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Quasi-symplectic methods for Langevin-type equations

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Langevin type equations are an important and fairly large class of systems close to Hamiltonian ones. The constructed mean-square and weak quasi-symplectic methods for such systems degenerate to symplectic methods when a system degenerates to a stochastic Hamiltonian one. In addition, quasi-symplectic methods' law of phase volume contractivity is close to the exact law. The methods derived are based on symplectic schemes for stochastic Hamiltonian systems. Mean-square symplectic methods were obtained in Milstein *et al.* (2002, *SIAM J. Numer. Anal.*, **39**, 2066–2088; 2003, *SIAM J. Numer. Anal.*, **40**, 1583–1604) while symplectic methods in the weak sense are constructed in this paper. Special attention is paid to Hamiltonian systems with separable Hamiltonians and with additive noise. Some numerical tests of both symplectic and quasi-symplectic methods are presented. They demonstrate superiority of the proposed methods in comparison with standard ones.

Keywords: Langevin equations; stochastic Hamiltonian systems; symplectic and quasi-symplectic numerical methods; mean-square and weak schemes.

1. Introduction

During the last 15–20 years a lot of attention in deterministic numerical analysis has been paid to symplectic integration of Hamiltonian systems (see e.g. Sanz-Serna & Calvo, 1994; Hairer *et al.*, 1993, 2002 and references therein). This interest is motivated by the fact that symplectic integrators in comparison with the usual numerical schemes allow us to simulate Hamiltonian systems on very long time intervals with high accuracy. The phase flows of some classes of stochastic systems (stochastic Hamiltonian systems) possess the property of preserving symplectic structure (symplecticness) (see Bismut, 1981 and also Milstein *et al.*, 2002). For instance, systems of this type describe synchrotron oscillations of particles in storage rings under the influence of external fluctuating electromagnetic fields

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(Seeßelberg *et al.*, 1994). Another popular model from this class is the Kubo oscillator (Kubo *et al.*, 1985) which is used in the theory of magnetic resonance and laser physics. In Milstein *et al.* (2002, 2003) mean-square symplectic methods for stochastic Hamiltonian systems were proposed. These methods have significant advantages over standard schemes for stochastic differential equations (SDEs) (Milstein, 1995; Kloeden & Platen, 1992).

It is natural to expect that making use of numerical methods, which are close, in a sense, to symplectic ones, also has some advantages when applying to stochastic systems close to Hamiltonian ones. An important and fairly large class of such systems is Langevin type equations which can be written as the following system of Ito SDEs:

$$\begin{gathered} \mathrm{d}P = f(t, Q)\,\mathrm{d}t - \nu \tilde{f}(t, P, Q)\,\mathrm{d}t + \sum_{r=1}^{m} \sigma_r(t, Q)\,\mathrm{d}w_r(t), \;\; P(t_0) = p, \\ \mathrm{d}Q = g(P)\,\mathrm{d}t, \;\; Q(t_0) = q, \end{gathered} \tag{1.1}$$

where P, Q, f, $\tilde{f}$, g, σ_r are n-dimensional column vectors, ν is a parameter, and $w_r(t)$, $r = 1, \ldots, m$, are independent standard Wiener processes. It is not difficult to verify that this system has the same form in the sense of Stratonovich.

The Langevin type equations (1.1) have the widespread occurrence in models from physics, chemistry, and biology. They are used in dissipative particle dynamics (see e.g. Ripoll *et al.*, 2001 and references therein), in molecular simulations (see e.g. Skeel, 1999; Izaguirre *et al.*, 2001 and references therein), for studying lattice dynamics in strongly anharmonic crystals (Gornostyrev *et al.*, 1996), descriptions of noise-induced transport in stochastic ratchets (Landa, 1998), investigations of the dispersion of passive tracers in turbulent flows (see Thomson, 1987; Sawford, 2001 and references therein), etc. In this paper we construct special numerical methods (we call them quasi-symplectic) which preserve some specific properties of the Langevin type equations.

In Section 2, we construct mean-square quasi-symplectic methods for Langevin equations which are an important particular case of (1.1) when $f(t, q) = f(q)$, $\tilde{f}(t, p, q) = \Gamma p$, Γ is an $n \times n$-dimensional constant matrix, $g(p) = M^{-1}p$, M is a positive definite matrix, and $\sigma_r(t, q) = \sigma_r$, $r = 1, \ldots, m$, are constant vectors. The proposed methods are such that they degenerate to symplectic methods when the system degenerates to a Hamiltonian one and their law of phase volume contractivity is close to the exact one. To construct numerical methods, we use the splitting technique (see e.g. Sanz-Serna & Calvo, 1994; Strang, 1968; Yanenko, 1971) and some ideas of Suris (1991), where methods for deterministic second-order differential equations with similar properties were obtained. In Section 3, we generalize mean-square methods of Section 2 to the Langevin type equations (1.1) and also to more general systems.

Mean-square methods are necessary for direct simulation of stochastic trajectories. Besides, they are the basis for the construction of weak methods which are important for many practical applications. As is known (see e.g. Milstein, 1995; Kloeden & Platen, 1992; Pardoux & Talay, 1985), weak methods are relevant to calculate expectations of functionals of a solution to SDEs by the Monte Carlo technique, and they are simpler than mean-square ones in many respects. An important advantage of weak approximations is that they give an opportunity to avoid the problem of simulating complicated random variables.

Before constructing weak schemes for Langevin type equation, we derive symplectic methods in the weak sense for stochastic Hamiltonian systems. Consider the Cauchy

problem for the system of SDEs in the sense of Stratonovich

$$\begin{aligned} \mathrm{d}P &= f(t, P, Q)\,\mathrm{d}t + \sum_{r=1}^{m} \sigma_r(t, P, Q) \circ \mathrm{d}w_r(t), \quad P(t_0) = p, \\ \mathrm{d}Q &= g(t, P, Q)\,\mathrm{d}t + \sum_{r=1}^{m} \gamma_r(t, P, Q) \circ \mathrm{d}w_r(t), \quad Q(t_0) = q, \end{aligned} \tag{1.2}$$

where P, Q, f, g, σ_r, γ_r are n-dimensional column vectors with the components P^i, Q^i, f^i, g^i, σ_r^i, γ_r^i, $i = 1, \dots, n$, and $w_r(t)$, $r = 1, \dots, m$, are independent standard Wiener processes.

We denote by $X(t; t_0, x) = (P^{\mathsf{T}}(t; t_0, p, q), Q^{\mathsf{T}}(t; t_0, p, q))^{\mathsf{T}}$, $t_0 \leqslant t \leqslant t_0 + T$, the solution of (1.2). A more detailed notation is $X(t; t_0, x; \omega)$, where ω is an elementary event. It is known that $X(t; t_0, x; \omega)$ is a phase flow (diffeomorphism) for almost every ω. See its properties in, for example, Bismut (1981) and Ikeda & Watanabe (1981). If there are functions $H_r(t, p, q)$, $r = 0, \dots, m$, such that (Bismut, 1981; Milstein *et al.*, 2002)

$$\begin{gathered} f^i = -\partial H_0/\partial q^i, \quad g^i = \partial H_0/\partial p^i, \\ \sigma_r^i = -\partial H_r/\partial q^i, \quad \gamma_r^i = \partial H_r/\partial p^i, \quad i = 1, \dots, n, \quad r = 1, \dots, m, \end{gathered} \tag{1.3}$$

then the phase flow of (1.2) preserves symplectic structure:

$$\mathrm{d}P \wedge \mathrm{d}Q = \mathrm{d}p \wedge \mathrm{d}q, \tag{1.4}$$

i.e. the sum of the oriented areas of projections onto the coordinate planes $(p^1, q^1), \dots, (p^n, q^n)$ is an integral invariant (Arnold, 1989). To avoid confusion, we note that the differentials in (1.2) and (1.4) have different meaning. In (1.2) P, Q are treated as functions of time and p, q are fixed parameters, while differentiation in (1.4) is made with respect to the initial data p, q.

Let P_k, Q_k, $k = 0, \dots, N$, $t_{k+1} - t_k = h_{k+1}$, $t_N = t_0 + T$, be a method for (1.2) based on the one-step approximation $\bar{P} = \bar{P}(t + h; t, p, q)$, $\bar{Q} = \bar{Q}(t + h; t, p, q)$. We say that the method preserves symplectic structure if

$$\mathrm{d}\bar{P} \wedge \mathrm{d}\bar{Q} = \mathrm{d}p \wedge \mathrm{d}q. \tag{1.5}$$

In Section 4, weak symplectic methods for stochastic Hamiltonian systems with multiplicative noise are constructed. Section 5 is devoted to symplectic integrators for Hamiltonian systems with additive noise. Weak symplectic schemes for Hamiltonian systems with coloured noise are available in the preprint Milstein & Tretyakov (2002). The proposed symplectic methods are the basis for construction of efficient weak methods for systems close to Hamiltonian ones and, in particular, for Langevin type equations.

In Section 6, we derive quasi-symplectic methods in the weak sense for Langevin type equations using weak methods from Sections 4 and 5 together with the ideas of Sections 2 and 3. It is known (Tropper, 1977; Soize, 1994; Mattingly *et al.*, 2002) that the Langevin diffusion is ergodic and for many applications it is interesting to compute the mean of a given function with respect to the invariant law of the diffusion. Ergodicity of numerical methods was first investigated in Talay (1990) in the case of non-degenerate

noise and globally Lipschitz coefficients. For Langevin equations, noise is degenerate and the coefficients may not be globally Lipschitz. In this case, ergodicity of the numerical schemes is considered in Mattingly *et al.* (2002) and Talay (2002). To evaluate the mean values with respect to the invariant law, one has to integrate a system over very long time intervals, especially when dissipation is small. In such a situation, numerical methods based on symplectic integrators are fairly relevant.

We should note that finite-time convergence of new methods derived in this paper is proved under traditional conditions on the drift and diffusion coefficients which consist of the existence and boundedness of their derivatives up to a certain order. In particular, the traditional conditions contain a rather restrictive one, namely a global Lipschitz condition. However, the methods can undoubtedly be used much more widely. This fact is well known in practice for many other methods. Some theoretical results on the convergence of numerical methods for equations with locally Lipschitz coefficients are obtained in Higham *et al.* (2003), Mattingly *et al.* (2002) and Talay (2002).

In Section 7, we present numerical tests of both symplectic and quasi-symplectic methods. They clearly demonstrate the superiority of the proposed methods over very long time intervals in comparison with standard methods.

2. Quasi-symplectic mean-square methods for Langevin equations

Consider the Langevin equation

$$\begin{aligned} &\mathrm{d}P = f(Q)\,\mathrm{d}t - \nu\Gamma P\,\mathrm{d}t + \sum_{r=1}^{m}\sigma_r\,\mathrm{d}w_r(t), \quad P(t_0) = p,\\ &\mathrm{d}Q = M^{-1}P\,\mathrm{d}t, \quad Q(t_0) = q, \end{aligned} \tag{2.1}$$

where P, Q, f are n-dimensional column vectors, σ_r, $r = 1, \dots, m$, are n-dimensional constant column vectors, Γ is an $n \times n$-dimensional constant matrix, $\nu \geqslant 0$ is a parameter, M is a positive definite matrix, and $w_r(t)$, $r = 1, \dots, m$, are independent standard Wiener processes. If there is a scalar function $U_0(q)$ such that

$$f^i(q) = -\frac{\partial U_0}{\partial q^i}, \quad i = 1, \dots, n, \tag{2.2}$$

and if $\nu = 0$, then the system (2.1) is a Hamiltonian system with additive noise, i.e. its phase flow preserves symplectic structure (Bismut, 1981; Milstein *et al.*, 2002).

