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Explicit pseudo-symplectic methods for stochastic Hamiltonian systems

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Abstract We construct stochastic pseudo-symplectic methods and analyze their pseudo-symplectic orders for stochastic Hamiltonian systems with additive noises in this paper. All of these methods are explicit so that the numerical implementations become much easier than implicit methods. Through the numerical experiments, we find that these methods have desired properties in accuracy and stability as well as the preservation of the symplectic structure of the systems.

Keywords Stochastic Hamiltonian system · Pseudo-symplectic method · Explicit Runge–Kutta method

Mathematics Subject Classification 60H35 · 37M15 · 60H10

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1 Introduction

Hamiltonian systems perturbed by additive Gaussian noises are used to describe the traditional Hamiltonian systems driven by random forces, which may give rise to essential differences in dynamical evolutions (see e.g. [3,5,10]). In this paper, we consider a class of stochastic Hamiltonian systems of the form

$$
\begin{aligned}
dP &= f(P, Q)dt + \sum_{r=1}^{m} \sigma_r(t) dW_r(t), \quad P(t_0) = p, \\
dQ &= g(P, Q)dt + \sum_{r=1}^{m} \gamma_r(t) dW_r(t), \quad Q(t_0) = q, \\
f &= -\frac{\partial H}{\partial q}, \quad g = \frac{\partial H}{\partial p},
\end{aligned}
\tag{1.1}
$$

where $P,\ Q,\ f,\ g,\ \sigma_r,\ \gamma_r$ are n-dimensional column-vectors, W_r are independent standard Wiener processes on a probability space $(\Omega, \mathscr{F}, \mathbb{P})$, $r = 1, \ldots, m$, and H is a Hamiltonian.

The Hamiltonians are assumed to be in $\mathscr{C}_b^K$ for certain $K \in \mathbb{N}$, the function space consists of K-times continuous differentiable functions with bounded derivatives up to order K. As in the deterministic case, the solution

$$\varphi_t(p_0, q_0) = (P(t, p_0, q_0), Q(t, p_0, q_0))$$

of (1.1) preserves the symplectic structure (see e.g. [10], Theorem 4.1). That is, for $y_0 = (p_0, q_0)$,

$$\left(\frac{\partial \varphi_t}{\partial y_0}\right)^T J \left(\frac{\partial \varphi_t}{\partial y_0}\right) = J, \quad \text{where} \quad J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}.$$

To numerically solve the stochastic Hamiltonian system (1.1), much research is looking at the stochastic symplectic integrators (see, [3,6,8,9,11–13] and references therein). This interest is motivated by the fact that symplectic integrators, in comparison with usual numerical schemes, allow us to simulate Hamiltonian systems on a long time interval with high accuracy. However, the backward error analysis for showing the good long time behaviors of stochastic symplectic integrators for stochastic Hamiltonian systems does not exist in the literature and it is a challenging open problem. It is known that all of stochastic symplectic methods should be implicit for general stochastic Hamiltonian systems and thus more computation complexity will arise. Only for special stochastic Hamiltonian systems such as separable systems, explicit stochastic symplectic methods can be constructed (see [10]).

In this paper, we construct explicit stochastic pseudo-symplectic methods for system (1.1) that can preserve the symplectic properties in relatively long time frames with certain accuracy. For the deterministic Hamiltonian systems, Aubry and Chartier [2] have proposed the concept of pseudo-symplectic methods (see also [7]). A one-step numerical method $y_1 = \Phi_h(y_0)$ of order M, $\Phi_h = \varphi_h + \mathscr{O}(h^{M+1})$, is called a pseudo-symplectic method of order (M, N) with $N > M$, if it satisfies

$$\left(\frac{\partial \Phi_h}{\partial y_0}\right)^T J \left(\frac{\partial \Phi_h}{\partial y_0}\right) - J = \mathscr{O}(h^{N+1}).$$

This idea motivates the following definition of a stochastic pseudo-symplectic method, whose strong convergence rate should be consistent with the convergence of stochastic integral in the sense of $L^2(\Omega)$-norm. From the viewpoint of structure preservation, stochastic symplectic methods and stochastic pseudo-symplectic methods generally have good performance, although it is also worthy to mention that there are exceptions such as the Lie-Trotter splitting methods for the simulation of the invariant measure for stochastic Langevin equation in [1].

Definition 1.1 If a numerical method $y_1 = \Phi_h(y_0)$ of mean-square order M for the stochastic Hamiltonian system (1.1) satisfies

$$\left\| \left(\frac{\partial \Phi_h}{\partial y_0}\right)^T J \left(\frac{\partial \Phi_h}{\partial y_0}\right) - J \right\|_{L^2(\Omega)} := \left(\mathbb{E} \left\| \left(\frac{\partial \Phi_h}{\partial y_0}\right)^T J \left(\frac{\partial \Phi_h}{\partial y_0}\right) - J \right\|^2 \right)^{\frac{1}{2}}$$
$$= \mathscr{O}\left(h^{N+1}\right),$$

with $N > M$, then this method is called a pseudo-symplectic method of mean-square order (M, N), and N is called the pseudo-symplectic order. Here $\|\cdot\|$ denotes the Frobenius norm and $\mathbb{E}$ denotes the expectation.

The rest of this paper is organized as follows. We construct a series of pseudo-symplectic methods for (1.1) with additive noise in Sect. 2, and give the pseudo-symplectic orders. In Sect. 3, we give numerical experiments for the pseudo-symplectic mid-point method. Compared with the Euler method and the symplectic method, we find that the pseudo-symplectic methods can be used in long-time computations to nearly preserve the symplectic structure. Finally, in Sect. 4, a summary of our work is presented.

2 Pseudo-symplectic methods for stochastic Hamiltonian systems

In this section, we construct two explicit methods and a series of explicit Runge–Kutta methods for (1.1).

