0$, it holds that $\sup_{t_m \in [0,T]} \|(P(t_m), Q(t_m))^\top - (P_\tau(t_m), Q_\tau(t_m))^\top\|_{L^{2\mathfrak{p}}(\Omega)} \le C\tau$.

Let $e(t_m) := P(t_m) - P_\tau(t_m)$, and let $\tilde{e}(t_m) := Q(t_m) - Q_\tau(t_m)$. By (1.1) and (2.1), we have

$$\begin{aligned} &P(t) - \tilde{P}_{T_m}(t) \\ &\quad = e(t_m) + \int_{t_m}^{t_{m+1}} \left(\frac{\upsilon}{2}\bar{P}_{T_m}(s) + \bar{Q}^3_{T_m}(s)\right) ds + \int_{t_m}^{t} \left(\frac{\upsilon}{2}\tilde{P}_{T_m}(s) - \upsilon P(s) - Q^3(s)\right) ds. \end{aligned} \tag{3.6}$$

This, together with the Taylor formula, yields

$$\begin{aligned} |e(t_{m+1})|^2 = &\left|e(t_m) + \int_{t_m}^{t_{m+1}} \left(\frac{\upsilon}{2}\bar{P}_{T_m}(s) + \bar{Q}^3_{T_m}(s)\right) ds\right|^2 + \int_{t_m}^{t_{m+1}} (P(t) - \tilde{P}_{T_m}(t)) \\ &\times (\upsilon\tilde{P}_{T_m}(t) - 2\upsilon P(t) - 2Q^3(t))dt = |e(t_m)|^2 + J_m^1 + J_m^2 + J_m^3 + J_m^4, \end{aligned} \tag{3.7}$$

where

$$\begin{aligned} J_m^1 &:= \int_{t_m}^{t_{m+1}} e(t_m)(\upsilon\bar{P}_{T_m}(s) + 2\bar{Q}^3_{T_m}(s) + \upsilon\tilde{P}_{T_m}(s) - 2\upsilon P(s) - 2Q^3(s))ds, \\ J_m^2 &:= \left|\int_{t_m}^{t_{m+1}} \left(\frac{\upsilon}{2}\bar{P}_{T_m}(s) + \bar{Q}^3_{T_m}(s)\right) ds\right|^2, \\ J_m^3 &:= \int_{t_m}^{t_{m+1}} \int_{t_m}^{t_{m+1}} \left(\frac{\upsilon}{2}\bar{P}_{T_m}(s) + \bar{Q}^3_{T_m}(s)\right)(\upsilon\tilde{P}_{T_m}(t) - 2\upsilon P(t) - 2Q^3(t))dsdt, \\ J_m^4 &:= \int_{t_m}^{t_{m+1}} \int_{t_m}^{t} \left(\frac{\upsilon}{2}\tilde{P}_{T_m}(s) - \upsilon P(s) - Q^3(s)\right)(\upsilon\tilde{P}_{T_m}(t) - 2\upsilon P(t) - 2Q^3(t))dsdt. \end{aligned}$$

For the term J_m^1, it can be decomposed as

$$\begin{aligned} J_m^1 = &\int_{t_m}^{t_{m+1}} \upsilon e(t_m)(\bar{P}_{T_m}(s) - P(s))ds + \int_{t_m}^{t_{m+1}} \upsilon e(t_m)(\tilde{P}_{T_m}(s) - P(s))ds \\ &+ 2\int_{t_m}^{t_{m+1}} e(t_m)(\bar{Q}^3_{T_m}(s) - Q^3(s))ds =: J_m^{1,1} + J_m^{1,2} + J_m^{1,3}. \end{aligned}$$

Note that

$$\begin{aligned} &\bar{P}_{T_m}(s) - P(s) \\ &\quad = -e(t_m) + \int_{t_m}^{s} \left(\upsilon P(r) - \frac{\upsilon}{2}\bar{P}_{T_m}(r) - \bar{Q}^3_{T_m}(r) + Q^3(r)\right) dr - \sigma(W_s - W_{t_m}), \end{aligned} \tag{3.8}$$

$$\bar{Q}_{T_m}(s) - Q(s) = -\tilde{e}(t_m) + \int_{t_m}^{s} \left(\bar{P}_{T_m}(r) - P(r) + \frac{\upsilon}{2}\bar{Q}_{T_m}(r)\right) dr. \tag{3.9}$$

Combining (3.6) leads to

$$J_m^{1,1} = -\upsilon|e(t_m)|^2\tau + \upsilon\int_{t_m}^{t_{m+1}}\int_{t_m}^{s} e(t_m)\left(\upsilon P(r) - \frac{\upsilon}{2}\bar{P}_{T_m}(r)\right)drds$$
$$+\upsilon\int_{t_m}^{t_{m+1}}\int_{t_m}^{s} e(t_m)(-\bar{Q}^3_{T_m}(r) + Q^3(r))drds - \upsilon\int_{t_m}^{t_{m+1}} e(t_m)\sigma(W_s - W_{t_m})ds,$$
$$J_m^{1,2} = -\upsilon|e(t_m)|^2\tau + \upsilon\int_{t_m}^{t_{m+1}}\int_{t_m}^{t_{m+1}} e(t_m)\left(-\frac{\upsilon}{2}\bar{P}_{T_m}(r) - \bar{Q}^3_{T_m}(r)\right)drds$$
$$+\upsilon\int_{t_m}^{t_{m+1}}\int_{t_m}^{s} e(t_m)\left(-\frac{\upsilon}{2}\tilde{P}_{T_m}(r) + \upsilon P(r) + Q^3(r)\right)drds,$$

and

$$J_m^{1,3} = 2\int_{t_m}^{t_{m+1}} e(t_m)(\bar{Q}_{T_m}(s) - Q(s))(\bar{Q}^2_{T_m}(s) + \bar{Q}_{T_m}(s)Q(s) + Q^2(s))ds$$
$$= -2e(t_m)\tilde{e}(t_m)\int_{t_m}^{t_{m+1}}(\bar{Q}^2_{T_m}(s) + \bar{Q}_{T_m}(s)Q(s) + Q^2(s))ds$$
$$+2\int_{t_m}^{t_{m+1}}\int_{t_m}^{s} e(t_m)\left(\bar{P}_{T_m}(r) - P(r) + \frac{\upsilon}{2}\bar{Q}_{T_m}(r)\right)$$
$$\times(\bar{Q}^2_{T_m}(s) + \bar{Q}_{T_m}(s)Q(s) + Q^2(s))drds.$$

Hence, by the Hölder inequality and the Young inequality, we obtain

$$\begin{aligned} J_m^1 \le& -\frac{\upsilon\tau}{2}|e(t_m)|^2 + C(|e(t_m)|^2 + |\tilde{e}(t_m)|^2)\int_{t_m}^{t_{m+1}}(|Q(s)|^2 + |\bar{Q}_{T_m}(s)|^2)ds \\ &+ C\tau^2\int_{t_m}^{t_{m+1}}\left(|P(s)|^6 + |\bar{P}_{T_m}(s)|^6 + |\tilde{P}_{T_m}(s)|^2 + |Q(s)|^6 + |\bar{Q}_{T_m}(s)|^6 + 1\right)ds \\ &- \upsilon\int_{t_m}^{t_{m+1}} e(t_m)\sigma(W_s - W_{t_m})ds. \end{aligned} \tag{3.10}$$

For terms J_m^2, J_m^3, J_m^4, it follows from $(a+b)^2 = a^2 + 2ab + b^2, a, b\in\mathbb{R}$, that

$$\begin{aligned} &J_m^2 + J_m^3 + J_m^4 \\ &= \bigg|\frac{\upsilon}{2}\int_{t_m}^{t_{m+1}}(\bar{P}_{T_m}(t) - P(t))dt \\ &\quad + \frac{\upsilon}{2}\int_{t_m}^{t_{m+1}}(\tilde{P}_{T_m}(t) - P(t))dt + \int_{t_m}^{t_{m+1}}(\bar{Q}^3_{T_m}(t) - Q^3(t))dt\bigg|^2 \\ &\quad - \int_{t_m}^{t_{m+1}}\int_{t}^{t_{m+1}}\left(\frac{\upsilon}{2}\tilde{P}_{T_m}(s) - \upsilon P(s) - Q^3(s)\right)\left(\frac{\upsilon}{2}\tilde{P}_{T_m}(t) - \upsilon P(t) - Q^3(t)\right)dsdt \\ &\quad + \int_{t_m}^{t_{m+1}}\int_{t_m}^{t}\left(\frac{\upsilon}{2}\tilde{P}_{T_m}(s) - \upsilon P(s) - Q^3(s)\right)\left(\frac{\upsilon}{2}\tilde{P}_{T_m}(t) - \upsilon P(t) - Q^3(t)\right)dsdt \\ &= \bigg|\frac{\upsilon}{2}\int_{t_m}^{t_{m+1}}(\bar{P}_{T_m}(t) - P(t))dt + \frac{\upsilon}{2}\int_{t_m}^{t_{m+1}}(\tilde{P}_{T_m}(t) - P(t))dt \\ &\quad + \int_{t_m}^{t_{m+1}}(\bar{Q}^3_{T_m}(t) - Q^3(t))dt\bigg|^2, \end{aligned}$$