The system (2.1) can be written as the second-order differential equation with additive noise:

$$M\ddot{Q} = f(Q) - \nu\Gamma M\dot{Q} + \sum_{r=1}^{m}\sigma_r\dot{w}_r.$$

Let $D_0 \in R^d$, $d = 2n$, be a domain with finite volume. This domain may be random. We suppose that $D_0 = D_0(\omega)$ is independent of the Wiener processes $w_r(t)$, $t \in [t_0, t_0 + T]$. The transformation $(p, q) \mapsto (P, Q)$ maps D_0 into the domain D_t. The volume V_t of

the domain D_t is equal to

$$V_t = \int\limits_{D_t} \mathrm{d}P^1 \dots \mathrm{d}P^n \mathrm{d}Q^1 \dots \mathrm{d}Q^n$$
$$= \int\limits_{D_0} \left| \frac{D(P^1, \dots, P^n, Q^1, \dots, Q^n)}{D(p^1, \dots, p^n, q^1, \dots, q^n)} \right| \mathrm{d}p^1 \dots \mathrm{d}p^n \mathrm{d}q^1 \dots \mathrm{d}q^n. \tag{2.3}$$

In the case of the system (2.1) the Jacobian J is equal to (Bismut, 1981; Kunita, 1990; Milstein *et al.*, 2002)

$$J = \frac{D(P^1, \dots, P^n, Q^1, \dots, Q^n)}{D(p^1, \dots, p^n, q^1, \dots, q^n)} = \exp\left(-\nu \operatorname{tr}\Gamma \cdot (t - t_0)\right). \tag{2.4}$$

That is, the system (2.1) preserves phase volume for $\nu = 0$. If $\nu > 0$ and $\operatorname{tr}\Gamma > 0$ then phase volume contractivity takes place.

Our aim is to propose mean-square methods based on the one-step approximations

$$\bar{P} = \bar{P}(t + h; t, p, q),\ \bar{Q} = \bar{Q}(t + h; t, p, q)$$

such that

RL1. *The method applied to* (2.1)–(2.2) *degenerates to a symplectic method when* $\nu = 0$, *i.e.* $\mathrm{d}\bar{P} \wedge \mathrm{d}\bar{Q} = \mathrm{d}p \wedge \mathrm{d}q$ *for* $\nu = 0$ *and* f *from* (2.2);

RL2. *The Jacobian*

$$\bar{J} = \frac{D(\bar{P}, \bar{Q})}{D(p, q)}$$

does not depend on p, q.

As is understood, a method is convergent and, consequently, $\bar{J}$ is close to J at any rate. The requirement RL2 is natural since the Jacobian J of the original system (2.1) does not depend on p, q. RL2 reflects the structural properties of the system which are connected with the law of phase volume contractivity. It is often possible to reach a stronger property consisting of the equality $\bar{J} = J$. However, such a requirement is too restrictive in general. In the context of deterministic equations the requirement RL2 was introduced in Suris (1991).

To construct methods satisfying RL1–RL2, we use the splitting technique (see e.g. Sanz-Serna & Calvo, 1994; Strang, 1968). In connection with (2.1), introduce the systems

$$\begin{aligned} \mathrm{d}P_{\mathrm{I}} &= f(Q_{\mathrm{I}})\,\mathrm{d}t + \sum_{r=1}^{m} \sigma_r\,\mathrm{d}w_r(t), \quad P_{\mathrm{I}}(t_0) = p, \\ \mathrm{d}Q_{\mathrm{I}} &= M^{-1} P_{\mathrm{I}}\,\mathrm{d}t, \quad Q_{\mathrm{I}}(t_0) = q, \end{aligned} \tag{2.5}$$

$$\frac{\mathrm{d}P_{\mathrm{II}}}{\mathrm{d}t} = -\nu\Gamma P_{\mathrm{II}}, \quad P_{\mathrm{II}}(0) = p, \tag{2.6}$$

and denote their solutions as $P_{\mathrm{I}}(t; t_0, p, q)$, $Q_{\mathrm{I}}(t; t_0, p, q)$ and $P_{\mathrm{II}}(t; p)$, respectively. The system (2.5) with $f(q)$ from (2.2) is a Hamiltonian system with additive noise. The system (2.6) is a deterministic linear system with constant coefficients, and its solution $P_{\mathrm{II}}(t; p)$ can be found explicitly.

2.1 *First-order methods*

Introduce a discretization of the time interval $[t_0, t_0 + T]$, for definiteness the equidistant one:

$$t_{i+1} = t_i + h, \quad i = 0, \dots, N-1, \quad h = T/N.$$

Let $\bar{P}_{\rm I} = \bar{P}_{\rm I}(t_0 + h; t_0, p, q)$, $\bar{Q}_{\rm I} = \bar{Q}_{\rm I}(t_0 + h; t_0, p, q)$ be a one-step approximation of a symplectic first-order mean-square method for (2.5), (2.2) (any explicit or implicit method from Milstein *et al.*, 2002 can be used). Its Jacobian is equal to one, i.e.

$$\frac{D(\bar{P}_{\rm I}(t_0 + h; t_0, p, q), \bar{Q}_{\rm I}(t_0 + h; t_0, p, q))}{D(p, q)} = 1.$$

We construct the one-step approximation $\bar{P}$, $\bar{Q}$ for the solution of (2.1)–(2.2) as follows:

$$\begin{aligned} \bar{P} = \bar{P}(t_0 + h; t_0, p, q) &:= P_{\rm II}(h; \bar{P}_{\rm I}(t_0 + h; t_0, p, q)), \\ \bar{Q} = \bar{Q}(t_0 + h; t_0, p, q) &:= \bar{Q}_{\rm I}(t_0 + h; t_0, p, q). \end{aligned} \tag{2.7}$$

We have

$$\bar{J} = \frac{D(\bar{P}, \bar{Q})}{D(p, q)} = \frac{D(P_{\rm II}, \bar{Q}_{\rm I})}{D(\bar{P}_{\rm I}, \bar{Q}_{\rm I})} \frac{D(\bar{P}_{\rm I}, \bar{Q}_{\rm I})}{D(p, q)} = J. \tag{2.8}$$

Further, if $\nu = 0$, then $\bar{P} = \bar{P}_{\rm I}$, $\bar{Q} = \bar{Q}_{\rm I}$, i.e. the approximation (2.7) degenerates to the symplectic method for (2.1)–(2.2) with $\nu = 0$. Thus, the approximation $\bar{P}$, $\bar{Q}$ satisfies both requirements RL1 and RL2.

LEMMA 2.1 Let $\bar{P}_{\rm I}$, $\bar{Q}_{\rm I}$ be a one-step approximation corresponding to any first-order mean-square method for the system (2.5). Then $\bar{P}$, $\bar{Q}$ defined in (2.7) is a one-step approximation of the first-order mean-square method for the system (2.1).

Proof. Due to the assumption, we can write

$$\begin{aligned} \bar{P}_{\rm I} &= p + \sum_{r=1}^{m} \sigma_r \Delta w_r + h f(q) + r_1, \\ \bar{Q}_{\rm I} &= q + h M^{-1} p + r_2, \end{aligned} \tag{2.9}$$

where

$$\Delta w_r = \Delta w_r(h) = w_r(t_0 + h) - w_r(t_0)$$

and the remainders r_1 and r_2 are such that

$$|Er_i| = O(h^2), \quad Er_i^2 = O(h^3), \quad i = 1, 2.$$

We have

$$P_{\rm II}(h; p) = p - h\nu\Gamma p + \rho, \quad \rho = O(h^2). \tag{2.10}$$

Using (2.9), (2.10), and (2.7), we get

$$\bar{P} = p + \sum_{r=1}^{m} \sigma_r \Delta w_r + h\,(f(q) - \nu\Gamma p) + R, \tag{2.11}$$

where

$$R = r_1 + \rho - h\nu\Gamma \cdot (\bar{P}_{\mathrm{I}} - p).$$

It is not difficult to see that

$$|ER| = O(h^2), \quad ER^2 = O(h^3).$$

Denote by $\tilde{P}$, $\tilde{Q}$ the Euler one-step approximation applied to (2.1). It follows from (2.9) and (2.11) that

$$\left| E\left(\begin{bmatrix} \bar{P} \\ \bar{Q} \end{bmatrix} - \begin{bmatrix} \tilde{P} \\ \tilde{Q} \end{bmatrix} \right) \right| = O(h^2), \quad \left[E\left(\begin{bmatrix} \bar{P} \\ \bar{Q} \end{bmatrix} - \begin{bmatrix} \tilde{P} \\ \tilde{Q} \end{bmatrix} \right)^2 \right]^{1/2} = O(h^{3/2}).$$

Then, recalling that the Euler method has the first mean-square order of accuracy for systems with additive noise and using the main theorem on mean-square convergence from Milstein (1995, p. 12), we get the result.

Thus, due to (2.8), we obtain the following convergence theorem. □

THEOREM 2.1 Let $\bar{P}_{\mathrm{I}}$, $\bar{Q}_{\mathrm{I}}$ be a one-step approximation corresponding to a symplectic first-order mean-square method for the system (2.5), (2.2). Then $\bar{P}$, $\bar{Q}$ defined in (2.7) is a one-step approximation of the first-order mean-square method for the system (2.1) such that (i) it is symplectic when applied to (2.1)–(2.2) with $\nu = 0$, (ii) its phase volume changes according to the same law as the phase volume of (2.1) does, i.e. the Jacobians $\bar{J} = D(\bar{P}, \bar{Q})/D(p, q)$ and $J = D(P, Q)/D(p, q)$ are equal.

Let us take two concrete schemes for $\bar{P}_{\mathrm{I}}$, $\bar{Q}_{\mathrm{I}}$ from Milstein *et al.* (2002). The first one is explicit:

$$\begin{gathered} \mathcal{Q} = q + \alpha h M^{-1} p, \quad \mathcal{P} = p + h f(\mathcal{Q}), \\ \bar{Q}_{\mathrm{I}} = \mathcal{Q} + (1-\alpha) h M^{-1} \mathcal{P}, \quad \bar{P}_{\mathrm{I}} = \mathcal{P} + \sum_{r=1}^{m} \sigma_r \Delta w_r, \end{gathered} \tag{2.12}$$

where α is a parameter. The second method

$$\begin{aligned} \bar{P}_{\mathrm{I}} &= p + h f((1-\alpha)\bar{Q}_{\mathrm{I}} + \alpha q) + \sum_{r=1}^{m} \sigma_r \Delta w_r, \\ \bar{Q}_{\mathrm{I}} &= q + h M^{-1}(\alpha \bar{P}_{\mathrm{I}} + (1-\alpha) p). \end{aligned} \tag{2.13}$$

is implicit for $0 < \alpha < 1$. Substitution of $\bar{P}_{\mathrm{I}}$, $\bar{Q}_{\mathrm{I}}$ from (2.12) or (2.13) in (2.7) gives us the concrete one-step approximations for (2.1).

REMARK 2.1 Theorem 2·1 also holds for the method based on the following one-step approximation:

$$\begin{aligned}\bar{P} &= \bar{P}(t_0+h;\, t_0,\, p,\, q) := \bar{P}_{\rm I}(t_0+h;\, t_0,\, P_{\rm II}(h;\, p),\, q),\\ \bar{Q} &= \bar{Q}(t_0+h;\, t_0,\, p,\, q) := \bar{Q}_{\rm I}(t_0+h;\, t_0,\, P_{\rm II}(h;\, p),\, q).\end{aligned} \tag{2.14}$$

There is another possibility to propose methods for (2.1) satisfying RL1–RL2. It consists in direct application of symplectic methods. For instance, the parametric first-order family of implicit methods from Milstein *et al.* (2002) in application to (2.1) takes the form

$$\begin{aligned}\bar{P} &= p + hf((1-\alpha)\bar{Q} + \alpha q) - h\nu\Gamma\cdot(\alpha\bar{P} + (1-\alpha)p) + \sum_{r=1}^{m}\sigma_r\Delta w_r,\\ \bar{Q} &= q + hM^{-1}(\alpha\bar{P} + (1-\alpha)p).\end{aligned} \tag{2.15}$$

However, it satisfies the requirement RL2 for $\alpha = 0$ and $\alpha = 1$ only. Moreover, due to their specific structure, not all the symplectic methods (see, for example, the explicit method (2.12)) can be directly applied to the Langevin equation (2.1) itself. Thus, in the direct application of symplectic methods to (2.1) we have rather restrictive opportunities. Nevertheless, we can obtain in this way some new methods.

2.2 *Second-order methods*

In order to construct second-order methods for the Langevin equation (2.1) with the properties RL1 and RL2, we use ideas of the method of fractional steps (Yanenko, 1971; Sanz-Serna & Calvo, 1994; Strang, 1968). In the deterministic case (i.e. when $\sigma_r = 0$, $r = 1, \ldots, m$) a second-order method satisfying RL1 and RL2 can be based on the following one-step approximation:

$$\begin{aligned}\bar{P} = \bar{P}(t_0+h;\, t_0,\, p,\, q) &:= P_{\rm II}\left(\frac{h}{2};\, \bar{P}_{\rm I}\left(t_0+h;\, t_0,\, P_{\rm II}\left(\frac{h}{2};\, p\right),\, q\right)\right),\\ \bar{Q} = \bar{Q}(t_0+h;\, t_0,\, p,\, q) &:= \bar{Q}_{\rm I}\left(t_0+h;\, t_0,\, P_{\rm II}\left(\frac{h}{2};\, p\right),\, q\right),\end{aligned} \tag{2.16}$$

where $\bar{P}_{\rm I}$, $\bar{Q}_{\rm I}$ corresponds to a one-step approximation of a symplectic method for (2.5), (2.2) with $\sigma_r = 0$.