2.1 Stochastic pseudo-symplectic mid-point method and stochastic pseudo-symplectic trapezoidal method

Suppose that $0 = t_0 < t_1 \cdots < t_n = T$ is a partition of $[0, T]$ with $t_k = kh$, $k = 0, \ldots, n-1$, and $h = \frac{T}{n}$. Denote $\delta_k W_r := W_r(t_k + h) - W_r(t_k)$, $r = 1, \ldots, m$, $k = 0, \ldots, n-1$, and define

$$\begin{aligned}\widetilde{p} &= p + f(p,q)h + \sum_{r=1}^{m} \sigma_r(t_k)\delta_k W_r,\\ \widetilde{q} &= p + g(p,q)h + \sum_{r=1}^{m} \gamma_r(t_k)\delta_k W_r.\end{aligned} \tag{2.1}$$

For $\alpha \in [0, 1]$, define

$$\begin{aligned}\overline{P} &= p + \alpha h f(p,q) + (1-\alpha)hf(\tilde{p},\tilde{q}) + \sum_{r=1}^{m} \sigma_r(t_k)\delta_k W_r,\\ \overline{Q} &= q + \alpha h g(p,q) + (1-\alpha)hg(\tilde{p},\tilde{q}) + \sum_{r=1}^{m} \gamma_r(t_k)\delta_k W_r,\end{aligned} \tag{2.2}$$

and

$$\begin{aligned}\widehat{P} &= p + hf\,(\alpha\tilde{p} + (1-\alpha)p, (1-\alpha)\tilde{q} + \alpha q) + \sum_{r=1}^{m} \sigma_r(t_k)\delta_k W_r,\\ \widehat{Q} &= q + hg\,(\alpha\tilde{p} + (1-\alpha)p, (1-\alpha)\tilde{q} + \alpha q) + \sum_{r=1}^{m} \gamma_r(t_k)\delta_k W_r.\end{aligned} \tag{2.3}$$

Comparing the above two explicit methods (2.1)+(2.2) and (2.1)+(2.3) with Euler method and then applying Milstein's mean-square comparison theorem (see e.g. [10], theorem 1.2.5), we obtain the convergence of the two explicit methods with mean-square order 1. They are both shown to be pseudo-symplectic in the following theorem.

Theorem 2.1 *Assume that $H \in \mathscr{C}_b^2$, then there exists a positive constant $C_1 = C_1(H,\alpha)$ such that the methods (2.1)+(2.2) and (2.1)+(2.3) for the system (1.1) satisfy*

$$\left\| \left(\frac{\partial(\overline{P},\overline{Q})}{\partial(p,q)}\right)^T J \left(\frac{\partial(\overline{P},\overline{Q})}{\partial(p,q)}\right) - J \right\|_{L^2(\Omega)} = C_1 h^2 + \mathscr{O}(h^3). \tag{2.4}$$

Moreover, if $H \in \mathscr{C}_b^4$, then there exists a positive constant $C_2 = C_2(H)$ such that

$$\left\| \left(\frac{\partial(\overline{P},\overline{Q})}{\partial(p,q)}\right)^T J \left(\frac{\partial(\overline{P},\overline{Q})}{\partial(p,q)}\right) - J \right\|_{L^2(\Omega)} = |2\alpha - 1| C_2 h^2 + \mathscr{O}(h^3). \tag{2.5}$$

Proof We only prove the results for the method (2.1)+(2.2). Similar arguments can be applied to the method (2.1)+(2.3). Rewrite (2.1)+(2.2) as

$$\begin{aligned}\tilde{F} &:= \tilde{p} - p - f(p,q)h - \sum_{r=1}^{m} \sigma_r(t_k)\delta_k W_r = 0,\\ \tilde{G} &:= \tilde{q} - p - g(p,q)h - \sum_{r=1}^{m} \gamma_r(t_k)\delta_k W_r = 0,\end{aligned}$$

and

$$\overline{F} := \overline{P} - p - \alpha h f(p,q) - (1-\alpha) h f(\tilde{p},\tilde{q}) - \sum_{r=1}^{m} \sigma_r(t_k)\delta_k W_r,$$
$$\overline{G} := \overline{Q} - q - \alpha h g(p,q) - (1-\alpha) h g(\tilde{p},\tilde{q}) - \sum_{r=1}^{m} \gamma_r(t_k)\delta_k W_r.$$

Assume that H is twice differentiable. From the above equations we have

$$\frac{\partial(\overline{F},\overline{G})}{\partial(\overline{P},\overline{Q})} \cdot \frac{\partial(\overline{P},\overline{Q})}{\partial(p,q)} + \frac{\partial(\overline{F},\overline{G})}{\partial(\tilde{p},\tilde{q})} \cdot \frac{\partial(\tilde{p},\tilde{q})}{\partial(p,q)} + \frac{\partial(\overline{F},\overline{G})}{\partial(p,q)} = 0.$$

Simple calculations yield

$$\begin{aligned}
\frac{\partial(\overline{F},\overline{G})}{\partial(\overline{P},\overline{Q})} &= \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix},\\
\frac{\partial(\overline{F},\overline{G})}{\partial(\tilde{p},\tilde{q})} &= \begin{pmatrix} (1-\alpha)\tilde{H}_{pq}h & (1-\alpha)\tilde{H}_{qq}h \\ -(1-\alpha)\tilde{H}_{pp}h & -(1-\alpha)\tilde{H}_{pq}h \end{pmatrix},\\
\frac{\partial(\tilde{p},\tilde{q})}{\partial(p,q)} &= \begin{pmatrix} I - H_{pq}h & -H_{qq}h \\ H_{pp}h & I + H_{pq}h \end{pmatrix},\\
\frac{\partial(\overline{F},\overline{G})}{\partial(p,q)} &= \begin{pmatrix} -I + \alpha H_{pq}h & \alpha H_{qq}h \\ -\alpha H_{pp}h & -I - \alpha H_{pq}h \end{pmatrix},
\end{aligned}$$

where $\tilde{H}_{pp}$, $\tilde{H}_{pq}$ and $\tilde{H}_{qq}$ denote the second derivatives of H with respect to $\tilde{p}$ and $\tilde{q}$. Then

$$\frac{\partial(\overline{P},\overline{Q})}{\partial(p,q)} = -\frac{\partial(\overline{F},\overline{G})}{\partial(\tilde{p},\tilde{q})} \cdot \frac{\partial(\tilde{p},\tilde{q})}{\partial(p,q)} - \frac{\partial(\overline{F},\overline{G})}{\partial(p,q)} =: \begin{pmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{pmatrix}.$$

with

$$\begin{aligned}
\Sigma_{11} &= I - [\alpha H_{pq} + (1-\alpha)\widetilde{H}_{pq}]h + (1-\alpha)(\widetilde{H}_{pq}H_{pq} - \widetilde{H}_{qq}H_{pp})h^2,\\
\Sigma_{12} &= -[\alpha H_{qq} + (1-\alpha)\widetilde{H}_{qq}]h + (1-\alpha)(\widetilde{H}_{pq}H_{qq} - \widetilde{H}_{qq}H_{pq})h^2,\\
\Sigma_{21} &= [\alpha H_{pp} + (1-\alpha)\widetilde{H}_{pp}]h - (1-\alpha)(\widetilde{H}_{pp}H_{pq} - \widetilde{H}_{pq}H_{pp})h^2,\\
\Sigma_{22} &= I + [\alpha H_{pq} + (1-\alpha)\widetilde{H}_{pq}]h - (1-\alpha)(\widetilde{H}_{pp}H_{qq} - \widetilde{H}_{pq}H_{pq})h^2.
\end{aligned}$$