where the second equality uses the integral transformation. Using (3.6), (3.8), (3.9), the Hölder inequality, and the Young inequality, we derive that

$$
\begin{aligned}
J_m^2+J_m^3+J_m^4 \leq C\bigg[&\tau^2|e(t_m)|^2+C\tau|\tilde{e}(t_m)|^2\int_{t_m}^{t_{m+1}}(|\bar{Q}_{T_m}(s)|^4+|Q(s)|^4)ds\\
&+\tau^3\int_{t_m}^{t_{m+1}}\Big(|P(s)|^6+|\tilde{P}_{T_m}(s)|^2+|\bar{P}_{T_m}(s)|^6+|\bar{Q}_{T_m}(s)|^6+|Q(s)|^6\Big)ds\\
&+\tau\int_{t_m}^{t_{m+1}}|\sigma(W_t-W_{t_m})|^2dt\bigg].
\end{aligned}\tag{3.11}
$$

By the Taylor formula and

$$
Q(t)-\tilde{Q}_{T_m}(t)=\tilde{e}(t_m)-\int_{t_m}^{t_{m+1}}\Big(\bar{P}_{T_m}(s)+\frac{\upsilon}{2}\bar{Q}_{T_m}(s)\Big)\,ds+\int_{t_m}^{t}\Big(P(s)+\frac{\upsilon}{2}\tilde{Q}_{T_m}(s)\Big)\,ds,
$$

we derive that

$$
\begin{aligned}
|\tilde{e}(t_{m+1})|^2=&\left|\tilde{e}(t_m)-\int_{t_m}^{t_{m+1}}\Big(\bar{P}_{T_m}(s)+\frac{\upsilon}{2}\bar{Q}_{T_m}(s)\Big)\,ds\right|^2+\int_{t_m}^{t_{m+1}}(Q(t)-\tilde{Q}_{T_m}(t))\\
&\times(2P(t)+\upsilon\tilde{Q}_{T_m}(t))dt=|\tilde{e}(t_m)|^2+K_m^1+K_m^2+K_m^3+K_m^4,
\end{aligned}\tag{3.12}
$$

where

$$
\begin{aligned}
K_m^1&:=2\int_{t_m}^{t_{m+1}}\tilde{e}(t_m)(P(t)-\bar{P}_{T_m}(t))dt+\upsilon\int_{t_m}^{t_{m+1}}\tilde{e}(t_m)(\tilde{Q}_{T_m}(t)-\bar{Q}_{T_m}(t))dt,\\
K_m^2&:=\left|\int_{t_m}^{t_{m+1}}\Big(\bar{P}_{T_m}(s)+\frac{\upsilon}{2}\bar{Q}_{T_m}(s)\Big)\,ds\right|^2,\\
K_m^3&:=-\int_{t_m}^{t_{m+1}}\int_{t_m}^{t_{m+1}}\Big(\bar{P}_{T_m}(s)+\frac{\upsilon}{2}\bar{Q}_{T_m}(s)\Big)(2P(t)+\upsilon\tilde{Q}_{T_m}(t))dsdt,\\
K_m^4&:=\int_{t_m}^{t_{m+1}}\int_{t_m}^{t}\Big(P(s)+\frac{\upsilon}{2}\tilde{Q}_{T_m}(s)\Big)\Big(2P(t)+\upsilon\tilde{Q}_{T_m}(t)\Big)\,dsdt.
\end{aligned}
$$

For the term K_m^1, it follows from (3.8) that

$$
\tilde{Q}_{T_m}(t)-\bar{Q}_{T_m}(t)=-\int_{t_m}^{t}\frac{\upsilon}{2}\tilde{Q}_{T_m}(r)dr+\int_{t}^{t_{m+1}}\Big(\bar{P}_{T_m}(r)+\frac{\upsilon}{2}\bar{Q}_{T_m}(r)\Big)\,dr\tag{3.13}
$$

and from the Hölder inequality that

$$
\begin{aligned}
K_m^1\leq& C\tau(|e(t_m)|^2+|\tilde{e}(t_m)|^2)+2\int_{t_m}^{t_{m+1}}\tilde{e}(t_m)\sigma(W_t-W_{t_m})dt\\
&+C\tau^2\int_{t_m}^{t_{m+1}}(|P(s)|^2+|\bar{P}_{T_m}(s)|^2+|Q(s)|^6+|\bar{Q}_{T_m}(s)|^6+|\tilde{Q}_{T_m}(s)|^2+1)ds.
\end{aligned}\tag{3.14}
$$

For terms $K_m^i, i=2,3,4$, by (3.8), (3.13), and the integral transformation, we have

$$
\begin{aligned}
K_m^2+K_m^3+K_m^4=&\left|\int_{t_m}^{t_{m+1}}(\bar{P}_{T_m}(s)-P(s))ds+\frac{\upsilon}{2}\int_{t_m}^{t_{m+1}}(\bar{Q}_{T_m}(s)-\tilde{Q}_{T_m}(s))ds\right|^2\\
\leq& C\tau^2|e(t_m)|^2+C\tau^3\int_{t_m}^{t_{m+1}}(|\tilde{P}_{T_m}(s)|^2+|P(s)|^2+|\bar{P}_{T_m}(s)|^2\\
&+|Q(s)|^6+|\bar{Q}_{T_m}(s)|^6)ds+C\tau\int_{t_m}^{t_{m+1}}|\sigma(W_s-W_{t_m})|^2ds.
\end{aligned}\tag{3.15}
$$

Hence, adding (3.7) and (3.12) and combining (3.10), (3.11), (3.14), (3.15), and the Young inequality, we arrive at that for $\epsilon \in (0,1)$,

$$\begin{aligned}|e(t_{m+1})|^2 + |\tilde{e}(t_{m+1})|^2 \leq (|e(t_m)|^2 + |\tilde{e}(t_m)|^2)\bigg(1 + C\int_{t_m}^{t_{m+1}} (1 + (\tau+\epsilon)\times \\ (|\bar{Q}_{T_m}(s)|^4 + |Q(s)|^4))ds\bigg) + C\tau^2 \int_{t_m}^{t_{m+1}} \Gamma_m(s)ds + C\tau\int_{t_m}^{t_{m+1}} |W_s - W_{t_m}|^2 ds \\ + \sigma(2\tilde{e}(t_m) - ve(t_m))\int_{t_m}^{t_{m+1}} (t_{m+1}-s)dW_s,\end{aligned}$$

where $\Gamma_m(s) := \Gamma(P(s), Q(s), \bar{P}_{T_m}(s), \bar{Q}_{T_m}(s), \tilde{P}_{T_m}(s), \tilde{Q}_{T_m}(s)), s \in T_m$, is a polynomial with order no larger than 6, and the Fubini theorem is also used to obtain

$$\begin{aligned}M_m &:= \sigma(2\tilde{e}(t_m) - ve(t_m))\int_{t_m}^{t_{m+1}} (W_s - W_{t_m})ds \\ &= \sigma(2\tilde{e}(t_m) - ve(t_m))\int_{t_m}^{t_{m+1}} (t_{m+1}-s)dW_s.\end{aligned}$$

It follows that $\{M_j\}_{j\in\mathbb{N}}$ is a martingale with $M_0 = 0$. By iteration, we have

$$\begin{aligned}|e(t_{m+1})|^2 + |\tilde{e}(t_{m+1})|^2 \leq C\sum_{j=0}^{m}(|e(t_j)|^2 + |\tilde{e}(t_j)|^2)\int_{t_j}^{t_{j+1}} (1 + (\tau+\epsilon)(|\bar{Q}_{T_j}(s)|^4 \\ + |Q(s)|^4))ds + C\tau^2\sum_{j=0}^{m}\int_{t_j}^{t_{j+1}} \Gamma_j(s)ds \\ + C\tau\sum_{j=0}^{m}\int_{t_j}^{t_{j+1}} |W_s - W_{t_j}|^2 ds + \sum_{j=0}^{m} M_j.\end{aligned}$$