In the stochastic case the interconnection between terms in (2.1) is more complicated and a correction to (2.16) is needed to obtain second-order accuracy. Consider the following approximation for solution of (2.1):

$$\begin{aligned}\bar{P} = \bar{P}(t_0+h;\, t_0,\, p,\, q) &:= P_{\rm II}\left(\frac{h}{2};\, \bar{P}_{\rm I}\left(t_0+h;\, t_0,\, P_{\rm II}\left(\frac{h}{2};\, p\right),\, q\right)\right)\\ &\quad -\nu\sum_{r=1}^{m}\Gamma\sigma_r\left(I_{r0} - \frac{h}{2}\Delta w_r\right),\\ \bar{Q} = \bar{Q}(t_0+h;\, t_0,\, p,\, q) &:= \bar{Q}_{\rm I}\left(t_0+h;\, t_0,\, P_{\rm II}\left(\frac{h}{2};\, p\right),\, q\right),\end{aligned} \tag{2.17}$$

where $\bar{P}_{\rm I}$, $\bar{Q}_{\rm I}$ is a one-step approximation corresponding to a symplectic (explicit or implicit) second-order mean-square method for (2.5), (2.2) (such methods are available in Milstein *et al.*, 2002),

$$I_{r0} = \int_{t_0}^{t} (w_r(s) - w_r(t_0))\,\mathrm{d}s.$$

LEMMA 2.2 Let $\bar{P}_{\rm I}$, $\bar{Q}_{\rm I}$ be a one-step approximation corresponding to any second-order mean-square method for the system (2.5). Then $\bar{P}$, $\bar{Q}$ defined in (2.17) is a one-step approximation of the second-order mean-square method for the system (2.1).

Proof. Due to the assumption, we can write

$$\begin{aligned}
\bar{P}_{\rm I}(t_0+h; t_0, p, q) &= p + \sum_{r=1}^{m} \sigma_r \Delta w_r + h f(q) + \frac{h^2}{2} \sum_{i=1}^{n} \left(M^{-1} p\right)^i \frac{\partial f}{\partial q^i} + r_1, \\
\bar{Q}_{\rm I}(t_0+h; t_0, p, q) &= q + h M^{-1} p + \sum_{r=1}^{m} M^{-1} \sigma_r I_{r0} + \frac{h^2}{2} M^{-1} f(q) + r_2,
\end{aligned} \tag{2.18}$$

where the remainders r_1 and r_2 are such that

$$|E r_i| = O(h^3), \quad E r_i^2 = O(h^5), \quad i = 1, 2.$$

We also have

$$P_{\rm II}(h; p) = p - h\nu\Gamma p + \frac{h^2}{2}\nu^2\Gamma^2 p + \rho, \quad \rho = O(h^3). \tag{2.19}$$

We obtain from (2.17)–(2.19) that

$$\begin{aligned}
\bar{P} = p &+ \sum_{r=1}^{m} \sigma_r \Delta w_r + h\,(f(q) - \nu\Gamma p) - \nu \sum_{r=1}^{m} \Gamma \sigma_r I_{r0} \\
&+ \frac{h^2}{2} \left[\sum_{i=1}^{n} \left(M^{-1} p\right)^i \frac{\partial f}{\partial q^i} + \nu^2 \Gamma^2 p - \nu \Gamma f(q) \right] + R_1,
\end{aligned} \tag{2.20}$$

$$\bar{Q} = q + h M^{-1} p + \sum_{r=1}^{m} M^{-1} \sigma_r I_{r0} + \frac{h^2}{2} M^{-1} [f(q) - \nu\Gamma p] + R_2,$$

where R_1 and R_2 are such that

$$|E R_i| = O(h^3), \quad E R_i^2 = O(h^5), \quad i = 1, 2.$$

It is not difficult to show that the standard Taylor-type mean-square method of order $3/2$ for systems with additive noise (Milstein, 1995, p. 37) has the second order of accuracy when it is applied to (2.1). Comparing the one-step approximation of this standard method with (2.20), we obtain that the method based on (2.17) is of mean-square order 2. □

One can easily check that the approximation (2.17) satisfies our requirements RL1 and RL2. The following theorem summarizes the result.

THEOREM 2.2 Let $\bar{P}_{\rm I}$, $\bar{Q}_{\rm I}$ be a one-step approximation corresponding to a symplectic second-order mean-square method for the system (2.5), (2.2). Then $\bar{P}$, $\bar{Q}$ defined in (2.17) is a one-step approximation of the second-order mean-square method for the system (2.1)–(2.2) such that (i) it is symplectic when applied to (2.1)–(2.2) with $\nu = 0$, and (ii) its phase volume changes according to the same law as the phase volume of (2.1)–(2.2) does.

Let us give a concrete example of a method based on (2.17):

$$\mathcal{P}_1 = P_{\rm II}\left(\frac{h}{2}; P_k\right), \quad \mathcal{Q}_1 = Q_k + \frac{h}{2}M^{-1}\mathcal{P}_1,$$

$$\mathcal{P}_2 = \mathcal{P}_1 + \sum_{r=1}^{m}\sigma_r \Delta_k w_r + hf(\mathcal{Q}_1), \quad \mathcal{Q}_2 = Q_k + hM^{-1}\mathcal{P}_1 + \sum_{r=1}^{m} M^{-1}\sigma_r (I_{r0})_k + \frac{h^2}{2}M^{-1} f(\mathcal{Q}_1), \tag{2.21}$$

$$P_{k+1} = P_{\rm II}\left(\frac{h}{2}; \mathcal{P}_2\right) - \nu\sum_{r=1}^{m}\Gamma\sigma_r\left(I_{r0} - \frac{h}{2}\Delta w_r\right), \quad Q_{k+1} = \mathcal{Q}_2, \quad k = 0, \dots, N-1.$$

To obtain (2.21), we use one of the explicit symplectic second-order partitioned Runge–Kutta (PRK) methods from Milstein *et al.* (2002), which is a generalization of the Störmer–Verlet method.

The random variables $\Delta_k w_r$, $(I_{r0})_k$ have a Gaussian joint distribution, and they can be simulated at each step by $2m$ mutually independent $\mathcal{N}(0, 1)$-distributed random variables ξ_{rk} and η_{rk}, $r = 0, \dots, m$:

$$\Delta_k w_r = h^{1/2}\xi_{rk}, \quad (I_{r0})_k = h^{3/2}(\xi_{rk} + \eta_{rk}/\sqrt{3})/2. \tag{2.22}$$

In molecular dynamics several methods based on the deterministic Störmer–Verlet method are used for simulation of the Langevin equation (2.1) with diagonal matrix Γ (see Skeel, 1999; Izaguirre *et al.*, 2001 and references therein). Effective numerical methods for this type of Langevin equation can be constructed by the following splitting:

$$\mathrm{d}P_{\rm I} = -\nu\Gamma P_{\rm I}\,\mathrm{d}t + \sum_{r=1}^{m}\sigma_r\,\mathrm{d}w_r(t), \quad \mathrm{d}Q_{\rm I} = M^{-1}P_{\rm I}\,\mathrm{d}t, \quad \mathrm{d}P_{\rm II} = f(q)\,\mathrm{d}t.$$

Since $P_{\rm I}$, $Q_{\rm I}$ satisfy the linear system with additive noise, they can be simulated exactly. A number of concrete schemes satisfying our requirements RL1–RL2 can be derived using the exact $P_{\rm I}$, $Q_{\rm I}$ and a deterministic symplectic method. Such a second-order method based on the Störmer–Verlet scheme coincides with the method proposed in Skeel (1999).

2.3 *Third-order methods*

Using ideas of the method of fractional steps, as we did in the previous sections, it is possible to construct a third-order method for (2.1) which satisfies the requirements RL1

and RL2. But such a method contains two fractional steps at which we have to approximate the Hamiltonian system (2.5), (2.1) using a third-order symplectic method. This makes the method too complicated, and we will use another approach. In Suris (1991) a similar problem for deterministic second-order differential equations was solved by a modification of symplectic Runge–Kutta–Nyström (RKN) methods from Suris (1989). Here we modify the symplectic RKN method from Milstein *et al.* (2002) using some ideas of Suris (1991).

As a result, we obtain the method

$$\mathcal{Q}_1 = Q_k + \frac{7}{24}hM^{-1}P_k, \quad \mathcal{P}_1 = P_k + \frac{7}{24}h\,[\,f(\mathcal{Q}_1) - \nu\Gamma\mathcal{P}_1\,],$$

$$\begin{aligned}\mathcal{Q}_2 &= Q_k + \frac{25}{24}hM^{-1}P_k + \frac{h^2}{2}M^{-1}\,[\,f(\mathcal{Q}_1) - \nu\Gamma\mathcal{P}_1\,],\\ \mathcal{P}_2 &= P_k + \frac{2}{3}h\,[\,f(\mathcal{Q}_1) - \nu\Gamma\mathcal{P}_1\,] + \frac{3}{8}h\,[\,f(\mathcal{Q}_2) - \nu\Gamma\mathcal{P}_2\,],\end{aligned} \tag{2.23}$$

$$\begin{aligned}\mathcal{Q}_3 &= Q_k + hM^{-1}P_k + \frac{17}{36}h^2M^{-1}\,[\,f(\mathcal{Q}_1) - \nu\Gamma\mathcal{P}_1\,] + \frac{1}{36}h^2M^{-1}\,[\,f(\mathcal{Q}_2) - \nu\Gamma\mathcal{P}_2\,],\\ \mathcal{P}_3 &= P_k + \frac{2}{3}h\,[\,f(\mathcal{Q}_1) - \nu\Gamma\mathcal{P}_1\,] - \frac{2}{3}h\,[\,f(\mathcal{Q}_2) - \nu\Gamma\mathcal{P}_2\,] + h\,[\,f(\mathcal{Q}_3) - \nu\Gamma\mathcal{P}_3\,],\end{aligned}$$

$$\begin{aligned}P_{k+1} = \mathcal{P}_3 &+ \sum_{r=1}^{m}\sigma_r\,\Delta_k w_r - \nu\sum_{r=1}^{m}\Gamma\sigma_r\cdot(I_{r0})_k\\ &+ \sum_{r=1}^{m}\left[\sum_{i=1}^{n}(M^{-1}\sigma_r)^i\,\frac{\partial f}{\partial q^i}(\mathcal{Q}_3) + \nu^2\Gamma^2\sigma_r\right](I_{r00})_k,\end{aligned} \tag{2.24}$$

$$Q_{k+1} = \mathcal{Q}_3 + \sum_{r=1}^{m}M^{-1}\sigma_r\cdot(I_{r0})_k - \nu\sum_{r=1}^{m}M^{-1}\Gamma\sigma_r(I_{r00})_k, \quad k = 0,\dots,N-1,$$

where

$$(I_{r00})_k := \int_{t_k}^{t_k+h}\int_{t_k}^{\vartheta_1}(w_r(\vartheta_2) - w_r(t_k))\,\mathrm{d}\vartheta_2\,\mathrm{d}\vartheta_1.$$

The joint distribution of the random variables $\Delta_k w_r$, $(I_{r0})_k$, $(I_{r00})_k$ is Gaussian. They can be simulated at each step by $3m$ independent $\mathcal{N}(0,1)$-distributed random variables ξ_{rk}, η_{rk}, and ζ_{rk}, $r = 0,\dots,m$:

$$\begin{aligned}\Delta_k w_r &= h^{1/2}\xi_{rk}, \quad (I_{r0})_k = h^{3/2}(\xi_{rk} + \eta_{rk}/\sqrt{3})/2,\\ (I_{r00})_k &= h^{5/2}(\xi_{rk} + \sqrt{3}\eta_{rk}/2 - \zeta_{rk}/(2\sqrt{5}))/6.\end{aligned} \tag{2.25}$$

Using (2.25), the method (2.23)–(2.24) can be written in constructive form. This is implicit in the components $\mathcal{P}_1$, $\mathcal{P}_2$, $\mathcal{P}_3$ and can easily be resolved at each step since the dependence on $\mathcal{P}$ is linear.