Thus

$$\left(\frac{\partial(\overline{P},\overline{Q})}{\partial(p,q)}\right)^T J \left(\frac{\partial(\overline{P},\overline{Q})}{\partial(p,q)}\right) = \begin{pmatrix} \Sigma_{11}^T\Sigma_{21} - \Sigma_{21}^T\Sigma_{11} & \Sigma_{11}^T\Sigma_{22} - \Sigma_{21}^T\Sigma_{12} \\ \Sigma_{12}^T\Sigma_{21} - \Sigma_{22}^T\Sigma_{11} & \Sigma_{12}^T\Sigma_{22} - \Sigma_{22}^T\Sigma_{12} \end{pmatrix}.$$

In what follows we only estimate $\Sigma_{11}^T\Sigma_{21} - \Sigma_{21}^T\Sigma_{11}$, while an analogous idea can be applied to estimate the terms $\Sigma_{11}^T\Sigma_{22} - \Sigma_{21}^T\Sigma_{12}$, $\Sigma_{12}^T\Sigma_{21} - \Sigma_{22}^T\Sigma_{11}$ and $\Sigma_{12}^T\Sigma_{22} - \Sigma_{22}^T\Sigma_{12}$.

Direct calculations yield that

$$
\begin{aligned}
&\left\| \Sigma_{11}^T\Sigma_{21} - \Sigma_{21}^T\Sigma_{11} \right\|_{L^2(\Omega)} \\
&= \Big\| \alpha^2 (H_{pp}H_{pq} - H_{pq}H_{pp}) + (1-\alpha)^2 (\widetilde{H}_{pp}\widetilde{H}_{pq} - \widetilde{H}_{pq}\widetilde{H}_{pp}) \\
&\quad - (1-\alpha)^2 (H_{pp}\widetilde{H}_{pq} - H_{pq}\widetilde{H}_{pp}) \\
&\quad - (1-\alpha)^2 (\widetilde{H}_{pp}H_{pq} - \widetilde{H}_{pq}H_{pp}) \Big\|_{L^2(\Omega)} h^2 + \mathscr{O}(h^3).
\end{aligned}
$$

Thus (2.4) holds for certain C_1.

Now we assume that $H \in \mathscr{C}_b^4$. Expanding $\widetilde{H}_{pp}$ and $\widetilde{H}_{pq}$ at (p, q), we have

$$
\begin{aligned}
\widetilde{H}_{pp} &= H_{pp} + H_{ppp} \otimes (\widetilde{p} - p) + H_{ppq} \otimes (\widetilde{q} - q) + C_3 h, \\
\widetilde{H}_{pq} &= H_{pq} + H_{ppq} \otimes (\widetilde{p} - p) + H_{pqq} \otimes (\widetilde{q} - q) + C_4 h.
\end{aligned}
$$

Since $\widetilde{p} - p$ and $\widetilde{q} - q$ are both $O(h^{\frac{1}{2}})$, the coefficient of h^2 in the estimation of $\Sigma_{11}^T\Sigma_{21} - \Sigma_{21}^T\Sigma_{11}$ is $|2\alpha - 1| \left(\mathbb{E}\|H_{pp}H_{pq} - H_{pq}H_{pp}\|^2\right)^{\frac{1}{2}} + \mathscr{O}(h)$. So there exists a positive constant $\widetilde{C} = \widetilde{C}(H)$ such that

$$
\left\| \Sigma_{11}^T\Sigma_{21} - \Sigma_{21}^T\Sigma_{11} \right\|_{L^2(\Omega)} = |2\alpha - 1| \widetilde{C} h^2 + \mathscr{O}\left(h^3\right).
$$

This yields (2.5) and we complete the proof.

The expansion (2.4) implies that, for (1.1), the method (2.1)+(2.2) and (2.1)+(2.3) are of order (1, 2) if and only if $\alpha = \frac{1}{2}$. We call them the stochastic pseudo-symplectic mid-point method and stochastic pseudo-symplectic trapezoidal method, respectively. Moreover, the proof of Theorem 2.1 implies that the coefficients of h^3 in the estimation of $\Sigma_{11}^T\Sigma_{21} - \Sigma_{21}^T\Sigma_{11}$ could not vanish, even if $\alpha = \frac{1}{2}$. This shows that the method (2.1)+(2.2) and (2.1)+(2.3) for (1.1) could not be pseudo-symplectic with pseudo-symplectic order more than 2 for any $\alpha \in [0, 1]$.

2.2 Explicit Runge–Kutta methods

Among the numerical methods for stochastic Hamiltonian systems, Runge–Kutta methods belongs to an important class of methods. However, they may bring more complexity to the calculations because they can be implicit. We try to construct a class of explicit Runge–Kutta methods in this subsection. Set

$$\begin{aligned}
\mathscr{P}_1 &= p + \varphi_1, \quad \mathscr{Q}_1 = q + \psi_1, \\
\mathscr{P}_i &= p + h\sum_{j=1}^{i-1}\alpha_{ij} f(\mathscr{P}_j, \mathscr{Q}_j) + \varphi_i, \quad \mathscr{Q}_i = q + h\sum_{j=1}^{i-1}\alpha_{ij} g(\mathscr{P}_j, \mathscr{Q}_j) + \psi_i, \\
P &= p + h\sum_{i=1}^{s}\beta_i f(\mathscr{P}_i, \mathscr{Q}_i) + \eta, \quad Q = q + h\sum_{i=1}^{s}\beta_i g(\mathscr{P}_i, \mathscr{Q}_i) + \zeta,
\end{aligned} \tag{2.6}$$

with $i = 2, \ldots, s$, where $\varphi_i,\ \psi_i,\ \eta,\ \zeta,\ i = 1, \ldots, s$, are functions that are independent of p and q and parameters $\alpha_{ij},\ \beta_i,\ i = 2, \ldots, s,\ j = 1, \ldots, i-1$, need to be fixed.