For $t \in T_j$, denote $\lfloor t \rfloor := t_j$, $n_t := j$, and $\mathcal{Y}_{\lfloor t \rfloor} := |e(t_j)|^2 + |\tilde{e}(t_j)|^2$. Then we have

$$\begin{aligned}\mathcal{Y}_{\lfloor t \rfloor} &\leq \int_0^{\lfloor t \rfloor} (C\mathcal{Y}_{\lfloor s \rfloor}(1 + (\tau+\epsilon)(|\bar{Q}_{T_{n_s}}(s)|^4 + |Q(s)|^4)) + C\tau^2\Gamma_{n_s}(s) \\ &\quad + C\tau|W_s - W_{\lfloor s \rfloor}|^2)ds + \int_0^{\lfloor t \rfloor} \sigma(2\tilde{e}(\lfloor s \rfloor) - ve(\lfloor s \rfloor))(\lfloor s \rfloor + \tau - s)dW_s \\ &=: \int_0^{\lfloor t \rfloor} a_s ds + \int_0^{\lfloor t \rfloor} b_s dW_s.\end{aligned}$$

To obtain the desired strong convergence order, we need to utilize the stochastic Grönwall inequality (see [14, Corollary 2.5]). Now we verify condition (34) of [14, Corollary 2.5] as follows: For $\mathfrak{p}_0 \geq 2$,

$$\begin{aligned}&\langle \mathcal{Y}_{\lfloor t \rfloor}, a_t\rangle + \frac{1}{2}|b_t|^2 + \frac{\mathfrak{p}_0 - 2}{2}\frac{|\langle \mathcal{Y}_{\lfloor t \rfloor}, b_t\rangle|^2}{|\mathcal{Y}_{\lfloor t \rfloor}|^2} \\ &\leq C(1 + (\tau+\epsilon)(|\bar{Q}_{T_{n_t}}(t)|^4 + |Q(t)|^4))|\mathcal{Y}_{\lfloor t \rfloor}|^2 \\ &\quad + (C\tau^2\Gamma_{n_t}(t) + C\tau|W_t - W_{\lfloor t \rfloor}|^2 + (\lfloor t \rfloor + \tau - t)^2)^2.\end{aligned}$$

Thus, combining Proposition 2.4 and [21, Lemma 2.3, Corollary 2.2], we have that for $\mathfrak{p} > 0$ and some $\mathfrak{p}_0, \mathfrak{p}_1 > 0$,

$$\|\mathcal{Y}_{t_{m+1}}\|_{L^{\mathfrak{p}}(\Omega)} \leq \left\|\exp\left\{C\int_0^T (1+(\tau+\epsilon)(|\bar{Q}_{T_{n_s}}(s)|^4+|Q(s)|^4))ds\right\}\right\|_{L^{\mathfrak{p}_1}(\Omega)}$$
$$\times\left(\int_0^T \left\|\frac{C\tau^2\Gamma_{n_s}(s)+C\tau|W_s-W_{\lfloor s\rfloor}|^2+(\lfloor s\rfloor+\tau-s)^2}{\exp\{\int_0^s(1+(\tau+\epsilon)(|\bar{Q}_{T_{n_u}}(u)|^4+|Q(u)|^4))du\}}\right\|^2_{L^{\mathfrak{p}_0}(\Omega)} ds\right)^{\frac{1}{2}}.$$

By the convexity of the exponential function, we have

$$\mathbb{E}\left[\exp\left\{C\mathfrak{p}_1\int_0^T \left(1+(\tau+\epsilon)(|\bar{Q}_{T_{n_s}}(s)|^4+|Q(s)|^4)\right)ds\right\}\right]$$
$$\leq \frac{1}{T}\int_0^T \mathbb{E}[\exp(TC\mathfrak{p}_1(1+(\tau+\epsilon)(1+|\bar{Q}_{T_{n_s}}(s)|^4+|Q(s)|^4)))]ds =: \mathcal{I}_0. \tag{3.16}$$

Based on (2.9) and Proposition 2.4, there exist positive constants $\tilde{\tau}_0 := \tilde{\tau}_0(T)$ and $\tilde{\epsilon}_0 := \tilde{\epsilon}_0(T)$ such that $CT\mathfrak{p}_1(\tilde{\tau}_0+\tilde{\epsilon}_0) \leq C_e e^{-\sigma^2 T}$, where C_e is given in (2.9). Then for $\tau \in (0,\tilde{\tau}_0)$ and $\epsilon \in (0,\tilde{\epsilon}_0)$, we have $\mathcal{I}_0 \leq C$. This finishes the proof of Step 1.

Step 2. Show that for any $T>0$, there exist $\tilde{\tau}_0 := \tilde{\tau}_0(T) \in (0,1)$ and $C := C(T) > 0$ such that for any $\tau \in (0,\tilde{\tau}_0)$ and $\mathfrak{p}>0$, it holds that $\sup_{t_m\in[0,T]} \|(P_\tau(t_m),Q_\tau(t_m))^\top - (P_m,Q_m)^\top\|_{L^{2\mathfrak{p}}(\Omega)} \leq C\tau$.

Denote $e_1(t_m) := P_\tau(t_m)-P_m$ and $\tilde{e}_1(t_m) := Q_\tau(t_m)-Q_m$. By (2.3) and (2.5), we have that for $t\in T_m$,

$$\tilde{P}_{T_m}(t)-\tilde{P}_{T_m,t}$$
$$= e_1(t_m) - \int_{t_m}^{t_{m+1}} \left(\frac{\upsilon}{2}\bar{P}_{T_m}(s)+\bar{Q}^3_{T_m}(s)+\tau^{-1}\mathcal{A}^m_\tau\right)ds - \frac{\upsilon}{2}\int_{t_m}^t (\tilde{P}_{T_m}(s)-\tilde{P}_{T_m,s})ds.$$

It follows from the Taylor formula that $|\tilde{P}_{T_m}(t)-\tilde{P}_{T_m,t}|^2 = |e_1(t_m)|^2+I_{m,1}+I_{m,2}+I_{m,3}-\upsilon\int_{t_m}^t(\tilde{P}_{T_m}(s)-\tilde{P}_{T_m,s})^2ds,\ t\in T_m$, where $I_{m,1} := e_1(t_m)\int_{t_m}^{t_{m+1}} -2\big(\bar{Q}^3_{T_m}(s)-Q^3_m\big)ds$ and

$$I_{m,2} := e_1(t_m)\int_{t_m}^{t_{m+1}}(-\upsilon(\bar{P}_{T_m}(s)-P_m)-\upsilon P_m-2Q^3_m-2\tau^{-1}\mathcal{A}^m_\tau)ds,$$
$$I_{m,3} := \left|\int_{t_m}^{t_{m+1}}\left(\frac{\upsilon}{2}(\bar{P}_{T_m}(s)-P_m)+\bar{Q}^3_{T_m}(s)-Q^3_m+\frac{\upsilon}{2}\bar{P}_m+Q^3_m+\tau^{-1}\mathcal{A}^m_\tau\right)ds\right|^2.$$

From (2.2), we have

$$\bar{P}_{T_m}(s)-P_m = -\frac{\upsilon}{2}\int_{t_m}^s \bar{P}_{T_m}(r)dr - \int_{t_m}^s \bar{Q}^3_{T_m}(r)dr + e_1(t_m), \tag{3.17}$$
$$\bar{Q}_{T_m}(s)-Q_m = \int_{t_m}^s \bar{P}_{T_m}(r)dr + \frac{\upsilon}{2}\int_{t_m}^s \bar{Q}_{T_m}(r)dr + \tilde{e}_1(t_m). \tag{3.18}$$

This, together with (2.5), (3.1), (3.17), (3.18), the Hölder inequality, and the Young inequality, yields

$$I_{m,1}+I_{m,2}+I_{m,3} \leq C(|e_1(t_m)|^2+|\tilde{e}_1(t_m)|^2)\int_{t_m}^{t_{m+1}}(1+|\bar{Q}_{T_m}(s)|^2+|Q_m|^2)ds$$
$$+C\tau^2\int_{t_m}^{t_{m+1}}(1+|\bar{P}_{T_m}(r)|^6+|\bar{Q}_{T_m}(r)|^6+|Q_m|^6$$
$$+(|\tau^{-1}\mathcal{A}^m_\tau|^{2a}+|\tau^{-1}\mathcal{B}^m_\tau|^{2b})|\Theta^m_1|^2)dr.$$

From (2.2) and (2.3), we obtain

$$\tilde{Q}_{T_m}(t) - \tilde{Q}_{T_m,t} = \tilde{e}_1(t_m) + \int_{t_m}^{t_{m+1}} \left(\bar{P}_{T_m}(s) + \frac{\upsilon}{2}\bar{Q}_{T_m}(s) - \tau^{-1}\mathcal{B}_\tau^m\right) ds - \frac{\upsilon}{2}\int_{t_m}^{t} (\tilde{Q}_{T_m}(s) - \tilde{Q}_{T_m,s})ds.$$