For $\nu = 0$ the method (2.23)–(2.24) coincides with the third-order symplectic method from Milstein *et al.* (2002) and so it satisfies the requirement RL1. For $\sigma_r = 0$, $r = 1, \dots, m$ (deterministic case), the RKN method (2.23)–(2.24) satisfies conditions set up in Suris (1991, Section 5). These conditions ensure that the Jacobian of the deterministic RKN method depends on $\nu\Gamma$ and h only, more precisely (Suris, 1991, Section 5)

$$\bar{J}_0 = \bar{J}_0(h, \nu\Gamma) := \frac{D(\mathcal{P}_3, \mathcal{Q}_3)}{D(P_k, Q_k)} = \frac{\det(I - \frac{3}{8}h\nu\Gamma)\det(I + \frac{25}{24}h\nu\Gamma)}{\det(I + \frac{7}{24}h\nu\Gamma)\det(I + \frac{3}{8}h\nu\Gamma)\det(I + h\nu\Gamma)},$$

where I is the $n \times n$ unit matrix.

We have

$$\bar{J} := \frac{D(P_{k+1}, Q_{k+1})}{D(P_k, Q_k)} = \frac{D(P_{k+1}, Q_{k+1})}{D(\mathcal{P}_3, \mathcal{Q}_3)}\frac{D(\mathcal{P}_3, \mathcal{Q}_3)}{D(P_k, Q_k)} = \bar{J}_0,$$

i.e. the Jacobian $\bar{J}$ does not depend on the initial data P_k, Q_k. Further, it is possible to adopt the proof of the corresponding theorem in Milstein *et al.* (2002) and prove that the method (2.23)–(2.24) is of mean-square order 3. Thus, we obtain the following theorem.

THEOREM 2.3 The method (2.23)–(2.24) for the system (2.1) is of mean-square order 3 and it is such that (i) it is symplectic when applied to (2.1)–(2.2) with $\nu = 0$ and (ii) the Jacobian $D(P_{k+1}, Q_{k+1})/D(P_k, Q_k)$ (i.e. the change of phase volume per step) does not depend on P_k, Q_k.

REMARK 2.2 A method of mean-square order 7/2 for (2.1) contains complicated Ito integrals, and it is not efficient with respect to simulation of the random variables used.

REMARK 2.3 All the methods of this section can be carried over to non-autonomous Langevin equations.

3. Quasi-symplectic mean-square methods for general Langevin type equations

Here we generalize the methods of Section 2 to the Langevin type system (cf. (1.1))

$$\begin{gathered} \mathrm{d}P = f(t, Q)\,\mathrm{d}t - \nu\tilde{f}(t, P, Q)\,\mathrm{d}t + \sum_{r=1}^{m}\sigma_r(t, Q)\,\mathrm{d}w_r(t),\ \ P(t_0) = p, \\ \mathrm{d}Q = g(P)\,\mathrm{d}t,\ \ Q(t_0) = q, \end{gathered} \tag{3.1}$$

where P, Q, f, $\tilde{f}$, g, σ_r are n-dimensional column vectors, ν is a parameter, and $w_r(t)$, $r = 1, \dots, m$, are independent standard Wiener processes.

If there are Hamiltonians $H_0(t, p, q) = V_0(p) + U_0(t, q)$ and $H_r(t, q)$, $r = 1, \dots, m$, such that

$$f^i = -\partial H_0/\partial q^i,\ \ g^i = \partial H_0/\partial p^i,\ \ \sigma_r^i = -\partial H_r/\partial q^i,\quad i = 1, \dots, n, \tag{3.2}$$

and if $\nu = 0$, then (3.1) is a Hamiltonian system with multiplicative noise (Bismut, 1981; Milstein *et al.*, 2002, 2003).

Our aim is to construct methods for (3.1) such that they inherit the properties RL1–RL2 of the specific methods for the Langevin equation (2.1). More precisely, we require

RLT1. *The methods become symplectic when the system degenerates to a Hamiltonian one*;

RLT2. *The methods degenerate to those satisfying the requirement* RL2 *from Section* 2 *when the system degenerates to the Langevin equation* (2.1).

We recall that the Euler method for general systems with multiplicative noise is of order $1/2$. But due to specific features of system (3.1), the Euler method (and other usual methods of order $1/2$) applied to (3.1) is of order 1. Therefore, we start with methods of order 1.

3.1 *First-order methods based on splitting*

In connection with (3.1), introduce the systems (cf. (2.5)–(2.6))

$$\begin{aligned} \mathrm{d}P_{\mathrm{I}} &= f(t, Q_{\mathrm{I}})\,\mathrm{d}t + \sum_{r=1}^{m} \sigma_r(t, Q_{\mathrm{I}})\,\mathrm{d}w_r(t), \quad P_{\mathrm{I}}(t_0) = p, \\ \mathrm{d}Q_{\mathrm{I}} &= g(P_{\mathrm{I}})\,\mathrm{d}t, \quad Q_{\mathrm{I}}(t_0) = q, \end{aligned} \tag{3.3}$$

$$\frac{\mathrm{d}P_{\mathrm{II}}}{\mathrm{d}t} = -\nu \tilde{f}(t, P_{\mathrm{II}}, q), \quad P_{\mathrm{II}}(t_0) = p, \tag{3.4}$$

and denote their solutions as $P_{\mathrm{I}}(t; t_0, p, q)$, $Q_{\mathrm{I}}(t; t_0, p, q)$ and $P_{\mathrm{II}}(t; t_0, p, q)$, respectively.

The system (3.3), (3.2) is a Hamiltonian system with separable Hamiltonians. Symplectic integrators for such systems are proposed in Milstein *et al.* (2003). The system (3.4) is deterministic.

Let $\bar{P}_{\mathrm{I}}, \bar{Q}_{\mathrm{I}}$ be a one-step approximation corresponding to a symplectic method for (3.3), (3.2) and $\bar{P}_{\mathrm{II}}$ be a one-step approximation of a deterministic method for (3.4). Introduce the approximation for (3.1) as follows:

$$\begin{aligned} \bar{P} = \bar{P}(t_0 + h; t_0, p, q) &:= \bar{P}_{\mathrm{II}}(t_0 + h; t_0, \bar{P}_{\mathrm{I}}(t_0 + h; t_0, p, q), \bar{Q}_{\mathrm{I}}(t_0 + h; t_0, p, q)), \\ \bar{Q} = \bar{Q}(t_0 + h; t_0, p, q) &:= \bar{Q}_{\mathrm{I}}(t_0 + h; t_0, p, q). \end{aligned} \tag{3.5}$$

Clearly, the approximation (3.5) satisfies the requirements RLT1 and RLT2. Further, using arguments similar to those in the proof of Lemma 2.1, we prove the following theorem.

THEOREM 3.1 Let $\bar{P}_{\mathrm{I}}, \bar{Q}_{\mathrm{I}}$ be a one-step approximation corresponding to a symplectic first-order mean-square method for the system (3.3), (3.2) and $\bar{P}_{\mathrm{II}}$ be a one-step approximation corresponding to a first-order deterministic method for the system (3.4). Then $\bar{P}, \bar{Q}$ defined in (3.5) is a one-step approximation of the first-order mean-square method for the system (3.1) such that (i) it is symplectic when applied to (3.1)–(3.2) with $\nu = 0$ and (ii) it satisfies the requirement RL2 from Section 2 when (3.1) degenerates to the Langevin equation (2.1).

Let us give a concrete example of a first-order splitting method (to this end we use a PRK method from Milstein *et al.*, 2003):

$$\mathcal{Q}_1 = Q_k + \alpha h g(P_k), \quad \mathcal{P}_1 = P_k + h f(t_k + \alpha h, \mathcal{Q}_1),$$

$$\mathcal{Q}_2 = \mathcal{Q}_1 + (1-\alpha) h g(\mathcal{P}_1), \ \mathcal{P}_2 = \mathcal{P}_1 + \sum_{r=1}^{m} \sigma_r(t_k, \mathcal{Q}_2) \Delta_k w_r, \tag{3.6}$$

$$Q_{k+1} = \mathcal{Q}_2, \ P_{k+1} = \mathcal{P}_2 - h\nu \tilde{f}(t_k, \mathcal{P}_2, \mathcal{Q}_2).$$

REMARK 3.1 Theorem 3.1 also holds for the method based on the one-step approximation

$$\begin{aligned} \bar{P} &:= \bar{P}_{\mathrm{I}}(t_0 + h; t_0, \bar{P}_{\mathrm{II}}(t_0 + h; t_0, p, q), q), \\ \bar{Q} &:= \bar{Q}_{\mathrm{I}}(t_0 + h; t_0, \bar{P}_{\mathrm{II}}(t_0 + h; t_0, p, q), q). \end{aligned} \tag{3.7}$$

REMARK 3.2 The discussion in the end of Section 2.1 is also valid here: there are first-order implicit symplectic methods which directly applied to (3.1) give the methods satisfying the requirements RLT1–RLT2.

The particular case of system (3.1), when $\tilde{f}(t, p, q) = \Gamma(q)p$, Γ is an $m \times m$-dimensional matrix, is of a special interest, in particular due to its application in dissipative particle dynamics (see e.g. Ripoll *et al.*, 2001 and references therein). In this case the system (3.4) becomes a deterministic linear system with constant coefficients, which can be solved exactly. If in addition to $\tilde{f}(t, p, q) = \Gamma(q)p$ the system (3.1) is with additive noise (i.e. $\sigma_r(t, q) = \sigma_r(t)$, $r = 1, \ldots, q$) and $g(p) = M^{-1}p$, then the method (3.9) (see Section 3.2) becomes of mean-square order 2. An important example of such systems is the Van der Pol oscillator under external excitations:

$$\ddot{Q} = -\omega^2 Q + \varepsilon^2 (1 - Q^2)\dot{Q} + \sigma \dot{w}.$$

Further, our approach can easily be applied to a more general system of Stratonovich SDEs:

$$\begin{aligned} \mathrm{d}P &= \Big(f(t, P, Q) - \nu \tilde{f}(t, P, Q) \Big) \mathrm{d}t + \sum_{r=1}^{m} \sigma_r(t, P, Q) \circ \mathrm{d}w_r(t), \ P(t_0) = p, \\ \mathrm{d}Q &= (g(t, P, Q) - \nu \tilde{g}(t, P, Q)) \, \mathrm{d}t + \sum_{r=1}^{m} \gamma_r(t, P, Q) \circ \mathrm{d}w_r(t), \ Q(t_0) = q, \end{aligned} \tag{3.8}$$

where $\nu \geqslant 0$ is a parameter, P, Q and all the coefficients are n-dimensional column vectors, and f, g, σ_r, γ_r satisfy (1.3). For $\nu = 0$ it coincides with the general Hamiltonian system (1.2). As usual, we can split (3.8) in two parts: in the Hamiltonian system (1.2) and the deterministic system, and then use a relation like (3.5) or (3.7) to approximate (3.8). In such an approximation we have $\bar{P}_{\mathrm{I}}$, $\bar{Q}_{\mathrm{I}}$ corresponding to a full implicit symplectic method from Milstein *et al.* (2003). As a result, we obtain the approximation $\bar{P}$, $\bar{Q}$ for (3.8) which satisfies the requirements RLT1–RLT2. Such a method for (3.8) based on an approximation of this kind has the mean-square order $1/2$.