We first construct a 2-stage explicit Runge–Kutta method

$$\begin{aligned}
\mathscr{P}_1 &= p + \varphi_1, \quad \mathscr{Q}_1 = q + \psi_1, \\
\mathscr{P}_2 &= p + h\alpha_{21} f(\mathscr{P}_1, \mathscr{Q}_1) + \varphi_2, \quad \mathscr{Q}_2 = q + h\alpha_{21} g(\mathscr{P}_1, \mathscr{Q}_1) + \psi_2, \\
P &= p + h\beta_1 f(\mathscr{P}_1, \mathscr{Q}_1) + h\beta_2 f(\mathscr{P}_2, \mathscr{Q}_2) + \eta, \\
Q &= q + h\beta_1 g(\mathscr{P}_1, \mathscr{Q}_1) + h\beta_2 g(\mathscr{P}_2, \mathscr{Q}_2) + \zeta.
\end{aligned} \tag{2.7}$$

Let

$$\begin{aligned}
\varphi_1 &= \sum_{r=1}^{m}\sigma_r(\lambda_1 J_{r0} + \mu_1\delta_k W_r), \quad \psi_1 = \sum_{r=1}^{m}\gamma_r(\lambda_1 J_{r0} + \mu_1\delta_k W_r), \\
\varphi_2 &= \sum_{r=1}^{m}\sigma_r(\lambda_2 J_{r0} + \mu_2\delta_k W_r), \quad \psi_2 = \sum_{r=1}^{m}\gamma_r(\lambda_2 J_{r0} + \mu_2\delta_k W_r), \\
\eta &= \sum_{r=1}^{m}\sigma_r\delta_k W_r + \sum_{r=1}^{m}\sigma_r^{'} I_{0r}, \quad \zeta = \sum_{r=1}^{m}\gamma_r\delta_k W_r + \sum_{r=1}^{m}\gamma_r^{'} I_{0r},
\end{aligned} \tag{2.8}$$

where

$$\delta_k W_r := h^{\frac{1}{2}}\xi_{rk},\ (J_{r0})_k := h^{\frac{1}{2}}\left(\frac{\xi_{rk}}{2} + \frac{\eta_{rk}}{\sqrt{12}}\right),\ (I_{0r})_k := h^{\frac{3}{2}}\left(\frac{\xi_{rk}}{2} - \frac{\eta_{rk}}{\sqrt{12}}\right) \tag{2.9}$$

with ξ_{rk} and $\eta_{rk}, r = 1, 2, \ldots, m, k = 0, 1, \ldots, n-1$, being a sequence of independent $N(0, 1)$-distributed random variables and where the parameters satisfy

$$\begin{aligned}
&\beta_1 + \beta_2 = 1,\ \alpha_{21}\beta_2 = \frac{1}{2},\ \sum_{i=1}^{3}\alpha_i\lambda_i = 1,\ \sum_{i=1}^{3}\alpha_i\mu_i = 0, \\
&\sum_{i=1}^{3}\alpha_i(\lambda_i J_{r0} + \mu_i\delta_k W_r)(\lambda_i J_{l0} + \mu_i\delta_k W_l) = \frac{h}{2}\delta_{rl}.
\end{aligned} \tag{2.10}$$

It turns out that the method (2.7)–(2.9), satisfying (2.10), is mean-square convergent of order $\frac{3}{2}$ (see e.g. [10]). We don't consider any higher order scheme here due to the fact that schemes with mean-square order higher than $\frac{3}{2}$ need to simulate the multiple Wiener intergral (see e.g. [13]). The following theorem shows that (2.7) is pseudo-symplectic of pseudo-symplectic order 2, with appropriate assumptions on the Hamiltonian H.

Theorem 2.2 *Assume that* $H \in \mathscr{C}_b^4$ *and the parameters in the 2-stage explicit Runge–Kutta method* (2.7)–(2.9) *satisfy the condition* (2.10)*, then this method is pseudo-symplectic of order* $(\frac{3}{2}, 2)$ *provided* $\beta_1 = \frac{1}{2},\ \beta_2 = \frac{1}{2}$ *and* $\alpha_{21} = 1$.

Proof Rewrite (2.7) as

$$\begin{aligned} F_1 &:= \mathscr{P}_1 - p - \varphi_1 = 0, \quad G_1 := \mathscr{Q}_1 - q - \psi_1 = 0,\\ F_2 &:= \mathscr{P}_2 - p - h\alpha_{21} f(\mathscr{P}_1, \mathscr{Q}_1) - \varphi_2 = 0,\\ G_2 &:= \mathscr{Q}_2 - q - h\alpha_{21} g(\mathscr{P}_1, \mathscr{Q}_1) - \psi_2 = 0,\\ F &:= P - p - h\beta_1 f(\mathscr{P}_1, \mathscr{Q}_1) - h\beta_2 f(\mathscr{P}_2, \mathscr{Q}_2) - \eta = 0,\\ G &:= Q - q - h\beta_1 g(\mathscr{P}_1, \mathscr{Q}_1) - h\beta_2 g(\mathscr{P}_2, \mathscr{Q}_2) - \zeta = 0. \end{aligned}$$

The above formulations immediately yield

$$\begin{aligned} &\frac{\partial(F,G)}{\partial(P,Q)} \cdot \frac{\partial(P,Q)}{\partial(p,q)} + \frac{\partial(F,G)}{\partial(\mathscr{P}_2,\mathscr{Q}_2)} \cdot \frac{\partial(\mathscr{P}_2,\mathscr{Q}_2)}{\partial(p,q)}\\ &+ \frac{\partial(F,G)}{\partial(\mathscr{P}_1,\mathscr{Q}_1)} \cdot \frac{\partial(\mathscr{P}_1,\mathscr{Q}_1)}{\partial(p,q)} + \frac{\partial(F,G)}{\partial(p,q)} = 0,\\ &\frac{\partial(F_2,G_2)}{\partial(\mathscr{P}_2,\mathscr{Q}_2)} \cdot \frac{\partial(\mathscr{P}_2,\mathscr{Q}_2)}{\partial(p,q)} + \frac{\partial(F_2,G_2)}{\partial(\mathscr{P}_1,\mathscr{Q}_1)} \cdot \frac{\partial(\mathscr{P}_1,\mathscr{Q}_1)}{\partial(p,q)} + \frac{\partial(F_2,G_2)}{\partial(p,q)} = 0,\\ &\frac{\partial(F_1,G_1)}{\partial(\mathscr{P}_1,\mathscr{Q}_1)} \cdot \frac{\partial(\mathscr{P}_1,\mathscr{Q}_1)}{\partial(p,q)} + \frac{\partial(F_1,G_1)}{\partial(p,q)} = 0. \end{aligned}$$