By virtue of the Taylor formula, we have $|\tilde{Q}_{T_m}(t) - \tilde{Q}_{T_m,t}|^2 = |\tilde{e}_1(t_m)|^2 + \hat{I}_{m,1} + \hat{I}_{m,2} + \hat{I}_{m,3} - \upsilon\int_{t_m}^t (\tilde{Q}_{T_m}(s) - \tilde{Q}_{T_m,s})^2 ds$, where $\hat{I}_{m,1} := \upsilon\tilde{e}_1(t_m)\int_{t_m}^{t_{m+1}} \left(\bar{Q}_{T_m}(s) - Q_m\right)ds$ and

$$\hat{I}_{m,2} := 2\tilde{e}_1(t_m)\int_{t_m}^{t_{m+1}} \left(\bar{P}_{T_m}(s) - P_m + P_m + \frac{\upsilon}{2}Q_m - \tau^{-1}\mathcal{B}_\tau^m\right) ds,$$

$$\hat{I}_{m,3} := \left|\int_{t_m}^{t_{m+1}} \left(\bar{P}_{T_m}(s) - P_m + \frac{\upsilon}{2}(\bar{Q}_{T_m}(s) - Q_m) + P_m + \frac{\upsilon}{2}Q_m - \tau^{-1}\mathcal{B}_\tau^m\right) ds\right|^2.$$

Then combining (3.2), (3.17), and (3.18), we have

$$\hat{I}_{m,1} + \hat{I}_{m,2} + \hat{I}_{m,3} \le C\tau(|e_1(t_m)|^2 + |\tilde{e}_1(t_m)|^2) + C\tau^2\int_{t_m}^{t_{m+1}} (1 + |\bar{P}_{T_m}(r)|^2 + |\bar{Q}_{T_m}(r)|^6 + (|\tau^{-1}\mathcal{A}_\tau^m|^{2a} + |\tau^{-1}\mathcal{B}_\tau^m|^{2b})|\Theta_2^m|^2)dr.$$

Hence, utilizing the Young inequality, we arrive at that for $\epsilon \in (0,1)$,

$$|e_1(t_{m+1})|^2 + |\tilde{e}_1(t_{m+1})|^2 \le (|e_1(t_m)|^2 + |\tilde{e}_1(t_m)|^2) \times \left(1 + C\int_{t_m}^{t_{m+1}} (C(\epsilon) + (\epsilon+\tau)(|\bar{Q}_{T_m}(s)|^4 + |Q_m|^4))ds\right) + C\tau^2\int_{t_m}^{t_{m+1}} \tilde{\Gamma}_m(s)ds,$$

where $\tilde{\Gamma}_m(s) := \tilde{\Gamma}(P_m, Q_m, \bar{P}_{T_m}(s), \bar{Q}_{T_m}(s), \tau^{-1}\mathcal{A}_\tau^m, \tau^{-1}\mathcal{B}_\tau^m), s \in T_m$, is a polynomial. Then by iteration, we have

$$|e_1(t_{m+1})|^2 + |\tilde{e}_1(t_{m+1})|^2 \le C\sum_{j=0}^{m}(|e_1(t_j)|^2 + |\tilde{e}_1(t_j)|^2) \times \int_{t_j}^{t_{j+1}} (1 + (\tau+\epsilon)(|\bar{Q}_{T_j}(s)|^4 + |Q_j|^4))ds + C\tau^2\sum_{j=0}^{m}\int_{t_j}^{t_{j+1}} \tilde{\Gamma}_j(s)ds.$$

By the discrete Grönwall inequality and taking $\mathfrak{p}$th moment, we obtain

$$\||e_1(t_{m+1})|^2 + |\tilde{e}_1(t_{m+1})|^2\|_{L^{\mathfrak{p}}(\Omega)} \le C\tau^2\left\|\int_0^T \tilde{\Gamma}_{n_s}(s)ds\right\|_{L^{2\mathfrak{p}}(\Omega)} \times \left\|\exp\left\{C\int_0^T (1 + (\epsilon+\tau)(|\bar{Q}_{T_{n_s}}(s)|^4 + |Q_{n_s}|^4)ds)\right\}\right\|_{L^{2\mathfrak{p}}(\Omega)}.$$

By Proposition 2.4(ii) and the preservation of the Hamiltonian for (2.2), we also have

$$\mathbb{E}\left[\exp\left\{\frac{H(\bar{P}_{T_j}(s), \bar{Q}_{T_j}(s))}{e^{\sigma^2 t_j}}\right\}\right] = \mathbb{E}\left[\exp\left\{\frac{H(P_\tau(t_j), Q_\tau(t_j))}{e^{\sigma^2 t_j}}\right\}\right] \le \exp\{H(P_0, Q_0) + Ct_j\}.$$

Then similar to the proof of (3.16), using the convexity of the exponential function and Proposition 2.3, there exist positive constants $\tilde{\tau}_0 := \tilde{\tau}_0(T)$ and $\tilde{\epsilon}_0 := \tilde{\epsilon}_0(T)$ such that when $\tau \in (0, \tilde{\tau}_0)$ and $\epsilon \in (0, \tilde{\epsilon}_0)$, $\sup_{t_m \in [0,T]} \||e_1(t_{m+1})|^2 + |\tilde{e}_1(t_{m+1})|^2\|_{L^{\mathfrak{p}}(\Omega)} \le C(T)\tau^2$. This finishes the proof. ∎

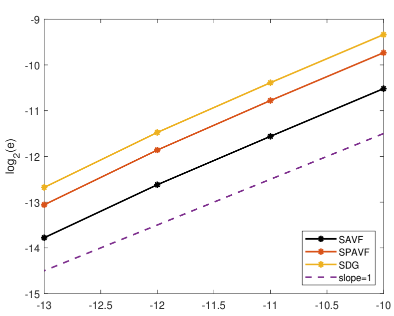
4. Numerical experiments. In this section, we first present some numerical experiments to verify our theoretical results on the strong and weak convergence orders. In addition, the long-time performance in calculating the ergodic limit is also illustrated by numerical experiments. Then we investigate extensions of our strategy to obtain the second-order method that preserves both the ergodicity and the exponential integrability, and to obtain the conformal symplectic method.

4.1. Convergence order and long-time performance. We first consider the strong convergence order. Take $T = 1$, $\sigma = 1$, and $\upsilon = 10$. The step sizes of the numerical solution for the proposed splitting methods are taken as $\tau_i = 2^{-i}, i = 10, 11, 12, 13$. The exact solution is realized by using the same numerical scheme with small step size $\tau = 2^{-15}$. Define error function $e(\tau_i, n) = \{\frac{1}{n}\sum_{k=1}^{n}(|P^k_{T/\tau_i+1} - P^k(T)|^2 + |Q^k_{T/\tau_i+1} - Q^k(T)|^2)\}^{\frac{1}{2}}$, where $\{P^k_{n+1}, Q^k_{n+1}\}$ and $\{P^k(t), Q^k(t)\}$ are the solutions in the kth sample. We take $n = 5000$ sample paths to simulate the expectation based on the Monte Carlo method. It is observed from Figure 2(a) that the mean square strong convergence order is 1 for the SAVF, SDG, and SPAVF schemes, which verifies our theoretical result in Theorem 3.1.

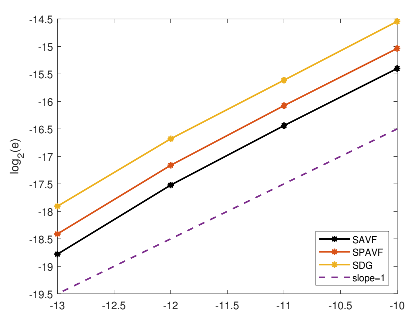
Then we consider the weak convergence order. Take the same parameters as above. Define error function $e'(\tau_i, n) = |\frac{1}{n}\sum_{k=1}^{n}(g(P^k_{T/\tau_i+1}, Q^k_{T/\tau_i+1}) - g(P^k(T), Q^k(T)))|$, where the test function $g(p, q) = \sin(p)\sin(q)$. It is observed from Figure 2(b) that the weak convergence order of these numerical schemes is also 1, which confirms the result in Theorem 3.2.

Below we test the long-time performance of the proposed methods. We take $n = 1000$ sample paths for the Monte Carlo simulation. We take time step $\tau = 1.25\times 10^{-6}$ to compute the reference solution and time step $\tau = 10^{-5}$ to compute the numerical solution. In Figure 3(a), we compute the strong error for $t \in [0, 1000]$ of the proposed SAVF scheme, which illustrates that the proposed scheme has a stable strong error in the long-time simulation. Similar performance holds for the long-time weak error, as shown in Figure 3(b). Here, we take $g(p, q) = \sin(1 + (p^2 + q^2)^{\frac{1}{2}})$.