3.2 *Methods of order* 3/2

Using the fractional step method, we propose the following approximation for (3.1):

$$\begin{aligned}
&\bar{P}(t_0+h;\,t_0,\,p,\,q)\\
&:=\bar{P}_{\mathrm{II}}\left(t_0+\frac{h}{2};\,t_0,\,\bar{P}_{\mathrm{I}}\left(t_0+h;\,t_0,\,\bar{P}_{\mathrm{II}}\left(t_0+\frac{h}{2};\,t_0,\,p,\,q\right),\,q\right),\right.\\
&\qquad\left.\bar{Q}_{\mathrm{I}}\left(t_0+h;\,t_0,\,\bar{P}_{\mathrm{II}}\left(t_0+\frac{h}{2};\,t_0,\,p,\,q\right),\,q\right)\right)\\
&-\nu\sum_{r=1}^{m}\sum_{i=1}^{n}\sigma_r^i\frac{\partial\tilde{f}}{\partial p^i}(t_0,\,p,\,q)\left[I_{r0}-\frac{h}{2}\Delta w_r\right]-\frac{h^2}{4}\nu\frac{\partial\tilde{f}}{\partial t}(t_0,\,p,\,q),\\
&\bar{Q}(t_0+h;\,t_0,\,p,\,q):=\bar{Q}_{\mathrm{I}}\left(t_0+h;\,t_0,\,\bar{P}_{\mathrm{II}}\left(t_0+\frac{h}{2};\,t_0,\,p,\,q\right),\,q\right),
\end{aligned}\tag{3.9}$$

where $\bar{P}_{\mathrm{I}}$, $\bar{Q}_{\mathrm{I}}$ is a one-step approximation corresponding to a symplectic method of order 3/2 for (3.3), (3.2) (such methods are available in Milstein *et al.*, 2003) and $\bar{P}_{\mathrm{II}}$ is a one-step approximation of a second-order deterministic method for (3.4).

By argument similar to those exploited in previous sections, we prove the following theorem.

THEOREM 3.2 Let $\bar{P}_{\mathrm{I}}$, $\bar{Q}_{\mathrm{I}}$ be a one-step approximation corresponding to a symplectic mean-square method of order 3/2 for the system (3.3), (3.2), and $\bar{P}_{\mathrm{II}}$ be a one-step approximation corresponding to a second-order deterministic method for the system (3.4). Then $\bar{P}$, $\bar{Q}$ defined in (3.9) is the one-step approximation of mean-square method of order 3/2 for the system (3.1) which satisfies the requirements RLT1–RLT2.

4. Symplectic methods in the weak sense for Hamiltonian systems with multiplicative noise

Let us recall some facts from the theory of numerical integration of SDEs in the weak sense. Further details are available in Milstein (1995) and Kloeden & Platen (1992). Consider the system of SDEs in the Ito sense

$$\mathrm{d}X=a(t,\,X)\,\mathrm{d}t+\sum_{r=1}^{m}b_r(t,\,X)\,\mathrm{d}w_r(t),\;\;X(t_0)=X_0,\tag{4.1}$$

where $X, a(t, x^1, \ldots, x^d), b_r(t, x^1, \ldots, x^d)$ are d-dimensional column vectors and $w_r(t)$, $r = 1, \ldots, m$, are independent standard Wiener processes.

Suppose the functions $a(t, x)$ and $b_r(t, x)$ are defined and continuous for $t \in [t_0, t_0 + T]$, $x \in R^d$ and satisfy a uniform (global) Lipschitz condition: for all $t \in [t_0, t_0 + T]$, $x, y \in R^d$ there exists a constant $L > 0$ such that

$$|a(t,x)-a(t,y)|+\sum_{r=1}^{m}|b_r(t,x)-b_r(t,y)|\leqslant L\,|x-y|\,.\tag{4.2}$$

DEFINITION 4.1 If for some method we have

$$\left|EF(\bar{X}_k) - EF(X(t_k))\right| \leqslant Kh^l,$$

for F from a sufficiently large class of functions, where the constant K does not depend on k and h, then we say that $\bar{X}_k$ approximates the solution $X(t_k)$ of (4.1) in the weak sense with (weak) order of accuracy l (or $O(h^l)$).

DEFINITION 4.2 A function $F(x)$, $x \in R^d$, is said to belong to the class $\mathbf{F}$, $F \in \mathbf{F}$, if there are constants $K > 0$ and $\varkappa \geqslant 0$ such that the inequality

$$|F(x)| \leqslant K \cdot (1 + |x|^{\varkappa})$$

holds for any $x \in R^d$.

The following general convergence theorem is proved in Milstein (1995) (see also Kloeden & Platen, 1992).

THEOREM 4.1 Suppose that

(1) the coefficients of (4.1) are continuous, satisfy a Lipschitz condition (4.2) and together with their partial derivatives of order up to $2l + 2$ belong to the class $\mathbf{F}$;

(2) the following inequalities hold:

$$\left|E\left(\prod_{j=1}^{s}\Delta^{i_j} - \prod_{j=1}^{s}\bar{\Delta}^{i_j}\right)\right| \leqslant K(x)h^{l+1},\ s = 1, \ldots, 2l+1, \tag{4.3}$$

$$E\prod_{j=1}^{2l+2}|\bar{\Delta}^{i_j}| \leqslant K(x)h^{l+1},\ l > 0,\ K(x) \in \mathbf{F}, \tag{4.4}$$

where $\Delta^i := X^i_{t,x}(t+h) - x^i$ and $\bar{\Delta}^i := \bar{X}^i_{t,x}(t+h) - x^i$;

(3) the function $F(x)$ together with its partial derivatives up to order $2l + 2$ belong to the class $\mathbf{F}$;

(4) for a sufficiently large number $\bar{m}$, the moments $E|X_k|^{\bar{m}}$ exist and are uniformly bounded with respect to N, $k = 0, \ldots, N$.

Then the method X_k approximates the solution $X(t_k)$ with the weak order l.

We assume the conditions on certain smoothness of the drift and diffusion coefficients and boundedness of their derivatives to be fulfilled. At the same time we underline once again (see Introduction) that these traditional requirements are not necessary.

4.1 *Implicit first-order methods for general stochastic Hamiltonian systems*

In this section weak symplectic methods for the stochastic Hamiltonian system (1.2), (1.3) are constructed. All the methods in this section are fully implicit (i.e. implicit in both deterministic and stochastic components). Let us recall that in the case of deterministic general Hamiltonian systems symplectic Runge–Kutta (RK) methods are

all implicit (Sanz-Serna & Calvo, 1994). The standard implicit methods for SDEs with multiplicative noise (see Milstein, 1995; Kloeden & Platen, 1992) contain implicitness in deterministic terms only. Meanwhile, to construct symplectic methods for general stochastic Hamiltonian systems, fully implicit methods are needed. Such mean-square methods are proposed in Milstein *et al.* (2003). Increments of Wiener processes in these implicit schemes are substituted by some truncated random variables. As a result, general mean-square symplectic methods are obtained in Milstein *et al.* (2003). We should note that the problem in obtaining *fully* implicit *weak* methods is much simpler because standard weak schemes exploit bounded random variables for their construction.

On the basis of a symplectic method of mean-square order $1/2$ from Milstein *et al.* (2003), we propose the weak method

$$\begin{aligned} P_{k+1} &= P_k + hf(t_k + \beta h, \alpha P_{k+1} + (1-\alpha)P_k, (1-\alpha)Q_{k+1} + \alpha Q_k) \\ &\quad + h\left(\frac{1}{2} - \alpha\right)\sum_{r=1}^{m}\sum_{j=1}^{n}\left(\frac{\partial \sigma_r}{\partial p^j}\sigma_r^j - \frac{\partial \sigma_r}{\partial q^j}\gamma_r^j\right) + h^{1/2}\sum_{r=1}^{m}\sigma_r\xi_{rk}, \\ Q_{k+1} &= Q_k + hg(t_k + \beta h, \alpha P_{k+1} + (1-\alpha)P_k, (1-\alpha)Q_{k+1} + \alpha Q_k) \\ &\quad + h\left(\frac{1}{2} - \alpha\right)\sum_{r=1}^{m}\sum_{j=1}^{n}\left(\frac{\partial \gamma_r}{\partial p^j}\sigma_r^j - \frac{\partial \gamma_r}{\partial q^j}\gamma_r^j\right) + h^{1/2}\sum_{r=1}^{m}\gamma_r\xi_{rk}, \end{aligned} \tag{4.5}$$

where σ_r, γ_r, $r = 1, \ldots, m$, and their derivatives are calculated at $(t_k, \alpha P_{k+1} + (1-\alpha)P_k, (1-\alpha)Q_{k+1} + \alpha Q_k)$, the parameters $\alpha, \beta \in [0, 1]$, and ξ_{rk} are i.i.d. random variables with the law

$$P(\xi = \pm 1) = 1/2. \tag{4.6}$$

Note that if $\alpha = \beta = 1/2$ the method (4.5) becomes the derivative-free (midpoint) method. The method requires solution of a nonlinear equation at each step (its solvability is proved within the next theorem).

THEOREM 4.2 The implicit method (4.5) for the system (1.2), (1.3) is symplectic and of the first weak order.

Proof. The symplecticness is proved in the same way as in Theorem 3.2 from Milstein *et al.* (2003). Let us prove convergence of the method. Denote by $\bar{X} = \bar{X}(t + h; t, x) = (\bar{P}^{\mathsf{T}}, \bar{Q}^{\mathsf{T}})^{\mathsf{T}}$ the one-step approximation corresponding to the method (4.5):

$$\begin{aligned} \bar{P} &= p + hf(t + \beta h, \alpha\bar{P} + (1-\alpha)p, (1-\alpha)\bar{Q} + \alpha q) \\ &\quad + h\left(\frac{1}{2} - \alpha\right)\sum_{r=1}^{m}\sum_{j=1}^{n}\left(\frac{\partial \sigma_r}{\partial p^j}\sigma_r^j - \frac{\partial \sigma_r}{\partial q^j}\gamma_r^j\right) + h^{1/2}\sum_{r=1}^{m}\sigma_r\xi_r, \\ \bar{Q} &= q + hg(t + \beta h, \alpha\bar{P} + (1-\alpha)p, (1-\alpha)\bar{Q} + \alpha q) \\ &\quad + h\left(\frac{1}{2} - \alpha\right)\sum_{r=1}^{m}\sum_{j=1}^{n}\left(\frac{\partial \gamma_r}{\partial p^j}\sigma_r^j - \frac{\partial \gamma_r}{\partial q^j}\gamma_r^j\right) + h^{1/2}\sum_{r=1}^{m}\gamma_r\xi_r, \end{aligned} \tag{4.7}$$

where σ_r, γ_r, $r = 1, \dots, m$, and their derivatives are calculated at $(t, \alpha\bar{P} + (1-\alpha)p, (1-\alpha)\bar{Q} + \alpha q)$.

Using the Lipschitz condition (4.2), one can prove (cf. Lemma 2.4 in Milstein *et al.*, 2003) that there are constants $K > 0$ and $h_0 > 0$ such that for any $h \leqslant h_0$, $t_0 \leqslant t \leqslant t_0 + T$, $x = (p^{\mathsf{T}}, q^{\mathsf{T}})^{\mathsf{T}} \in R^d$, $d = 2n$, the equation (4.7) has a unique solution $\bar{X}$ which satisfies the inequality

$$|\bar{X} - x| \leqslant K(1 + |x|)\sqrt{h}, \tag{4.8}$$

and this solution can be found by the method of simple iteration with $x = (p^{\mathsf{T}}, q^{\mathsf{T}})^{\mathsf{T}}$ as the initial approximation.

The condition (4.4) with $l = 1$ of Theorem 4.1 holds for the approximation (4.7) due to (4.8). Let us check the fulfillment of condition (4.3) with $l = 1$. To this end, introduce the weak Euler approximation $\hat{X} = (\hat{P}^{\mathsf{T}}, \hat{Q}^{\mathsf{T}})^{\mathsf{T}}$ for the Stratonovich system (1.2), (1.3):

$$\begin{aligned}
\hat{P} &= p + hf + \frac{h}{2}\sum_{r=1}^{m}\sum_{j=1}^{n}\left(\frac{\partial \sigma_r}{\partial p^j}\sigma_r^j + \frac{\partial \sigma_r}{\partial q^j}\gamma_r^j\right) + h^{1/2}\sum_{r=1}^{m}\sigma_r\xi_r, \\
\hat{Q} &= q + hg + \frac{h}{2}\sum_{r=1}^{m}\sum_{j=1}^{n}\left(\frac{\partial \gamma_r}{\partial p^j}\sigma_r^j + \frac{\partial \gamma_r}{\partial q^j}\gamma_r^j\right) + h^{1/2}\sum_{r=1}^{m}\gamma_r\xi_r,
\end{aligned} \tag{4.9}$$

where f, g and σ_r, γ_r, $r = 1, \dots, m$, and their derivatives are calculated at (t, p, q).