Successively, we can get

$$\frac{\partial(\mathscr{P}_1,\mathscr{Q}_1)}{\partial(p,q)} = \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix}, \quad \frac{\partial(\mathscr{P}_2,\mathscr{Q}_2)}{\partial(p,q)} = \begin{pmatrix} I - \alpha_{21} H_{pq}^{(1)} h & -\alpha_{21} H_{qq}^{(1)} h \\ \alpha_{21} H_{pp}^{(1)} h & I + \alpha_{21} H_{pq}^{(1)} h \end{pmatrix},$$

and

$$\begin{aligned} \frac{\partial(P,Q)}{\partial(p,q)} &= - \frac{\partial(F,G)}{\partial(\mathscr{P}_2,\mathscr{Q}_2)} \cdot \frac{\partial(\mathscr{P}_2,\mathscr{Q}_2)}{\partial(p,q)} - \frac{\partial(F,G)}{\partial(\mathscr{P}_1,\mathscr{Q}_1)} \cdot \frac{\partial(\mathscr{P}_1,\mathscr{Q}_1)}{\partial(p,q)} - \frac{\partial(F,G)}{\partial(p,q)}\\ &=: \begin{pmatrix} \Theta_{11} & \Theta_{12} \\ \Theta_{21} & \Theta_{22} \end{pmatrix}, \end{aligned}$$

with

$$\Theta_{11} = I - (\beta_1 H_{pq}^{(1)} + \beta_2 H_{pq}^{(2)})h + \alpha_{21}\beta_2 (H_{pq}^{(2)} H_{pq}^{(1)} - H_{qq}^{(2)} H_{pp}^{(1)})h^2,$$

$$\Theta_{12} = -(\beta_1 H^{(1)}_{qq} + \beta_2 H^{(2)}_{qq})h + \alpha_{21}\beta_2(H^{(2)}_{pq} H^{(1)}_{qq} - H^{(2)}_{qq} H^{(1)}_{pq})h^2,$$
$$\Theta_{21} = (\beta_1 H^{(1)}_{pp} + \beta_2 H^{(2)}_{pp})h - \alpha_{21}\beta_2(H^{(2)}_{pp} H^{(1)}_{pq} - H^{(2)}_{pq} H^{(1)}_{pp})h^2,$$
$$\Theta_{22} = I + (\beta_1 H^{(1)}_{pq} + \beta_2 H^{(2)}_{pq})h - \alpha_{21}\beta_2(H^{(2)}_{pp} H^{(1)}_{qq} - H^{(2)}_{pq} H^{(1)}_{pq})h^2.$$

We have

$$\left(\frac{\partial(P,Q)}{\partial(p,q)}\right)^T J \left(\frac{\partial(P,Q)}{\partial(p,q)}\right) = \begin{pmatrix} \Theta_{11}^T\Theta_{21} - \Theta_{21}^T\Theta_{11} & \Theta_{11}^T\Theta_{22} - \Theta_{21}^T\Theta_{12} \\ \Theta_{12}^T\Theta_{21} - \Theta_{22}^T\Theta_{11} & \Theta_{12}^T\Theta_{22} - \Theta_{22}^T\Theta_{12} \end{pmatrix}, \tag{2.11}$$

Next we only focus on the estimate for $\Theta_{11}^T\Theta_{21} - \Theta_{21}^T\Theta_{11}$. An analogous idea can be applied to estimate the other elements of the above matrix.

Direct calculations yield that

$$\begin{aligned} &\left(\mathbb{E}\left\|\Theta_{11}^T\Theta_{21} - \Theta_{21}^T\Theta_{11}\right\|^2\right)^{\frac{1}{2}} \\ &= \Big(\mathbb{E}\Big\| - \beta_1^2(H^{(1)}_{pq}H^{(1)}_{pp} - H^{(1)}_{pp}H^{(1)}_{pq}) - \beta_2^2(H^{(2)}_{pq}H^{(2)}_{pp} - H^{(2)}_{pp}H^{(2)}_{pq}) \\ &\quad + (\alpha_{21}\beta_2 - \beta_2\beta_1)((H^{(2)}_{pq}H^{(1)}_{pp} - H^{(2)}_{pp}H^{(1)}_{pq}) + (H^{(1)}_{pq}H^{(2)}_{pp} - H^{(1)}_{pp}H^{(1)}_{pq}))\Big\|^2\Big)^{\frac{1}{2}} h^2 \\ &\quad + \mathscr{O}(h^{\frac{5}{2}}). \end{aligned}$$

Therefore, (2.4) holds for some C_1. Due to

$$H^{(2)}_{pq} = H^{(1)}_{pq} + H^{(1)}_{ppq} \otimes (P_2 - P_1) + H^{(1)}_{pqq} \otimes (Q_2 - Q_1) + O(h),$$
$$H^{(2)}_{pq} = H^{(1)}_{pq} + H^{(1)}_{ppq} \otimes (P_2 - P_1) + H^{(1)}_{pqq} \otimes (Q_2 - Q_1) + O(h),$$

and the relationship of p, q, P_1, Q_1, P_2, Q_2, we obtain

$$\begin{aligned} &\left\|\Theta_{11}^T\Theta_{21} - \Theta_{21}^T\Theta_{11}\right\|_{L^2(\Omega)} \\ &= \left|(\beta_1+\beta_2)^2 - 2\alpha_{21}\beta_2\right| \cdot \left\|H^{(1)}_{pq}H^{(1)}_{pp} - H^{(1)}_{pp}H^{(1)}_{pq}\right\|_{L^2} h^2 \\ &\quad + \left|\alpha_{21}\beta_2 - \beta_1\beta_2 - \beta_2^2\right| \cdot \left\|\mathbb{M} - \mathbb{M}^T\right\|_{L^2} h^{\frac{5}{2}} + \mathscr{O}\left(h^3\right), \end{aligned}$$

for some matrix $\mathbb{M}$ which is generally not symmetric. The above analysis implies that the 2-stage explicit RK method (2.7) is pseudo-symplectic of order $(\frac{3}{2}, 2)$ under the condition (2.10), which yields $\beta_2 = \frac{1}{2}$, $\beta_1 = \frac{1}{2}$ and $\alpha_{21} = 1$.

For general s-stage explicit Runge–Kutta method (2.6) with

$$\varphi_i = \sum_{r=1}^m \sigma_r(\lambda_i J_{r0} + \mu_i \delta_k W_r),\ \ \psi_i = \sum_{r=1}^m \gamma_r(\lambda_i J_{r0} + \mu_i \delta_k W_r),\ i = 2, \ldots, s, \tag{2.12}$$

it is convergent of mean-square order $\frac{3}{2}$ when the parameters satisfy (see e.g. [10])

$$\sum_{i=1}^{s}\beta_i = 1, \quad \sum_{i=1}^{s}\sum_{j=1}^{i-1}\beta_i\alpha_{ij} = \frac{1}{2},$$
$$\sum_{i=1}^{s}\beta_i\lambda_i = 1, \quad \sum_{i=1}^{s}\beta_i\mu_i = 0,$$
$$\sum_{i=1}^{s}\beta_i(\lambda_i J_{r0} + \mu_i\delta_k W_r)(\lambda_i J_{l0} + \mu_i\delta_k W_l) = \frac{h}{2}\delta_{rl}. \tag{2.13}$$

The following theorem shows that (2.6) satisfying (2.13) is pseudo-symplectic of pseudo-symplectic order 2. The proof is similar to that of Theorem 2.2 and thus we omit it.