To examine the numerical ergodicity for the proposed splitting methods, we compute the empirical distribution at different times as follows. We set $\sigma = 1$, $\upsilon = 15$, and the initial values $P(0) = 0, Q(0) = 0$ and compute over $n = 5000$ sample paths until $T = 512$ with $\tau = 2^{-8}$ via the SAVF scheme. We plot the empirical distribution at different times $t = 0, 2, 256$ in Figure 4, which shows that the empirical distribution converges to the reference Gibbs distribution as time increases. This indicates the

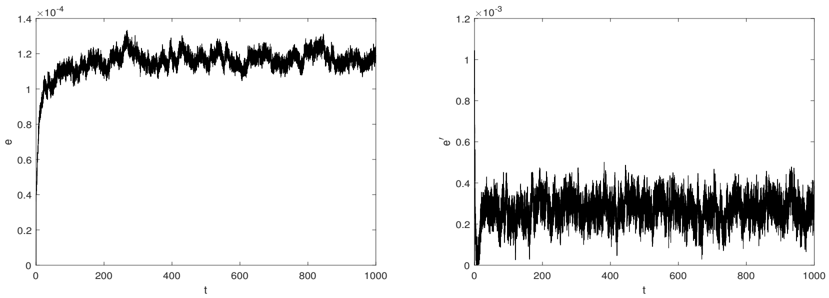


(a) Strong order



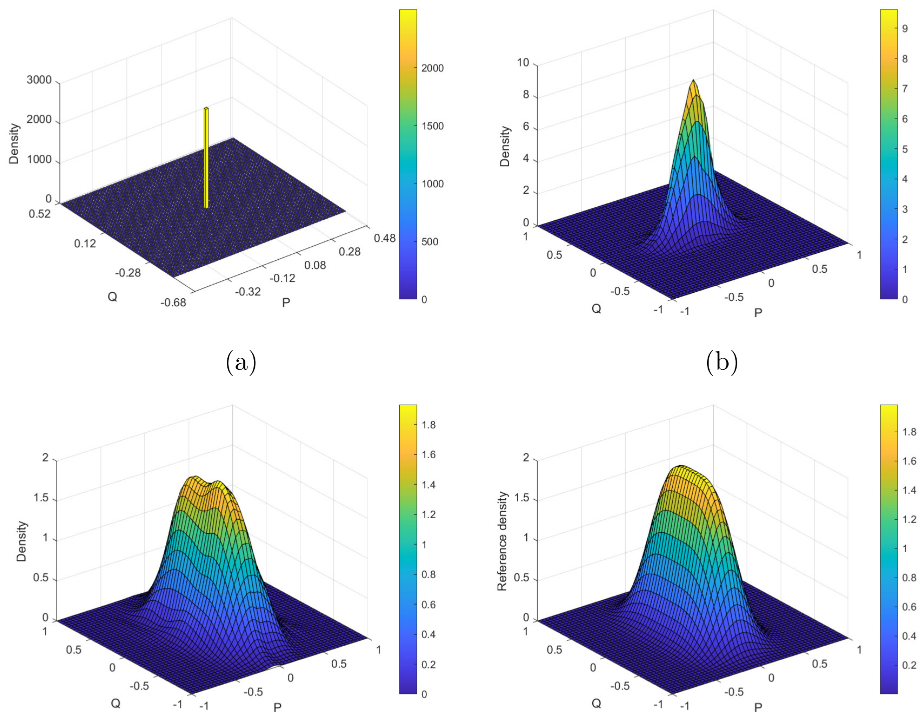
(b) Weak order

FIG. 2. *Convergence order in* log-log *scale.*



(a) Strong error (b) Weak error

FIG. 3. *Long-time error.*



(a) (b)

(c) (d)

FIG. 4. *The empirical distribution at times* $t = 0$ (a), $t = 2$ (b), and $t = 256$ (c). (d) *The reference distribution* $\rho(p,q) = \frac{\sqrt{\upsilon}}{\sigma\sqrt{\pi}\int_{\mathbb{R}} e^{-\upsilon q^4/(2\sigma^2)}dq} e^{-\frac{2\upsilon}{\sigma^2}(\frac{p^2}{2}+\frac{q^4}{4})}$*; see* [19, *p.* 183].

ergodicity of the numerical solution. The differences between the numerical distribution and reference distribution at times $t = 2, 256$ are plotted in Figure 5, from which we see that the error becomes smaller by increasing the number of sample paths.

The mean square displacement of $(P(t), Q(t))$ is defined as

$$MSD(t) := \mathbb{E}[|(P(t), Q(t)) - (P(0), Q(0))|^2], \tag{4.1}$$

which characterizes the diffusion behavior and motion properties of molecules in a quantitative way. It tends to an equilibrium as time grows to infinity, as shown

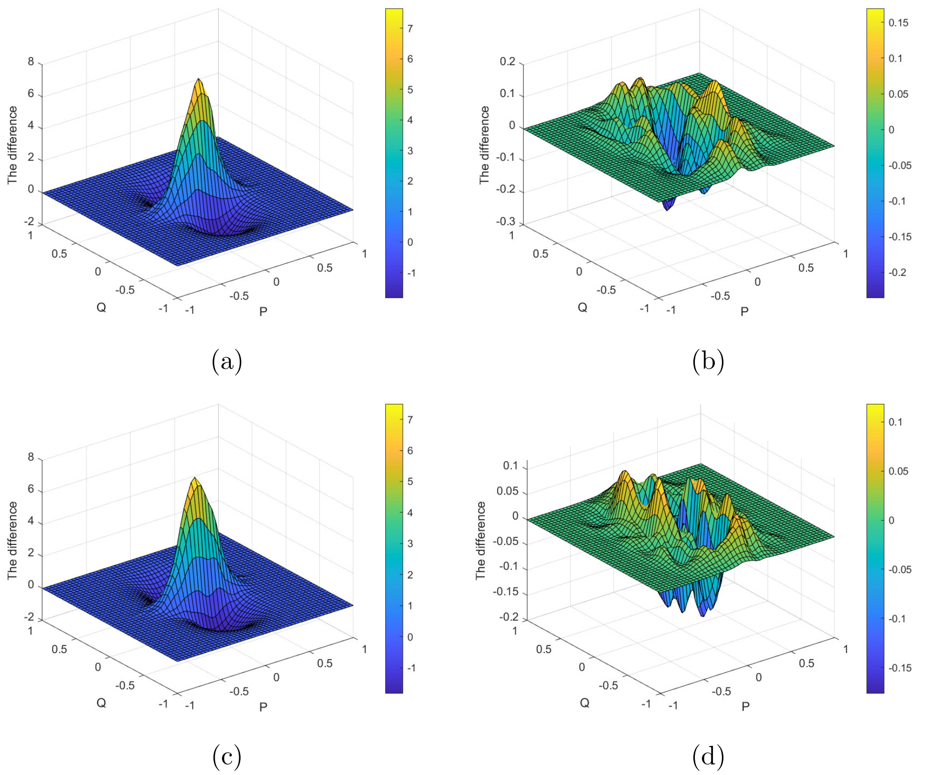


FIG. 5. *The difference between numerical distribution and the reference distribution at times* $t = 2$ (a) *and* $t = 256$ (b) *for* $n = 5000$ *sample paths and at times* $t = 2$ (c) *and* $t = 256$ (d) *for* $n = 10000$ *sample paths.*

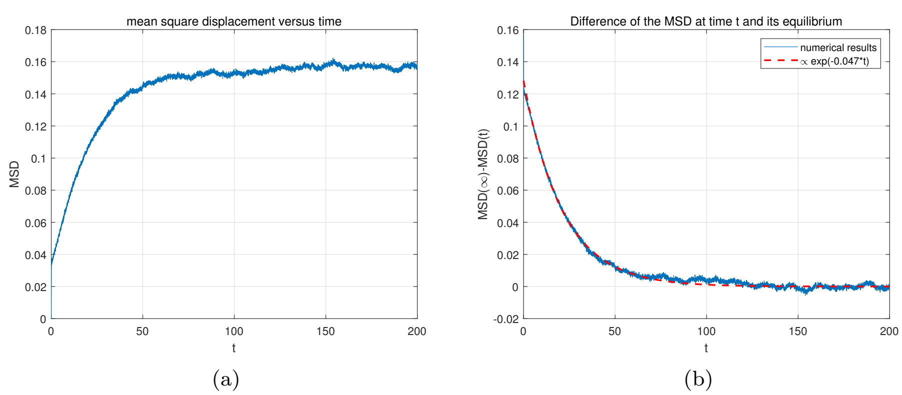


FIG. 6. *Mean square displacement* (a) *and* $MSD(\infty) - MSD(t)$ (b).

in Figure 6(a). To see the convergence rate more clearly, we take time $T = 512$ to simulate $MSD(\infty)$ and compute the evolution of $MSD(\infty)-MSD(t)$ with respect to time in Figure 6(b). It is indicated in Figure 6(b) that the mean square displacement approaches an equilibrium with an exponential rate.