Expanding the terms in the right-hand side of (4.7) around (t, p, q) and using (4.8) and the corresponding conditions on smoothness and boundedness of the coefficients, it is not difficult to obtain that

$$\left|E\left(\prod_{j=1}^{s}\hat{\Delta}^{i_j} - \prod_{j=1}^{s}\bar{\Delta}^{i_j}\right)\right| \leqslant K(x)h^2, \ s = 1, 2, 3, \ i_j = 1, \dots, 2n, \ K(x) \in \mathbf{F}, \tag{4.10}$$

where $\bar{\Delta}^i := \bar{X}^i - x^i$, $\hat{\Delta}^i := \hat{X}^i - x^i$.

Taking into account (4.10) and the fact that the Euler approximation (4.9) satisfies (4.3) with $l = 1$ (Milstein, 1995; Kloeden & Platen, 1992), we get that the approximation (4.7) satisfies (4.3) with $l = 1$ as well.

Finally, to check the fourth condition of Theorem 4.1, we use Lemma 9.1 from Milstein (1995, p. 114) which ensures existence and uniform boundedness of the moments $E|\bar{X}_k|^{\bar{m}}$ under the conditions (i) $|E\bar{\Delta}| \leqslant K(1 + |x|)h$ and (ii) $|\bar{\Delta}| \leqslant M(\xi)(1 + |x|)\sqrt{h}$ with $M(\xi)$ having moments of all orders. The inequalities (4.10) and $|E\hat{\Delta}| \leqslant K(1 + |x|)h$ imply fulfillment of the condition (i), while the condition (ii) holds here due to (4.8). □

REMARK 4.1 In the case of separable Hamiltonians at noise, i.e. when $H_r(t, p, q) =$

$U_r(t,q)+V_r(t,p)$, $r=1,\dots m$, the method (4.5) with $\alpha=1,\ \beta=0$ acquires the form

$$\begin{aligned} P_{k+1} &= P_k + f(t_k, P_{k+1}, Q_k)h \\ &\quad + \frac{h}{2}\sum_{r=1}^{m}\sum_{j=1}^{n}\frac{\partial\sigma_r}{\partial q^j}(t_k, Q_k)\cdot\gamma_r^j(t_k, P_{k+1}) + h^{1/2}\sum_{r=1}^{m}\sigma_r(t_k, Q_k)\xi_{rk}, \\ Q_{k+1} &= Q_k + g(t_k, P_{k+1}, Q_k)h \\ &\quad - \frac{h}{2}\sum_{r=1}^{m}\sum_{j=1}^{n}\frac{\partial\gamma_r}{\partial p^j}(t_k, P_{k+1})\cdot\sigma_r^j(t_k, Q_k) + h^{1/2}\sum_{r=1}^{m}\gamma_r(t_k, P_{k+1})\xi_{rk} \end{aligned} \tag{4.11}$$

with not too complicated implicitness. Besides, when the Hamiltonians are such that $H_0(t,p,q)=V_0(t,p)+U_0(t,q)$ and $H_r(t,p,q)=\Gamma_r^{\top}(t)p+U_r(t,q)$, $r=1,\dots m$, $\Gamma_r(t)$ are n-dimensional vectors, one obtains fully explicit symplectic methods.

REMARK 4.2 As is known (Milstein, 1995; Kloeden & Platen, 1992), there are effective methods of weak order 2 for general systems of SDEs. These methods applied to (1.2), (1.3) are not symplectic. We have not constructed a symplectic method of weak order 2 for the general Hamiltonian system (1.2), (1.3), and this question requires further investigation. In the next section a symplectic method of weak order 2 is proposed for a particular case of (1.2), (1.3).

4.2 *Explicit first-order methods in the case of separable Hamiltonians*

In this and the next sections we consider a special case of the Hamiltonian system (1.2), (1.3) such that

$$H_0(t,p,q)=V_0(p)+U_0(t,q),\ \ H_r(t,p,q)=U_r(t,q),\ \ r=1,\dots m. \tag{4.12}$$

In this case we get the following system:

$$\begin{gathered} \mathrm{d}P = f(t,Q)\,\mathrm{d}t + \sum_{r=1}^{m}\sigma_r(t,Q)\,\mathrm{d}w_r(t),\ \ P(t_0)=p, \\ \mathrm{d}Q = g(P)\,\mathrm{d}t,\ \ Q(t_0)=q, \end{gathered} \tag{4.13}$$

with

$$f^i=-\partial U_0/\partial q^i,\ \ g^i=\partial V_0/\partial p^i,\ \ \sigma_r^i=-\partial U_r/\partial q^i,\ \ r=1,\dots m,\ \ i=1,\dots,n. \tag{4.14}$$

Recall that the system (4.13) has the same form in the sense of Stratonovich. Due to specific features of the system (4.13), (4.14) we have succeeded in construction of explicit PRK methods of a higher order.

On the basis of the mean-square PRK method (4.6) from Milstein *et al.* (2003) we obtain the weak PRK method for (4.13):

$$\begin{gathered} \mathcal{Q}_1 = Q_k + \alpha h g(P_k),\ \ \mathcal{P}_1 = P_k + h f(t_k+\alpha h, \mathcal{Q}_1), \\ \mathcal{Q}_2 = \mathcal{Q}_1 + (1-\alpha)h g(\mathcal{P}_1), \end{gathered} \tag{4.15}$$

$$P_{k+1} = \mathcal{P}_1 + h^{1/2} \sum_{r=1}^{m} \sigma_r(t_k, \mathcal{Q}_2)\xi_{rk}, \quad Q_{k+1} = \mathcal{Q}_2, \ k = 0, \dots, N-1, \tag{4.16}$$

where $0 \leqslant \alpha \leqslant 1$ is a parameter and ξ_{rk} are i.i.d. random variables with the law (4.6).

THEOREM 4.3 The explicit method (4.15)–(4.16) for the system (4.13), (4.14) is symplectic and of the first weak order.

Proof. Due to (4.14), $\partial\sigma_r^i/\partial q^j = \partial\sigma_r^j/\partial q^i$. Using this, we obtain $\mathrm{d}P_{k+1} \wedge \mathrm{d}Q_{k+1} = d\mathcal{P}_1 \wedge \mathrm{d}\mathcal{Q}_2$. It is easy to prove that $\mathrm{d}\mathcal{P}_1 \wedge \mathrm{d}\mathcal{Q}_2 = \mathrm{d}\mathcal{P}_1 \wedge \mathrm{d}\mathcal{Q}_1 = \mathrm{d}P_k \wedge \mathrm{d}Q_k$. Therefore the method (4.15)–(4.16) is symplectic. The order of convergence is proved as in Theorem 4.2 (even simpler). □

4.3 *Explicit second-order method in the case of separable Hamiltonians*

Introduce the explicit PRK method for the system (4.13), (4.14):

$$\mathcal{Q}_1 = Q_k + \frac{h}{2} g(P_k), \quad \mathcal{P}_1 = P_k + hf\left(t_k + \frac{h}{2}, \mathcal{Q}_1\right) + h^{1/2} \sum_{r=1}^{m} \sigma_r\left(t_k + \frac{h}{2}, \mathcal{Q}_1\right)\xi_{rk},$$
$$P_{k+1} = \mathcal{P}_1, \quad Q_{k+1} = \mathcal{Q}_1 + \frac{h}{2} g(\mathcal{P}_1), \ k = 0, \dots, N-1, \tag{4.17}$$

where ξ_{rk} are i.i.d. random variables with the law

$$P(\xi = 0) = 2/3, \quad P(\xi = \pm\sqrt{3}) = 1/6. \tag{4.18}$$

It follows from Lemma 4.1 from Milstein *et al.* (2003) that this method is symplectic. Comparing (4.17) with the standard Taylor type second-order weak method from Milstein (1995, p. 115) applied to (4.13), we prove the following theorem.

THEOREM 4.4 The explicit method (4.17) for the system (4.13), (4.14) is symplectic and of the second weak order.

5. Symplectic methods in the weak sense for Hamiltonian systems with additive noise

Consider Hamiltonian systems with additive noise

$$\begin{aligned} \mathrm{d}P &= f(t, P, Q)\,\mathrm{d}t + \sum_{r=1}^{m} \sigma_r(t)\,\mathrm{d}w_r(t), \ P(t_0) = p, \\ \mathrm{d}Q &= g(t, P, Q)\,\mathrm{d}t + \sum_{r=1}^{m} \gamma_r(t)\,\mathrm{d}w_r(t), \ Q(t_0) = q, \end{aligned} \tag{5.1}$$

where f and g satisfy (1.3).

The first-order method for (5.1) follows from the method (4.5).

5.1 *Implicit second-order methods in the case of general Hamiltonian system*

On the basis of a mean-square symplectic method of order $3/2$ from Milstein *et al.* (2002), we construct the weak method:

$$\begin{aligned}
\mathcal{P}_1 &= P_k + \frac{\alpha}{2} h f\left(t_k + \frac{\alpha}{2}h, \mathcal{P}_1, \mathcal{Q}_1\right) + \lambda_1 h^{1/2} \sum_{r=1}^{m} \sigma_r \left(t_k + \frac{h}{2}\right) \xi_{rk}, \\
\mathcal{Q}_1 &= Q_k + \frac{\alpha}{2} h g\left(t_k + \frac{\alpha}{2}h, \mathcal{P}_1, \mathcal{Q}_1\right) + \lambda_1 h^{1/2} \sum_{r=1}^{m} \gamma_r \left(t_k + \frac{h}{2}\right) \xi_{rk}, \\
\mathcal{P}_2 &= P_k + \alpha h f\left(t_k + \frac{\alpha}{2}h, \mathcal{P}_1, \mathcal{Q}_1\right) + \frac{1-\alpha}{2} h f\left(t_k + \frac{1+\alpha}{2}h, \mathcal{P}_2, \mathcal{Q}_2\right) \\
&\quad + \lambda_2 h^{1/2} \sum_{r=1}^{m} \sigma_r \left(t_k + \frac{h}{2}\right) \xi_{rk}, \\
\mathcal{Q}_2 &= Q_k + \alpha h g\left(t_k + \frac{\alpha}{2}h, \mathcal{P}_1, \mathcal{Q}_1\right) + \frac{1-\alpha}{2} h g\left(t_k + \frac{1+\alpha}{2}h, \mathcal{P}_2, \mathcal{Q}_2\right) \\
&\quad + \lambda_2 h^{1/2} \sum_{r=1}^{m} \gamma_r \left(t_k + \frac{h}{2}\right) \xi_{rk}, \\
P_{k+1} &= P_k + h\left[\alpha f\left(t_k + \frac{\alpha}{2}h, \mathcal{P}_1, \mathcal{Q}_1\right) + (1-\alpha) f\left(t_k + \frac{1+\alpha}{2}h, \mathcal{P}_2, \mathcal{Q}_2\right)\right] \\
&\quad + h^{1/2} \sum_{r=1}^{m} \sigma_r \left(t_k + \frac{h}{2}\right) \xi_{rk}, \\
Q_{k+1} &= Q_k + h\left[\alpha g\left(t_k + \frac{\alpha}{2}h, \mathcal{P}_1, \mathcal{Q}_1\right) + (1-\alpha) g\left(t_k + \frac{1+\alpha}{2}h, \mathcal{P}_2, \mathcal{Q}_2\right)\right] \\
&\quad + h^{1/2} \sum_{r=1}^{m} \gamma_r \left(t_k + \frac{h}{2}\right) \xi_{rk},
\end{aligned} \tag{5.2}$$

where the parameters α, λ_1, λ_2 are such that

$$\alpha\lambda_1 + (1-\alpha)\lambda_2 = \frac{1}{2}, \ \alpha\lambda_1^2 + (1-\alpha)\lambda_2^2 = \frac{1}{2}, \tag{5.3}$$

and ξ_{rk} are i.i.d. random variables with the law (4.18).

For example, the following set of parameters satisfies (5.3):

$$\alpha = \frac{1}{2}, \ \lambda_1 = 0, \ \lambda_2 = 1. \tag{5.4}$$

The symplecticness follows from Lemma 3.5 of Milstein *et al.* (2002). The order of convergence is proved similarly to the proof of Theorem 4.2 comparing (5.2) with the standard Taylor type second-order weak method from Milstein (1995, p. 115) applied to (5.1).

THEOREM 5.1 The implicit method (5.2), (5.3) for the system (5.1) is symplectic and of the second weak order.