Theorem 2.3 *If the parameters in the s-stage explicit Runge–Kutta method* (2.6) *satisfy* (2.13)*, then it is pseudo-symplectic of order* $(\frac{3}{2}, 2)$ *provided*

$$\sum_{j=1}^{k-1}\beta_k\alpha_{kj} + \sum_{j\geq k+1}^{s}\beta_j\alpha_{jk} - \beta_k\left(\sum_{i=1}^{s}\beta_i\right) = 0, \quad k = 2, \ldots, s. \tag{2.14}$$

Notice that for $s = 2$, combining (2.13) and (2.14), this method is of order $(\frac{3}{2}, 2)$ if and only if $\beta_1 = \frac{1}{2}$, $\beta_2 = \frac{1}{2}$ and $\alpha_{21} = 1$, as shown in Theorem 2.2. For $s > 2$, this method could be of order $(\frac{3}{2}, 2)$ with many admissible parameters. One can construct higher order explicit pseudo-symplectic methods based on the explicit Runge–Kutta method (2.6) through appropriate choice of the parameters.

3 Numerical experiments

In this section, we give numerical experiments to simulate stochastic Hamiltonian system (1.1). We take both linear and nonlinear oscillators as well as a stochastic nonlinear Schrödinger equation as examples.

3.1 Stochastic harmonic oscillator

We first consider a linear harmonic oscillator with additive noise (see e.g. [10]):

$$\begin{aligned} dP &= Qdt, & P(0) &= p_0, \\ dQ &= -Pdt + \gamma dW(t), & Q(0) &= q_0, \end{aligned} \tag{3.1}$$

with Hamiltonians $H_0(p, q) = \frac{1}{2}(p^2 + q^2)$ and $H_1(p, q) = -\gamma p$, which represents kinetic energy and thermal energy, respectively, caused by the stochastic perturbation. The exact solution of this system is

$$\begin{pmatrix} P(t_{k+1}) \\ Q(t_{k+1}) \end{pmatrix} = \begin{pmatrix} \cos h & \sin h \\ -\sin h & \cos h \end{pmatrix} \begin{pmatrix} P(t_k) \\ Q(t_k) \end{pmatrix} + \gamma \begin{pmatrix} \int_{t_k}^{t_{k+1}} \sin(t_{k+1}-t)dW(t) \\ \int_{t_k}^{t_{k+1}} \cos(t_{k+1}-t)dW(t) \end{pmatrix}, \tag{3.2}$$

with $h := t_{k+1} - t_k$, $k = 0, 1, \ldots, N-1$. We simulate the linear harmonic oscillator (3.1) by the pseudo-symplectic mid-point method, i.e., the method (2.1)+(2.2),

$$\begin{aligned} \tilde{P}_k &= P_k + hQ_k, \\ \tilde{Q}_k &= Q_k - hP_k + \gamma\delta_k W, \\ P_{k+1} &= P_k + \frac{h}{2}(Q_k + \tilde{Q}_k), \\ Q_{k+1} &= Q_k - \frac{h}{2}(P_k + \tilde{P}_k) + \gamma\delta_k W, \end{aligned} \tag{3.3}$$

compared with the (forward) Euler method and the symplectic mid-point method. For simplicity, we take $p_0 = q_0 = 0$ and $\gamma = 1$ in the simulations.

Since the period of free oscillations of (3.1) is 2π, the left part and the right parts of Fig. 1, corresponding to the time interval [0, 128] and [0, 1280], approximately contain 20 oscillations and 200 oscillations of (3.1). From these graphs, it is clear that the Euler method is unsuitable for the simulation of the Hamiltonian system (3.1) on a long time interval, since the amplitude of oscillations simulated by Euler method is about 50000 times greater than the exact amplitude after 200 oscillations. In contrast, the pseudo-symplectic method as well as symplectic method does much better than Euler method in reproducing oscillations of the system (3.1). Although the pseudo-symplectic method is not so accurate as the symplectic method, the norm of its error still keeps within 5% of the norm of the exact solution after 200 oscillations.

Figure 2 represents the evolution of domains in the phase plane of system (3.1). The initial domain is the unit circle with center at the origin. We plot images of this circle, which are obtained by the exact solution (3.2) and the three methods. The exact graphs are unit circles shifted from the origin due to the effect of noise. The images for Euler method are also circles but the radius increased, while for the symplectic and pseudo-symplectic methods, the images become ellipse. In spite of the fact that pseudo-symplectic method and Euler method are both explicit and have the same mean-square order of accuracy, pseudo-symplectic method is much better than Euler method and does more or less as well as symplectic method.

3.2 Nonlinear stochastic oscillator

Next, we consider the following double well problem (see e.g. [3]):

$$\begin{aligned} dP &= (Q - Q^3)dt + \sigma dW(t), \quad & P(0) = p_0, \\ dQ &= Pdt, & Q(0) = q_0. \end{aligned} \tag{3.4}$$