4.2. Second-order property-preserving method. Based on our strategy, one can apply the Strang splitting technique to obtain the second-order weak convergence method that preserves both the ergodicity and the exponential integrability. To be specific, the Strang splitting technique yields the following evolution operator:

$$\begin{aligned}&\mathcal{P}_\tau^{\frac{1}{2}(\mathcal{L}_1+\mathcal{L}_2+\frac{1}{2}(\mathcal{L}_3-\mathcal{L}_3')),\frac{1}{2}(\mathcal{L}_3+\mathcal{L}_3')+\mathcal{L}_4,\frac{1}{2}(\mathcal{L}_1+\mathcal{L}_2+\frac{1}{2}(\mathcal{L}_3-\mathcal{L}_3'))}\\&\quad=e^{\frac{\tau}{2}(\mathcal{L}_1+\mathcal{L}_2+\frac{1}{2}(\mathcal{L}_3-\mathcal{L}_3'))}e^{\tau(\frac{1}{2}(\mathcal{L}_3+\mathcal{L}_3')+\mathcal{L}_4)}e^{\frac{\tau}{2}(\mathcal{L}_1+\mathcal{L}_2+\frac{1}{2}(\mathcal{L}_3-\mathcal{L}_3'))}.\end{aligned}$$

Then one can construct second-order numerical methods associated with this splitting. For example, we have the following Strang SAVF scheme:

$$\begin{aligned}\bar{P}_{T_n,t_{n+\frac{1}{2}}}&=P_n-\frac{\tau\upsilon}{8}(\bar{P}_{T_n,t_{n+\frac{1}{2}}}+P_n)-\frac{\tau}{2}\int_0^1(Q_n+\lambda(\bar{Q}_{T_n,t_{n+\frac{1}{2}}}-Q_n))^3d\lambda,\\\bar{Q}_{T_n,t_{n+\frac{1}{2}}}&=Q_n+\frac{\tau}{4}(\bar{P}_{T_n,t_{n+\frac{1}{2}}}+P_n)+\frac{\tau\upsilon}{8}(\bar{Q}_{T_n,t_{n+\frac{1}{2}}}+Q_n),\\\tilde{P}_{T_n,t_{n+1}}&=e^{-\frac{\upsilon\tau}{2}}\bar{P}_{T_n,t_{n+\frac{1}{2}}}+\sigma\int_{t_n}^{t_{n+1}}e^{-\frac{\upsilon}{2}(t_{n+1}-t)}dW_t,\\\tilde{Q}_{T_n,t_{n+1}}&=e^{-\frac{\upsilon\tau}{2}}\bar{Q}_{T_n,t_{n+\frac{1}{2}}},\\P_{n+1}&=\tilde{P}_{T_n,t_{n+1}}-\frac{\tau\upsilon}{8}(P_{n+1}+\tilde{P}_{T_n,t_{n+1}})\\&\quad-\frac{\tau}{2}\int_0^1(\tilde{Q}_{T_n,t_{n+1}}+\lambda(Q_{n+1}-\tilde{Q}_{T_n,t_{n+1}}))^3d\lambda,\\Q_{n+1}&=\tilde{Q}_{T_n,t_{n+1}}+\frac{\tau}{4}(P_{n+1}+\tilde{P}_{T_n,t_{n+1}})+\frac{\tau\upsilon}{8}(Q_{n+1}+\tilde{Q}_{T_n,t_{n+1}}).\end{aligned}$$

By the similar proof to that of Proposition 2.2, we can first show that the sequence $\{(P_{3n},Q_{3n})\}_{n\in\mathbb{N}_+}$ is ergodic. Then combining (A.3) and the preservation of energy for the AVF scheme, one can also derive (A.4) for the considered numerical solution and thus prove the ergodicity of the numerical solution $\{(P_n,Q_n)\}_{n\in\mathbb{N}_+}$. The exponential integrability of the numerical solution can be obtained in a similar way as Proposition 2.3, and thus the proof is omitted.

We employ the numerical experiment to illustrate the weak convergence order. Take $g(p,q)=\sin((p^2+q^2)^{\frac{1}{2}})$, $n=5000$, and $T=100$. The step sizes of the numerical solution for the Strang SAVF scheme are taken as $\tau_i=2^{-i}, i=10,11,12,13$. The exact solution is realized by using the same numerical scheme with small step size $\tau=2^{-15}$. It is observed from Figure 7 that the weak convergence order is 2.

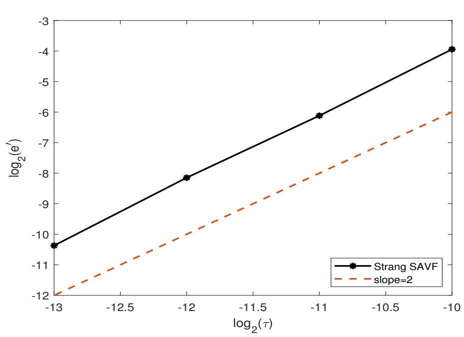
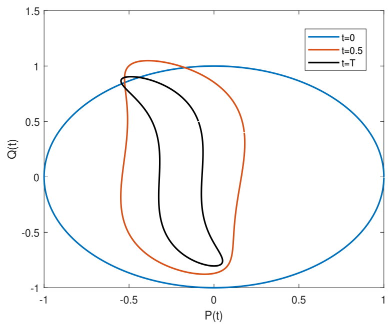
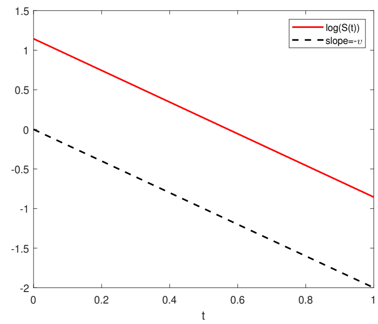


FIG. 7. *Weak order for the Strang SAVF scheme.*



(a) The curve in the phase space



(b) The logarithm of area

FIG. 8. *Evolution for area of domain in the phase space.*

4.3. Conformal symplectic splitting-based method. When one applies the symplectic method to the Hamiltonian subsystem (2.2) and solves the stochastic subsystem exactly, the corresponding splitting method (2.4) can be proved to preserve the conformal symplectic structure: $\mathrm{d}P_{n+1} \wedge \mathrm{d}Q_{n+1} = e^{-\upsilon\tau}\mathrm{d}P_n \wedge \mathrm{d}Q_n$, $n \in \mathbb{N}$. To illustrate this by a numerical experiment, we use the symplectic Euler method to solve subsystem (2.2) and obtain the one-step mapping (2.5) as follows:

$$\begin{aligned}\bar{P}_{T_n,t_{n+1}} &= P_n - \tau\left(Q_n^3 + \frac{\upsilon}{2}\bar{P}_{T_n,t_{n+1}}\right),\\ \bar{Q}_{T_n,t_{n+1}} &= Q_n + \tau\left(\bar{P}_{T_n,t_{n+1}} + \frac{\upsilon}{2}Q_n\right).\end{aligned}$$

Further solving subsystem (2.3) exactly derives the conformal symplectic splitting scheme (2.4). Set $T = 1$, $\upsilon = 2$, and $\tau = 10^{-4}$. We let the initial values be on the unit circle and plot the curve of the numerical solution using the above conformal symplectic splitting scheme. As shown in Figure 8(a), the area of the curve in the phase space decreases as time grows. We plot the logarithm of the area $S(t)$ of the curve as time t increases in Figure 8(b), which verifies that $S(t) = \pi exp(-\upsilon t)$.

Appendix A. Some proofs. This section is devoted to presenting some auxiliary proofs, including the proofs of (1.3) and Lemma 2.1.