5.2 *A third-order method in a particular case of Hamiltonian system*

In this section we propose a symplectic weak method of order 3 for the system with additive noise:

$$\begin{gathered} \mathrm{d}P = f(t,Q)\,\mathrm{d}t + \sum_{r=1}^{m}\sigma_r(t)\,\mathrm{d}w_r(t),\ \ f^i(t,Q) = -\frac{\partial U_0}{\partial q^i},\ \ P(t_0) = p, \\ \mathrm{d}Q = M^{-1}P\,\mathrm{d}t,\ \ Q(t_0) = q. \end{gathered} \tag{5.5}$$

On the basis of a symplectic mean-square method of order 3 from Milstein *et al.* (2002), we construct the weak method:

$$\begin{gathered} \mathcal{Q}_1 = Q_k + \frac{7}{24}hM^{-1}P_k,\ \ \mathcal{P}_1 = P_k + \frac{2}{3}hf\left(t_k + \frac{7h}{24}, \mathcal{Q}_1\right), \\ \mathcal{Q}_2 = \mathcal{Q}_1 + \frac{3}{4}hM^{-1}\mathcal{P}_1,\ \ \mathcal{P}_2 = \mathcal{P}_1 - \frac{2}{3}hf\left(t_k + \frac{25h}{24}, \mathcal{Q}_2\right), \\ \mathcal{Q}_3 = \mathcal{Q}_2 - \frac{1}{24}hM^{-1}\mathcal{P}_2,\ \ \mathcal{P}_3 = \mathcal{P}_2 + hf(t_k + h, \mathcal{Q}_3), \end{gathered} \tag{5.6}$$

$$\begin{aligned} P_{k+1} &= \mathcal{P}_3 + h^{1/2}\sum_{r=1}^{m}\sigma_r(t_k)\xi_{rk} + h^{3/2}\sum_{r=1}^{m}\sigma_r'(t_k)(\xi_r/2 - \eta_r)_k + h^{5/2}\sum_{r=1}^{m}\sigma_r''(t_k)\xi_{rk}/6 \\ &\quad + h^{5/2}\sum_{r=1}^{m}\sum_{i=1}^{n}(M^{-1}\sigma_r(t_k))^i\frac{\partial f}{\partial q^i}(t_k, \mathcal{Q}_3)\xi_{rk}/6, \\ Q_{k+1} &= \mathcal{Q}_3 + h^{3/2}\sum_{r=1}^{m}M^{-1}\sigma_r(t_k)(\xi_r/2 + \eta_r)_k + h^{5/2}\sum_{r=1}^{m}M^{-1}\sigma_r'(t_k)\xi_{rk}/6, \\ &\qquad k = 0, \ldots, N-1, \end{aligned} \tag{5.7}$$

where ξ_{rk}, η_{rk} are mutually independent random variables distributed by the laws

$$\begin{gathered} P(\xi = 0) = \frac{1}{3},\ \ P(\xi = \pm 1) = \frac{3}{10},\ \ P(\xi = \pm\sqrt{6}) = \frac{1}{30}, \\ P(\eta = \pm 1/\sqrt{12}) = \frac{1}{2}. \end{gathered} \tag{5.8}$$

The symplecticness of this method follows from Theorem 5.3 of Milstein *et al.* (2002). The order of convergence can be proved by standard arguments (Milstein, 1995, Section 10) using the fact that the corresponding mean-square method from Milstein *et al.* (2002) has the third order of convergence or by comparing the method (5.6)–(5.7) with the weak method of order 3 from Milstein (1995, p. 126) applied to (5.5).

THEOREM 5.2 The explicit method (5.6)–(5.7) for the system (5.5) is symplectic and of the third weak order.

6. Weak methods for Langevin type equations

Symplectic methods in the weak sense proposed in Sections 4 and 5 together with the ideas of Sections 2 and 3 allow us to derive efficient weak methods for Langevin type equations.

6.1 *Langevin equation: linear damping and additive noise*

In this section we propose weak methods for the Langevin equation (2.1), which satisfy the requirements RL1–RL2 from Section 2.

Using the splitting ideas presented in Section 2, we obtain the first-order method.

THEOREM 6.1 Let $\bar{P}_{\mathrm{I}}$, $\bar{Q}_{\mathrm{I}}$ be a one-step approximation corresponding to a symplectic method of first weak order for the system (2.5), (2.2). Then $\bar{P}$, $\bar{Q}$ defined in (2.7) or in (2.14) is a one-step approximation of the method of first weak order for the system (2.1) which satisfies the requirements RL1–RL2.

As for $\bar{P}_{\mathrm{I}}$, $\bar{Q}_{\mathrm{I}}$ appearing in the above theorem, one can take the approximation corresponding to the symplectic implicit method (4.5) or to the explicit one (4.15)–(4.16).

REMARK 6.1 The implicit method (4.5) can directly be applied to the Langevin equation (2.1). Of course, it satisfies the requirement RL1. The method (4.5) satisfies the requirement RL2 for $\alpha = 0$ and $\alpha = 1$ only (see also the discussion in the end of Section 2.1).

Now we construct a method of weak order 2. To this end, consider the following approximation for (2.1) (cf. (2.17)):

$$\begin{aligned} \bar{P} = \bar{P}(t_0 + h;\, t_0,\, p, q) &:= P_{\mathrm{II}}\left(\frac{h}{2};\, \bar{P}_{\mathrm{I}}\left(t_0 + h;\, t_0,\, P_{\mathrm{II}}\left(\frac{h}{2};\, p\right), q\right)\right), \\ \bar{Q} = \bar{Q}(t_0 + h;\, t_0,\, p, q) &:= \bar{Q}_{\mathrm{I}}\left(t_0 + h;\, t_0,\, P_{\mathrm{II}}\left(\frac{h}{2};\, p\right), q\right), \end{aligned} \tag{6.1}$$

where $\bar{P}_{\mathrm{I}}$, $\bar{Q}_{\mathrm{I}}$ is a one-step approximation corresponding to any symplectic weak second-order method for (2.5), (2.2) (for instance, one can use the implicit method (5.2) or the explicit method (4.17)), and $P_{\mathrm{II}}(t)$ is the exact solution of (2.6).

THEOREM 6.2 Let $\bar{P}_{\mathrm{I}}$, $\bar{Q}_{\mathrm{I}}$ be a one-step approximation corresponding to a symplectic method of second weak order for the system (2.5), (2.2). Then $\bar{P}$, $\bar{Q}$ defined in (6.1) is a one-step approximation of the method of second weak order for the system (2.1) which satisfies the requirements RL1–RL2.

To get a method of weak order 3 for (2.1), we modify the symplectic RKN method (5.6)–(5.7) as we did in Section 2.3 in the case of mean-square methods. On this way we obtain the following method

$$\mathcal{Q}_1 = Q_k + \frac{7}{24}hM^{-1}P_k, \quad \mathcal{P}_1 = P_k + \frac{7}{24}h\left[f(\mathcal{Q}_1) - \nu\Gamma\mathcal{P}_1\right],$$

$$\begin{aligned} \mathcal{Q}_2 &= Q_k + \frac{25}{24}hM^{-1}P_k + \frac{h^2}{2}M^{-1}\left[f(\mathcal{Q}_1) - \nu\Gamma\mathcal{P}_1\right], \\ \mathcal{P}_2 &= P_k + \frac{2}{3}h\left[f(\mathcal{Q}_1) - \nu\Gamma\mathcal{P}_1\right] + \frac{3}{8}h\left[f(\mathcal{Q}_2) - \nu\Gamma\mathcal{P}_2\right], \end{aligned} \tag{6.2}$$

$$\mathcal{Q}_3 = Q_k + hM^{-1}P_k + \frac{17}{36}h^2M^{-1}[f(\mathcal{Q}_1) - \nu\Gamma\mathcal{P}_1] + \frac{1}{36}h^2M^{-1}[f(\mathcal{Q}_2) - \nu\Gamma\mathcal{P}_2],$$
$$\mathcal{P}_3 = P_k + \frac{2}{3}h[f(\mathcal{Q}_1) - \nu\Gamma\mathcal{P}_1] - \frac{2}{3}h[f(\mathcal{Q}_2) - \nu\Gamma\mathcal{P}_2] + h[f(\mathcal{Q}_3) - \nu\Gamma\mathcal{P}_3],$$

$$\begin{aligned} P_{k+1} &= \mathcal{P}_3 + h^{1/2}\sum_{r=1}^{m}\sigma_r\xi_{rk} - \nu h^{3/2}\sum_{r=1}^{m}\Gamma\sigma_r\cdot(\xi_r/2+\eta_r)_k \\ &\quad + h^{5/2}\sum_{r=1}^{m}\left[\sum_{i=1}^{n}(M^{-1}\sigma_r)^i\frac{\partial f}{\partial q^i}(\mathcal{Q}_3) + \nu^2\Gamma^2\sigma_r\right]\xi_{rk}/6, \\ Q_{k+1} &= \mathcal{Q}_3 + h^{3/2}\sum_{r=1}^{m}M^{-1}\sigma_r\cdot(\xi_r/2+\eta_r)_k \\ &\quad - \nu h^{5/2}\sum_{r=1}^{m}M^{-1}\Gamma\sigma_r\xi_{rk}/6, \quad k=0,\dots,N-1, \end{aligned} \tag{6.3}$$

where ξ_{rk}, η_{rk} are mutually independent random variables distributed by the laws (5.8).

The weak order of this method can be proved by standard arguments (Milstein, 1995) and its phase volume contractivity properties are proved by the same arguments as those before Theorem 2.3.

THEOREM 6.3 The method (6.2)–(6.3) for the system (2.1) has third weak order and satisfies the requirements RL1–RL2.

REMARK 6.2 The methods given in this section can be carried over to non-autonomous Langevin equations. It is also possible to apply the presented approach to Langevin equations with coloured noise using symplectic methods from Milstein & Tretyakov (2002).

6.2 *Langevin type equation: nonlinear damping and multiplicative noise*

In this section we propose weak methods for the Langevin type equation (3.1) which satisfy the requirements RLT1–RLT2 from Section 3. As for first-order methods, we have the following theorem.

THEOREM 6.4 Let $\bar{P}_{\rm I}$, $\bar{Q}_{\rm I}$ be a one-step approximation corresponding to a symplectic method of first weak order for the system (3.3), (3.2), and $\bar{P}_{\rm II}$ be a one-step approximation corresponding to a first-order deterministic method for the system (3.4). Then $\bar{P}$, $\bar{Q}$ defined in (3.5) or (3.7) is a one-step approximation of the method of first weak order for the system (3.1) which satisfies the requirements RLT1–RLT2.

A concrete method based on $\bar{P}$, $\bar{Q}$ from the above theorem can be written using the implicit symplectic method (4.5) or the explicit one (4.15)–(4.16) for $\bar{P}_{\rm I}$, $\bar{Q}_{\rm I}$. Further, as in the case of mean-square methods, the proposed approach can be generalized to a more general system of the form (3.8) (see the comment in the end of Section 3.1).

By the method of fractional steps (as in Sections 2.2 and 3.2) we construct the second-order weak method for (3.1) on the basis of the symplectic method (4.17). The method has

the form

$$\mathcal{P}_1 = \bar{P}_{\rm II}\left(t_k + \frac{h}{2}; t_k, P_k, Q_k\right),\ \mathcal{Q}_1 = Q_k + \frac{h}{2}g(\mathcal{P}_1),$$
$$\mathcal{P}_2 = \mathcal{P}_1 + hf\left(t_k + \frac{h}{2}, \mathcal{Q}_1\right) + h^{1/2}\sum_{r=1}^{m}\sigma_r\left(t_k + \frac{h}{2}, \mathcal{Q}_1\right)\xi_{rk},\ \mathcal{Q}_2 = \mathcal{Q}_1 + \frac{h}{2}g(\mathcal{P}_2), \quad (6.4)$$

$$P_{k+1} = \bar{P}_{\rm II}\left(t_k + \frac{h}{2}; t_k, \mathcal{P}_2, \mathcal{Q}_2\right) - \frac{h^2}{4}\nu\frac{\partial\tilde{f}}{\partial t}(t_k, P_k, Q_k),\quad Q_{k+1} = \mathcal{Q}_2,\ k = 0, \ldots, N-1,$$

where ξ_{rk} are i.i.d. random variables with the law (4.18) and $\bar{P}_{\rm II}$ is a one-step approximation of any second-order deterministic method for system (3·4).

Using a specific approximation instead of $\bar{P}_{\rm II}$, it is possible to modify the method (6.4) in such a way that it will become a derivative-free method (i.e. the correction with the derivative $\partial\tilde{f}/\partial t$ can be incorporated in $\bar{P}_{\rm II}$) but we do not consider this here.

The following theorem holds for the method (6.4).