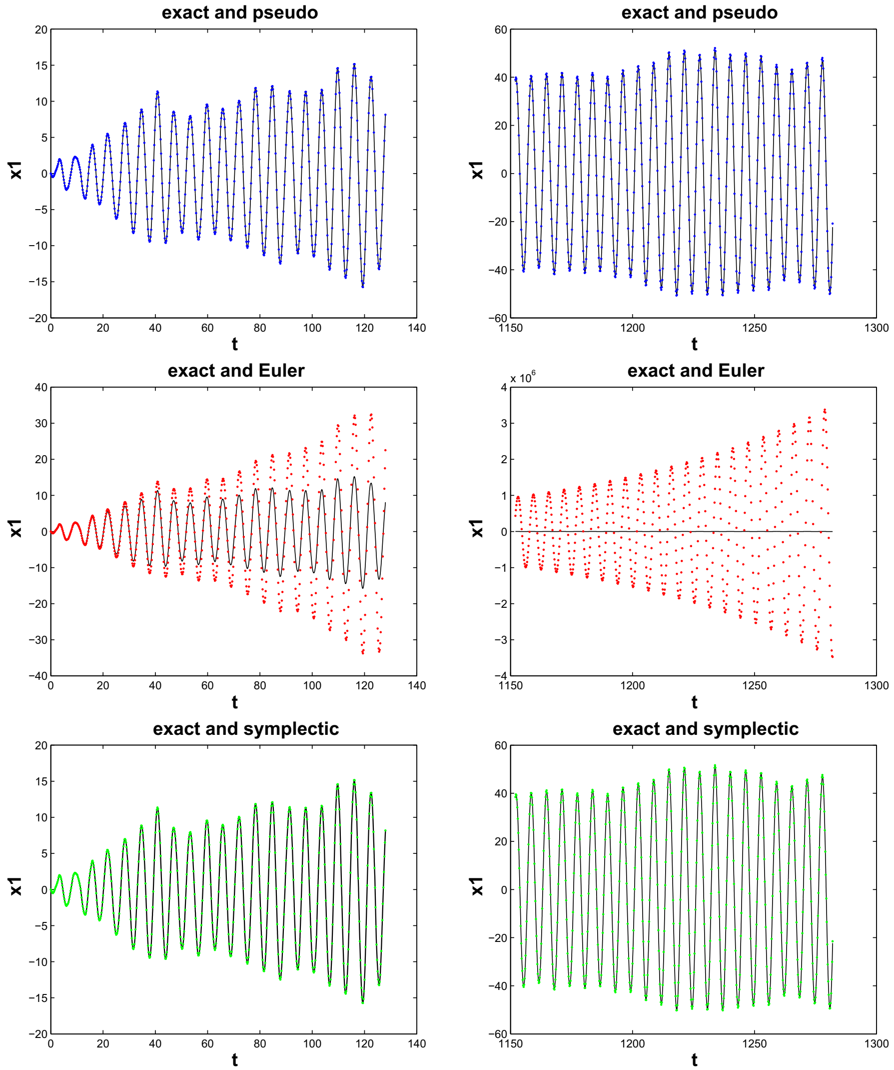

Fig. 1 Two sample trajectories of the solution obtained by the exact formula (3.2) (*solid line*) and pseudo-symplectic mid-point method, Euler method and symplectic mid-point method with $h = 0.02$

It is obvious that $H_0(p, q) := \frac{1}{2}(p^2 - q^2) + \frac{1}{4}q^4$ and $H_1(p, q) := -\sigma q$ are the Hamiltonians for this system. Since the system (3.4) is nonlinear, we can't explicitly express its solution. We test the pseudo-symplectic mid-point method

$$\begin{aligned}
\tilde{P}_{k+1} &= P_k + h(Q_k - Q_k^3) + \sigma \delta_k W, \\
\tilde{Q}_{k+1} &= Q_k + h P_k, \\
P_{k+1} &= P_k + \frac{h}{2}(Q_k - Q_k^3 + \tilde{Q}_{k+1} - \tilde{Q}_{k+1}^3) + \sigma \delta_k W,
\end{aligned}$$

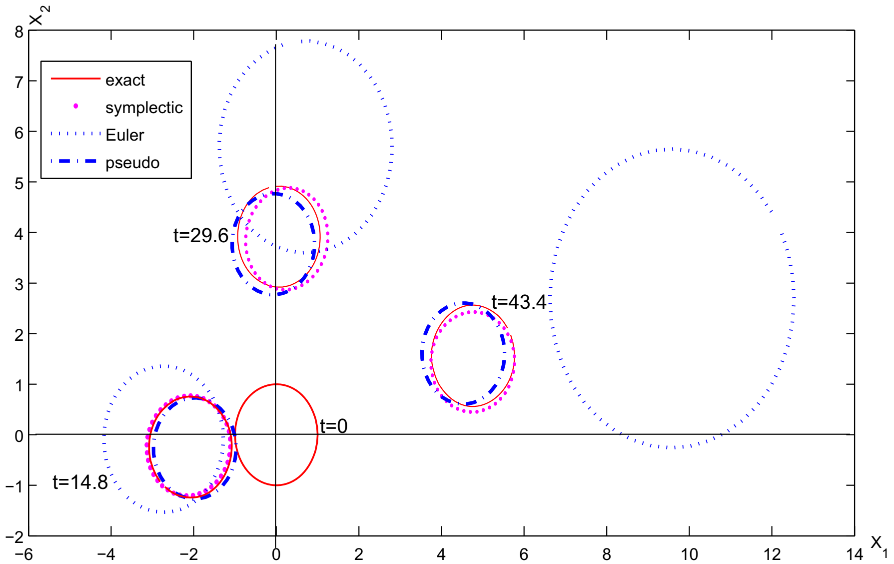

Fig. 2 The evolution of domains in the phase plane of system (3.1) obtained by the exact solution (3.2) and pseudo-symplectic mid-point method, symplectic mid-point method, and Euler methods with $h = 0.05$

$$Q_{k+1} = Q_k + \frac{h}{2}(P_k + \tilde{P}_{k+1}), \tag{3.5}$$

compared with symplectic mid-point method which is a fully implicit method, and both forward and backward Euler methods. We take $p_0 = q_0 = \sqrt{2}$ and $\sigma = 0.05$ in the simulations.

Figure 3 illustrates the numerical behavior of pseudo-symplectic mid-point method, symplectic mid-point method, and backward Euler methods applied to (3.4) in the time interval [0, 140]. These graphs indicate that the pseudo-symplectic method, compared with the symplectic method, does much better than backward Euler method in reproducing oscillations of the system (3.4).

3.3 Stochastic nonlinear Schrödinger equation

In this part, we consider the following focusing stochastic nonlinear Schrödinger equation with an additive noise:

$$\mathbf{i}du = -\Delta u dt - |u|^2 u dt + dW(t), \quad \text{in} \quad (0, T] \times \mathscr{O}; \quad u(0) = u_0 \tag{3.6}$$

under homogenous Dirichlet boundary condition. Here $T \in (0, \infty)$, $\mathscr{O} = (0, 1)$ and $W = \{W(t) : t \in [0, T]\}$ is a real-valued Φ-Wiener process on a stochastic basis $(\Omega, \mathscr{F}, \mathscr{F}_t, \mathbb{P})$ (see e.g. [4]), i.e., there exists an real-valued, orthonormal basis $\{e_k\}_{k=1}^{\infty}$ of $L_2(\mathscr{O})$ and a sequence of mutually independent, real-valued Brownian