Proof of (1.3). Denote $\mu(P(t),Q(t)) = (-Q^3(t) - \upsilon P(t), P(t))^\top$ and $\tilde{\sigma} = (\sigma, 0)^\top$. Then one can obtain $\mathcal{D}H(P(t),Q(t))\mu(P(t),Q(t)) = -\frac{\upsilon}{2}P^2(t) - \frac{\upsilon}{2}Q^4(t) - \frac{\upsilon^2}{2}P(t)Q(t)$, $tr(\mathcal{D}^2H(P(t),Q(t))\tilde{\sigma}\tilde{\sigma}^T) = \sigma^2$, and $|\tilde{\sigma}^T\mathcal{D}H(P(t),Q(t))|^2 = |\sigma(P(t) + \frac{\upsilon}{2}Q(t))|^2$. This gives that for $\beta > 0$,

$$\begin{aligned}\mathcal{E} :=& \mathcal{D}H(P(t),Q(t))\mu(P(t),Q(t)) + \frac{tr(\mathcal{D}^2H(P(t),Q(t))\tilde{\sigma}\tilde{\sigma}^T)}{2} + \frac{|\tilde{\sigma}^T\mathcal{D}H(P(t),Q(t))|^2}{2e^{\beta t}}\\ \le& -\upsilon H(P(t),Q(t)) + \sigma^2 H(P(t),Q(t)) + \frac{\sigma^2\upsilon^4}{64} + \frac{\sigma^2}{2}.\end{aligned}$$

Let $\bar{V} = \upsilon H(P(t),Q(t)) - (\frac{\sigma^2\upsilon^4}{64} + \frac{\sigma^2}{2})$, and let $\beta := \sigma^2$. Then using [9, Lemma 3.2], we derive that

$$\mathbb{E}\left[\exp\left\{\frac{H(P(t),Q(t))}{e^{\sigma^2 t}} + \int_0^t \frac{\upsilon H(P(r),Q(r)) - (\frac{\sigma^2\upsilon^4}{64} + \frac{\sigma^2}{2})}{e^{\sigma^2 r}}dr\right\}\right] \le e^{H(P_0,Q_0)},$$

which, together with (2.8) and (2.9), yields

$$\mathbb{E}\left[\exp\left\{\frac{C_e(|P(t)|^2+|Q(t)|^4)}{e^{\sigma^2 t}}\right\}\right] \le e^{(\upsilon C_H+\frac{\sigma^2\upsilon^4}{64}+\frac{\sigma^2}{2})t+C+H(P_0,Q_0)}.$$

This completes the proof by taking the supremum with $t\in[0,T]$. ◻

Proof of Lemma 2.1. We use the induction argument on $\mathfrak{p}\in\mathbb{N}_+$ to prove (2.6) and (2.7). We first prove the case of $\mathfrak{p}=1$. The Itô formula applied to $H+C_H$ and H can yield the same result, so without loss of generality, we suppose $H$to be positive here. By the Itô formula, we have

$$\begin{aligned} dH(\tilde P_{T_n,t},\tilde Q_{T_n,t}) &= \left(\tilde P_{T_n,t}+\frac{\upsilon}{2}\tilde Q_{T_n,t}\right)d\tilde P_{T_n,t}+\left(\tilde Q^3_{T_n,t}+\frac{\upsilon}{2}\tilde P_{T_n,t}\right)d\tilde Q_{T_n,t}+\frac{\sigma^2}{2}dt\\ &\le -\upsilon H(\tilde P_{T_n,t},\tilde Q_{T_n,t})dt+\frac{\sigma^2}{2}dt+\left(\tilde P_{T_n,t}+\frac{\upsilon}{2}\tilde Q_{T_n,t}\right)\sigma dW_t, \end{aligned}$$

which yields that $H(\tilde P_{T_n,t},\tilde Q_{T_n,t})\le e^{-\upsilon(t-t_n)}H(\tilde P_{T_n,t_n},\tilde Q_{T_n,t_n})+\frac{\sigma^2}{2}\int_{t_n}^t e^{-\upsilon(t-s)}ds+\int_{t_n}^t e^{-\upsilon(t-s)}(\tilde P_{T_n,s}+\frac{\upsilon}{2}\tilde Q_{T_n,s})\sigma dW_s$. By the preservation of the Hamiltonian for (2.5), we obtain $H(\tilde P_{T_n,t_n},\tilde Q_{T_n,t_n})=H(\bar P_{T_n,t_{n+1}},\bar Q_{T_n,t_{n+1}})=H(P_n,Q_n)$, and thus, by iteration, we arrive at

$$\begin{aligned} H(\tilde P_{T_n,t},\tilde Q_{T_n,t}) \le{}& e^{-\upsilon t}H(P_0,Q_0)+\frac{\sigma^2}{2}\int_0^t e^{-\upsilon(t-s)}ds\\ &+\int_0^t e^{-\upsilon(t-s)}\left(\tilde P_{T_{n_s},s}+\frac{\upsilon}{2}\tilde Q_{T_{n_s},s}\right)\sigma dW_s. \end{aligned}\tag{A.1}$$

Applying the maximal inequality and combining (2.9) gives that for any fixed $T>0$,

$$\begin{aligned} \mathbb{E}\left[\sup_{t\in[0,T]}(|\tilde P_{T_{n_t},t}|^2+|\tilde Q_{T_{n_t},t}|^4)\right] \le{}& C(H(P_0,Q_0)+1)\\ &+\int_0^T\mathbb{E}\left[\sup_{r\in[0,s]}|\tilde P_{T_{n_r},r}|^2+|\tilde Q_{T_{n_r},r}|^4\right]ds, \end{aligned}$$

which, together with the Grönwall inequality, leads to (2.6) with $\mathfrak{p}=1$. Then taking expectation on both sides of (A.1) and using (2.9) finishes the proof for $\mathfrak{p}=1$.

Assume that (2.6) and (2.7) hold for the case of $\mathfrak{p}-1$ with $\mathfrak{p}\ge 2$. Then we show the case of $\mathfrak{p}$. By the Itô formula, we have

$$\begin{aligned} &dH^{\mathfrak{p}}(\tilde P_{T_n,t},\tilde Q_{T_n,t})\\ &\quad\le -\upsilon\mathfrak{p}H^{\mathfrak{p}}(\tilde P_{T_n,t},\tilde Q_{T_n,t})dt+\mathfrak{p}(\mathfrak{p}-1)\sigma^2 H^{\mathfrak{p}-2}(\tilde P_{T_n,t},\tilde Q_{T_n,t})\\ &\qquad\times\left(\frac{\tilde P^2_{T_n,t}}{2}+\frac{\upsilon}{2}\tilde P_{T_n,t}\tilde Q_{T_n,t}+\frac{\upsilon^2}{8}\tilde Q^2_{T_n,t}\right)dt\\ &\qquad+\frac{1}{2}\mathfrak{p}\sigma^2 H^{\mathfrak{p}-1}(\tilde P_{T_n,t},\tilde Q_{T_n,t})dt+\sigma\mathfrak{p}H^{\mathfrak{p}-1}(\tilde P_{T_n,t},\tilde Q_{T_n,t})\left(\tilde P_{T_n,t}+\frac{\upsilon}{2}\tilde Q_{T_n,t}\right)dW_t. \end{aligned}$$

From the Young inequality, we derive that

$$\begin{aligned} dH^{\mathfrak{p}}(\tilde P_{T_n,t},\tilde Q_{T_n,t}) \le{}& -\upsilon\mathfrak{p}H^{\mathfrak{p}}(\tilde P_{T_n,t},\tilde Q_{T_n,t})dt+\mathfrak{p}\left(\mathfrak{p}-\frac{1}{2}\right)\sigma^2 H^{\mathfrak{p}-1}(\tilde P_{T_n,t},\tilde Q_{T_n,t})dt\\ &+C\mathfrak{p}(\mathfrak{p}-1)\sigma^2 H^{\mathfrak{p}-2}(\tilde P_{T_n,t},\tilde Q_{T_n,t})dt\\ &+\sigma\mathfrak{p}H^{\mathfrak{p}-1}(\tilde P_{T_n,t},\tilde Q_{T_n,t})\left(\tilde P_{T_n,t}+\frac{\upsilon}{2}\tilde Q_{T_n,t}\right)dW_t. \end{aligned}$$

Let $\gamma \in (0,1)$ be a small number to be determined later. The Young inequality gives

$$\begin{aligned} d(e^{\gamma\mathfrak{p}t}H^{\mathfrak{p}}(\tilde{P}_{T_n,t},\tilde{Q}_{T_n,t})) &\leq e^{\gamma\mathfrak{p}t}(\gamma\mathfrak{p}-\upsilon\mathfrak{p}+\epsilon\mathfrak{p})H^{\mathfrak{p}}(\tilde{P}_{T_n,t},\tilde{Q}_{T_n,t})dt + C(\epsilon)e^{\gamma\mathfrak{p}t}dt \\ &\quad + \sigma\mathfrak{p}H^{\mathfrak{p}-1}(\tilde{P}_{T_n,t},\tilde{Q}_{T_n,t})\Big(\tilde{P}_{T_n,t}+\frac{\upsilon}{2}\tilde{Q}_{T_n,t}\Big)e^{\gamma\mathfrak{p}t}dW_t. \end{aligned} \tag{A.2}$$