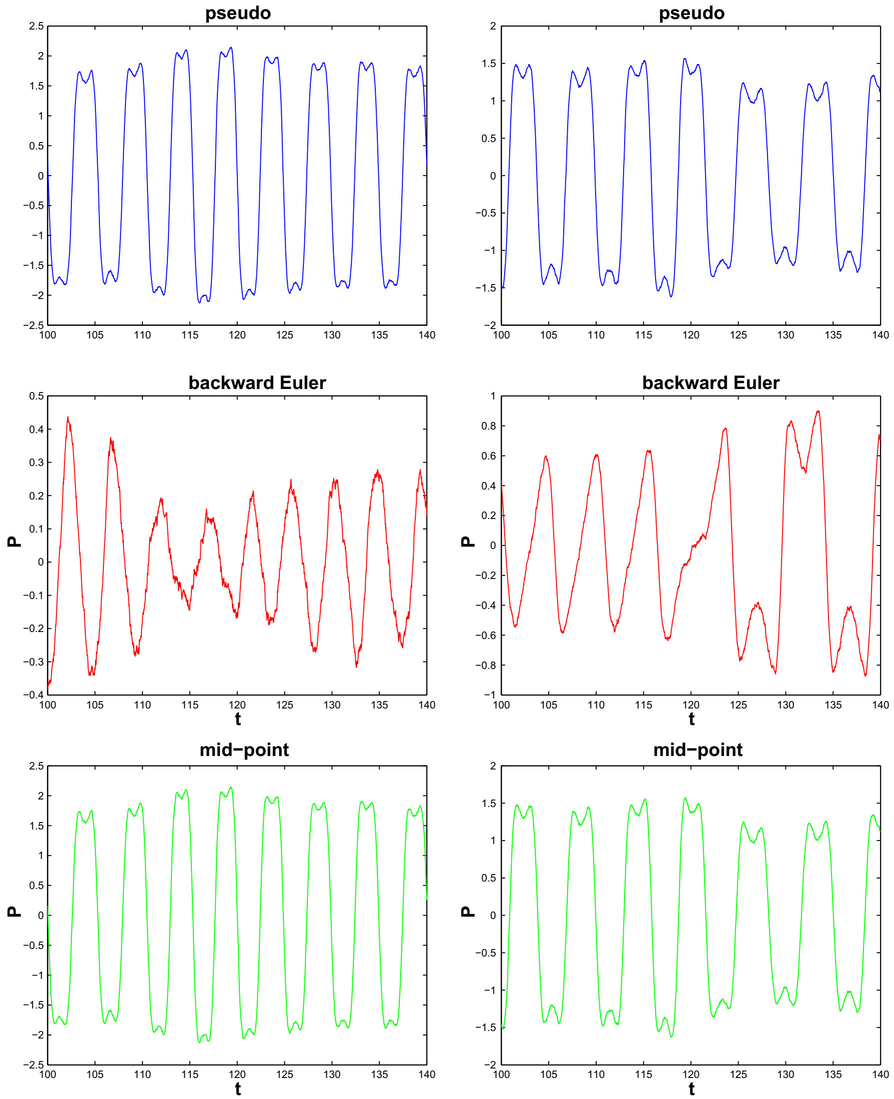

Fig. 3 Two sample trajectorys of the solution of (3.4) obtained by pseudo-symplectic mid-point method, backward Euler method and symplectic mid-point method with $h = 0.02$

motions $\{\beta_k\}_{k=1}^{\infty}$ such that

$$W(t) = \sum_{k=1}^{\infty} \Phi^{\frac{1}{2}} e_k \beta_k(t), \quad t \in [0, T].$$

This equation models the propagation of nonlinear dispersive waves in non-homogeneous or random media (see e.g. [4]).

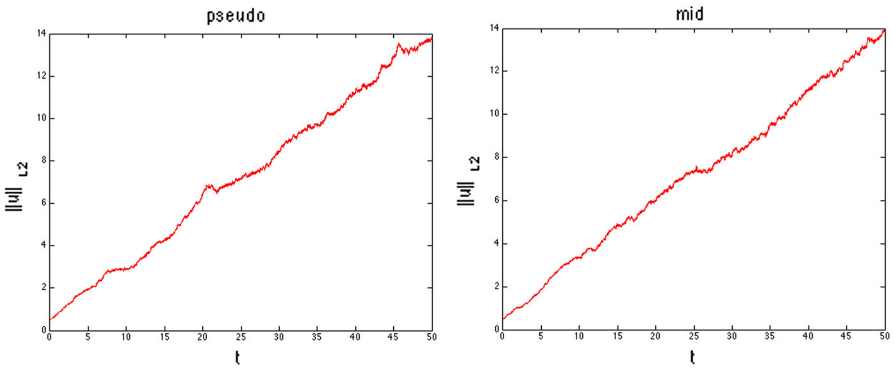

Fig. 4 The evolution of pseudo-symplectic mid-point method and symplectic mid-point method with $\delta x = 2^{-3}$ and $\delta t = 2^{-12}$

It is shown in [4] that the charge of this equation has the following evolution:

$$\|u(t)\|^2_{L_2(\mathscr{O})} = \|u_0\|^2_{L_2(\mathscr{O})} - 2\sum_{k=1}^{\infty} \Re\left[\int_0^t \int_{\mathscr{O}} \bar{u}(s)\Phi^{\frac{1}{2}} e_k dx d\beta(s)\right] + t\sum_{k=1}^{\infty} \|\Phi^{\frac{1}{2}} e_k\|^2_{L_2(\mathscr{O})}.$$

Here we will show that our numerical scheme recovers the charge evolution. To make it clear, we first truncate the noise with the first $M = 2^3$ terms and spatially discretize Eq. (3.6) by centered difference method with uniform step size $\delta x = \frac{1}{M}$, we obtain the M-dimensional stochastic Hamiltonian system

$$\begin{aligned} dP_{\delta x}(t) &= -\Delta_{\delta x} Q_{\delta x} dt - |Q_{\delta x}|^2 Q_{\delta x} dt - \Im\left[\left(\sum_{i=1}^{M} \Phi^{\frac{1}{2}} e_k d\beta_i(t)\right)_{\delta x}\right], \\ dQ_{\delta x}(t) &= \Delta_{\delta x} P_{\delta x} dt + |P_{\delta x}|^2 P_{\delta x} dt + \Re\left[\left(\sum_{i=1}^{M} \Phi^{\frac{1}{2}} e_k d\beta_i(t)\right)_{\delta x}\right], \end{aligned} \tag{3.7}$$

where $P_{\delta x}$ and $Q_{\delta x}$ are the real part and imaginary part of the numerical solution $u_{\delta x}$, respectively, and $\Delta_{\delta x}$ denotes the centered difference discretization of Δ. Here we take $\Phi^{\frac{1}{2}} e_k = \frac{1}{1+k^{2.6}} e_k$ with $e_k(x) = \sqrt{2}\sin(k\pi x)$, $1 \le k \le M$, $x \in \mathscr{O}$. Then we apply the proposed pseudo-symplectic scheme (2.3) with $\alpha = 1/2$ to numerically solve Eq. (3.7) with time step size $\delta t = 2^{-12}$. Figure 4 presents the evolution of charge for our numerical methods compared with symplectic methods.

4 Conclusions

In the present paper, a class of explicit pseudo-symplectic methods applicable to stochastic Hamiltonian systems with an additive multidimensional Wiener process is introduced. Compared to other methods, the main advantage of the proposed class of pseudo-symplectic methods is the significant reduction of the computational costs as well as the preservation of the symplectic structure of the systems over a relatively long time with certain accuracy. These theoretical results are verified by linear and nonlinear oscillators as well as spatially discrete stochastic nonlinear Schrödinger equation. For future research, the construction of explicit pseudo-symplectic schemes with higher pseudo-symplectic order for general stochastic Hamiltonian system with multiplicative noises may be of particular interest.

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