One can choose ϵ and γ so that $\gamma - \upsilon + \epsilon \leq -\frac{\upsilon}{2} < 0$. Notice that for any fixed $T > 0$,

$$\begin{aligned} &\mathbb{E}\left[\sup_{t\in[0,T]}\left|\int_0^t H^{\mathfrak{p}-1}(\tilde{P}_{T_{n_s},s},\tilde{Q}_{T_{n_s},s})\big(\tilde{P}_{T_{n_s},s}+\frac{\upsilon}{2}\tilde{Q}_{T_{n_s},s}\big)e^{-\gamma\mathfrak{p}(t-s)}dW_s\right|\right] \\ &\leq C\left(\mathbb{E}\left[\sup_{s\in[0,T]}H^{\mathfrak{p}-1}(\tilde{P}_{T_{n_s},s},\tilde{Q}_{T_{n_s},s})\right]\right)^{\frac{1}{2}}\left(\mathbb{E}\left[\int_0^T H^{\mathfrak{p}}(\tilde{P}_{T_{n_s},s},\tilde{Q}_{T_{n_s},s})ds\right]\right)^{\frac{1}{2}} + C(T) \\ &\leq C(T) + C(T)\mathbb{E}\left[\int_0^T H^{\mathfrak{p}}(\tilde{P}_{T_{n_s},s},\tilde{Q}_{T_{n_s},s})ds\right]. \end{aligned}$$

Hence, applying the Grönwall inequality yields (2.6). Furthermore, it follows from (A.2) that

$$\mathbb{E}[H^{\mathfrak{p}}(\tilde{P}_{T_n,t},\tilde{Q}_{T_n,t})] \leq e^{-\frac{\upsilon}{2}\mathfrak{p}(t-t_n)}\mathbb{E}[H^{\mathfrak{p}}(\tilde{P}_{T_n,t_n},\tilde{Q}_{T_n,t_n})] + Ce^{-\frac{\upsilon}{2}\mathfrak{p}(t-t_n)}(t-t_n). \tag{A.3}$$

Then combining the preservation of Hamiltonian for (2.5), we have

$$\mathbb{E}[H^{\mathfrak{p}}(P_{n+1},Q_{n+1})] \leq e^{-\frac{\upsilon}{2}\mathfrak{p}\tau}\mathbb{E}[H^{\mathfrak{p}}(P_n,Q_n)] + Ce^{-\frac{\upsilon}{2}\mathfrak{p}\tau}\tau, \tag{A.4}$$

which yields $\mathbb{E}[H^{\mathfrak{p}}(P_{n+1},Q_{n+1})] \leq e^{-\frac{\upsilon}{2}n\mathfrak{p}\tau}H^{\mathfrak{p}}(P_0,Q_0) + C$. Combining (2.9) finishes the proof of (2.7). ∎

REFERENCES

[1] A. Abdulle, G. Vilmart, and K. C. Zygalakis, *Long time accuracy of Lie-Trotter splitting methods for Langevin dynamics*, SIAM J. Numer. Anal., 53 (2015), pp. 1–16, https://doi.org/10.1137/140962644.

[2] N. Bou-Rabee and H. Owhadi, *Long-run accuracy of variational integrators in the stochastic context*, SIAM J. Numer. Anal., 48 (2010), pp. 278–297, https://doi.org/10.1137/090758842.

[3] W. Cai, H. Li, and Y. Wang, *Partitioned averaged vector field methods*, J. Comput. Phys., 370 (2018), pp. 25–42, https://doi.org/10.1016/j.jcp.2018.05.009.

[4] C. Chen, D. Cohen, R. D'Ambrosio, and A. Lang, *Drift-preserving numerical integrators for stochastic Hamiltonian systems*, Adv. Comput. Math., 46 (2020), 27, https://doi.org/10.1007/s10444-020-09771-5.

[5] C. Chen, T. Dang, and J. Hong, *An adaptive time-stepping fully discrete scheme for stochastic NLS equation: Strong convergence and numerical asymptotics*, Stochastic Process. Appl., 173 (2024), 104373, https://doi.org/10.1016/j.spa.2024.104373.

[6] C. Chen, J. Hong, and D. Jin, *Modified averaged vector field methods preserving multiple invariants for conservative stochastic differential equations*, BIT, 60 (2020), pp. 917–957, https://doi.org/10.1007/s10543-020-00803-6.

[7] W. T. Coffey and Y. P. Kalmykov, *The Langevin Equation*, 3rd ed., World Scientific Series in Contemporary Chemical Physics 27, World Scientific, River Edge, NJ, 2012, https://doi.org/10.1142/WSSCCP.

[8] S. Cox, M. Hutzenthaler, and A. Jentzen, *Local Lipschitz continuity in the initial value and strong completeness for nonlinear stochastic differential equations*, Mem. Amer. Math. Soc., 296 (2024), pp. v+90.

[9] J. Cui, J. Hong, and D. Sheng, *Density function of numerical solution of splitting AVF scheme for stochastic Langevin equation*, Math. Comp., 91 (2022), pp. 2283–2333, https://doi.org/10.1090/mcom/3752.

[10] L. Dai and X. Wang, *Order-one strong convergence of numerical methods for SDEs without globally monotone coefficients*, preprint, arXiv:2401.00385.

[11] D. T. Gillespie, *The chemical Langevin equation*, J. Chem. Phys., 113 (2000), pp. 297–306, https://doi.org/10.1063/1.481811, https://api.semanticscholar.org/CorpusID:44203273.

[12] J. Hong and L. Sun, *Symplectic Integration of Stochastic Hamiltonian Systems*, Lecture Notes in Mathematics 2314, Springer-Verlag, Berlin, 2022, https://doi.org/10.1007/978-981-19-7670-4.

[13] J. Hong and X. Wang, *Invariant Measures for Stochastic Nonlinear Schrödinger Equations: Numerical Approximations and Symplectic Structures*, Lecture Notes in Mathematics 2251, Springer-Verlag, Berlin, 2019, https://doi.org/10.1007/978-981-32-9069-3.

[14] A. Hudde, M. Hutzenthaler, and S. Mazzonetto, *A stochastic Gronwall inequality and applications to moments, strong completeness, strong local Lipschitz continuity, and perturbations*, Ann. Inst. Henri Poincaré Probab. Stat., 57 (2021), pp. 603–626, https://doi.org/10.1214/20-AIHP1064.

[15] M. Hutzenthaler, A. Jentzen, and X. Wang, *Exponential integrability properties of numerical approximation processes for nonlinear stochastic differential equations*, Math. Comp., 87 (2018), pp. 1353–1413, https://doi.org/10.1090/mcom/3146.

[16] B. Leimkuhler, C. Matthews, and G. Stoltz, *The computation of averages from equilibrium and nonequilibrium Langevin molecular dynamics*, IMA J. Numer. Anal., 36 (2016), pp. 13–79, https://doi.org/10.1093/imanum/dru056.

[17] J. C. Mattingly, A. M. Stuart, and D. J. Higham, *Ergodicity for SDEs and approximations: Locally Lipschitz vector fields and degenerate noise*, Stochastic Process. Appl., 101 (2002), pp. 185–232, https://doi.org/10.1016/S0304-4149(02)00150-3.

[18] G. N. Milstein and M. V. Tretyakov, *Computing ergodic limits for Langevin equations*, Phys. D, 229 (2007), pp. 81–95, https://doi.org/10.1016/j.physd.2007.03.011.

[19] G. A. Pavliotis, *Stochastic Processes and Applications: Diffusion Processes, the Fokker-Planck and Langevin Equations*, Texts in Applied Mathematics 60, Springer-Verlag, Berlin, 2014, https://doi.org/10.1007/978-1-4939-1323-7.

[20] G. R. W. Quispel and D. I. McLaren, *A new class of energy-preserving numerical integration methods*, J. Phys. A, 41 (2008), 045206, https://doi.org/10.1088/1751-8113/41/4/045206.

[21] D. Talay, *Stochastic Hamiltonian systems: Exponential convergence to the invariant measure, and discretization by the implicit Euler scheme*, Markov Process. Related Fields, 8 (2002), pp. 163–198.

[22] B. K. Tapley, *Geometric integration of ODEs using multiple quadratic auxiliary variables*, SIAM J. Sci. Comput., 44 (2022), pp. A2651–A2668, https://doi.org/10.1137/21M1442644.

[23] W. Zhou, L. Zhang, J. Hong, and S. Song, *Projection methods for stochastic differential equations with conserved quantities*, BIT, 56 (2016), pp. 1497–1518, https://doi.org/10.1007/s10543-016-0614-0.