THEOREM 6.5 The method (6.4) for the system (3.1) has the second weak order and satisfies the requirements RLT1–RLT2.

We note that for $\tilde{f}(t, p, q) = \Gamma(q)p$, $\Gamma - m \times m$ dimensional matrix, $P_{\rm II}(t)$ can be found explicitly. Consequently, we can put $P_{\rm II}$ instead of $\bar{P}_{\rm II}$ in (6.4) (see also the discussion after Remark 3.2).

7. Examples

The first example (Section 7.1) deals with testing weak symplectic methods by simulation of a model describing synchrotron oscillations of particles. In Section 7.2 we give a comparative analysis of Euler schemes and a quasi-symplectic method considering a stochastic linear oscillator with linear damping. Numerical tests of quasi-symplectic methods by simulating a stochastic oscillator with cubic restoring force are presented in Section 7.3.

7.1 *A model for synchrotron oscillations of particles in storage rings*

In Seeßelberg *et al.* (1994) a model describing synchrotron oscillations of particles in storage rings under the influence of external fluctuating electromagnetic fields was considered. This model can be written in the following form:

$$\begin{aligned} \mathrm{d}P &= -\omega^2\sin(Q)\,\mathrm{d}t - \sigma_1\cos(Q)\,\mathrm{d}w_1 - \sigma_2\sin(Q)\,\mathrm{d}w_2, \\ \mathrm{d}Q &= P\,\mathrm{d}t, \end{aligned} \quad (7.1)$$

where P and Q are scalars. The system (7.1) is of the form (4.13) and therefore its phase flow preserves symplectic structure.

Let us mention that a certain weak numerical method for the system (4.13) with $g(p) = M^{-1}p$ was proposed in Seeßelberg *et al.* (1994). In the absence of noise this method coincides with a deterministic symplectic method but in the stochastic case the method of Seeßelberg *et al.* (1994) is not symplectic (also see similar methods in Tretyakov & Tret'jakov, 1994). Here we demonstrate an efficiency of symplectic integrators proposed in the present paper in comparison with ordinary (nonsymplectic) methods for SDEs. We test four weak methods: two first-order methods (the Euler method, which is not symplectic, and the symplectic method (4.15)–(4.16)) and two second-order methods (a standard second-order weak method (Milstein, 1995; Kloeden & Platen, 1992) and the symplectic method (4.17)).

The weak Euler method for (7.1) takes the form

$$\begin{gathered} P_{k+1} = P_k - h\omega^2 \sin(Q_k) - h^{1/2}(\sigma_1 \cos(Q_k)\xi_{1k} + \sigma_2 \sin(Q_k)\xi_{2k}), \\ Q_{k+1} = Q_k + hP_k, \end{gathered} \tag{7.2}$$

where ξ_{1k}, ξ_{2k} are i.i.d random variables with the law (4.6).

In application to (7.1) the first-order symplectic method (4.15)–(4.16) with $\alpha = 1$ is written as

$$\begin{gathered} \mathcal{Q} = Q_k + hP_k, \\ P_{k+1} = P_k - h\omega^2 \sin(\mathcal{Q}) - h^{1/2}(\sigma_1 \cos(\mathcal{Q})\xi_{1k} + \sigma_2 \sin(\mathcal{Q})\xi_{2k}), \quad Q_{k+1} = \mathcal{Q}, \end{gathered} \tag{7.3}$$

where ξ_{1k}, ξ_{2k} are i.i.d random variables with the law (4.6).

The standard second-order method from Milstein (1995) and Kloeden & Platen (1992) applied to (7.1) has the form

$$\begin{aligned} P_{k+1} &= P_k - h^{1/2}(\sigma_1 \cos(Q_k)\xi_{1k} + \sigma_2 \sin(Q_k)\xi_{2k}) - h\omega^2 \sin(Q_k) \\ &\quad + \frac{h^{3/2}}{2}(\sigma_1 \sin(Q_k)\xi_{1k} - \sigma_2 \cos(Q_k)\xi_{2k})P_k - \frac{h^2}{2}\omega^2 \cos(Q_k)P_k, \\ Q_{k+1} &= Q_k + hP_k - \frac{h^{3/2}}{2}(\sigma_1 \cos(Q_k)\xi_{1k} + \sigma_2 \sin(Q_k)\xi_{2k}) - \frac{h^2}{2}\omega^2 \sin(Q_k), \end{aligned} \tag{7.4}$$

where ξ_{1k}, ξ_{2k} are i.i.d. random variables with the law (4.18).

The second-order symplectic method (4.17) is written for the system (7.1) as

$$\begin{gathered} \mathcal{Q}_1 = Q_k + \frac{h}{2}P_k, \quad \mathcal{P}_1 = P_k - h\omega^2 \sin(\mathcal{Q}_1) - h^{1/2}(\sigma_1 \cos(\mathcal{Q}_1)\xi_{1k} + \sigma_2 \sin(\mathcal{Q}_1)\xi_{2k}), \\ P_{k+1} = \mathcal{P}_1, \quad Q_{k+1} = \mathcal{Q}_1 + \frac{h}{2}\mathcal{P}_1, \end{gathered} \tag{7.5}$$

where ξ_{1k}, ξ_{2k} are i.i.d. random variables with the law (4.18).

Consider the quantity

$$\mathcal{E}(p, q) = \frac{p^2}{2} - \omega^2 \cos(q).$$

Its mean value $E\mathcal{E}(P(t), Q(t))$ is treated in physical literature (see e.g. Seeßelberg *et al.*, 1994 and references therein) as a mean energy of the system. Under the assumption $\sigma_1 =$

TABLE 1 *The model* (7.1)*. Simulation of* $E\mathcal{E}(P(t), Q(t))$ *with* $P(0) = 1$, $Q(0) = 0$, $\omega = 4$, $\sigma_1 = \sigma_2 = 0{\cdot}3$, $t = 200$ *for various time steps* h *by the Euler method* (7.2)*, the first-order symplectic method* (7.3)*, the standard second-order method* (7.4)*, and the second-order symplectic method* (7.5)*. The exact solution is* $-6{\cdot}5$*.* M *is a number of independent realizations in the Monte Carlo simulation. Note that the '*$\pm$*' reflects the Monte Carlo error only* (*cf.* (7.7))*, it does not reflect the error of a method*

h	M	(7.2)	(7.3)	(7.4)	(7.5)
0·1	10^5	$493{\cdot}3 \pm 0{\cdot}3$	$-6{\cdot}268 \pm 0{\cdot}059$	$462{\cdot}2 \pm 0{\cdot}6$	$-6{\cdot}316 \pm 0{\cdot}059$
0·05	10^5	$966{\cdot}1 \pm 0{\cdot}7$	$-6{\cdot}397 \pm 0{\cdot}059$	$0{\cdot}896 \pm 0{\cdot}094$	$-6{\cdot}421 \pm 0{\cdot}058$
0·01	$4 \cdot 10^6$	$234{\cdot}5 \pm 0{\cdot}06$	$-6{\cdot}503 \pm 0{\cdot}009$	$-6{\cdot}456 \pm 0{\cdot}009$	$-6{\cdot}502 \pm 0{\cdot}009$

$\sigma_2 = \sigma$ one can obtain that

$$E\mathcal{E}(P_{0,p,q}(t), Q_{0,p,q}(t)) = \mathcal{E}(p, q) + \frac{\sigma^2}{2}t. \tag{7.6}$$

In Table 1 we compare results produced by the four methods given above. We have two types of errors in numerical simulations here: error of a weak method used and a Monte Carlo error. The results in the table are approximations of $E\mathcal{E}(\bar{P}(t), \bar{Q}(t))$ calculated as

$$E\mathcal{E}(\bar{P}(t), \bar{Q}(t)) \doteq \frac{1}{M}\sum_{m=1}^{M} \mathcal{E}(\bar{P}^{(m)}(t), \bar{Q}^{(m)}(t)) \pm 2\sqrt{\frac{\bar{D}_M}{M}}, \tag{7.7}$$

where

$$\bar{D}_M = \frac{1}{M}\sum_{m=1}^{M}[\mathcal{E}(\bar{P}^{(m)}(t), \bar{Q}^{(m)}(t))]^2 - \left[\frac{1}{M}\sum_{m=1}^{M} \mathcal{E}(\bar{P}^{(m)}(t), \bar{Q}^{(m)}(t))\right]^2,$$

i.e. $E\mathcal{E}(\bar{P}(t), \bar{Q}(t))$ belongs to the interval defined in this formula with probability 0·95 (we recall that for sufficiently small h the sampling variance is sufficiently close to the variance of $\mathcal{E}(\bar{P}(t), \bar{Q}(t))$). Note that the '$\pm$' reflects the Monte Carlo error only, it does not reflect the error of a method.

The above experiments with the model (7.1) demonstrate superiority of symplectic methods in comparison with nonsymplectic ones. In Seeßelberg *et al.* (1994) the system (7.1) is also considered with coloured noise. In this case symplectic methods for Hamiltonian systems with coloured noise given in the preprint Milstein & Tretyakov (2002) can be exploited. We note that the authors of Seeßelberg *et al.* (1994) are interested in systems with small noise. Effective symplectic methods in the weak sense for Hamiltonian systems with small noise can be obtained using ideas from Milstein & Tretyakov (1997b) (see also Milstein *et al.*, 2002, 2003 where mean-square symplectic methods for Hamiltonian systems with small noise were obtained).

7.2 *Linear oscillator with linear damping under external random excitation*

Let us consider the linear oscillator with linear damping term and additive noise

$$\begin{aligned} \mathrm{d}X^1 &= \omega X^2\,\mathrm{d}t \\ \mathrm{d}X^2 &= (-\omega X^1 - \nu X^2)\,\mathrm{d}t + \frac{\sigma}{\omega}\,\mathrm{d}w(t), \end{aligned} \tag{7.8}$$

where $w(t)$ is a standard Wiener process, $\omega,\ \nu,\ \sigma$ are positive constants. The system (7.8) is dissipative, its invariant measure μ is Gaussian $\mathcal{N}(0, R)$ with the density

$$\rho(x) = (2\pi)^{-1}(\det R)^{-1/2}\exp\left\{-\frac{1}{2}(R^{-1}x, x)\right\}, \tag{7.9}$$

where $R = (\sigma^2/2\nu\omega^2)I$ is the covariance matrix for the two-dimensional process $X = (X^1, X^2)^\top$, I denotes the identity matrix.

The discrete system obtained by the explicit Euler scheme has the form

$$\begin{aligned} \bar{X}^1_{k+1} &= \bar{X}^1_k + \omega\bar{X}^2_k h \\ \bar{X}^2_{k+1} &= \bar{X}^2_k - (\omega\bar{X}^1_k + \nu\bar{X}^2_k)h + \frac{\sigma}{\omega}\Delta_k w. \end{aligned} \tag{7.10}$$

The eigenvalues of the homogeneous part of (7.10) are

$$\lambda_{1,2} = 1 - \frac{\nu h}{2} \pm h\sqrt{\frac{\nu^2}{4} - \omega^2}. \tag{7.11}$$

We consider the case when the damping term is small, and that is why we suppose that

$$\frac{\nu}{2} < \omega. \tag{7.12}$$

If (7.12) is fulfilled, then $|\lambda_{1,2}|^2 = 1 - \nu h + \omega^2 h^2$, and consequently (7.10) is asymptotically stable if and only if

$$h < \frac{\nu}{\omega^2}. \tag{7.13}$$

In this case, the system (7.10) possesses a unique invariant measure $\mu_h(x)$ with a Gaussian density $\rho_h(x)$ corresponding to the normal law $\mathcal{N}(0, R_h)$ with zero mean and the covariance matrix

$$R_h = \frac{\sigma^2}{\omega^2\varkappa}\begin{bmatrix} 1 - \nu h/2 + \omega^2 h^2/2 & -\omega h/2 \\ -\omega h/2 & 1 \end{bmatrix},$$

where

$$\varkappa := 2\nu - 2\omega^2 h - \nu^2 h + \frac{3\nu\omega^2 h^2}{2} - \frac{\omega^4 h^3}{2}.$$

Due to (7.12) and (7.13), it is possible to prove that $\varkappa > 0$. The elements of R_h can be represented as

$$R_h^{jj} = \frac{\sigma^2}{2\nu\omega^2}\left(1 + \frac{\omega^2 h}{\nu} + O(h\nu) + O\left(\frac{h^2}{\nu^2}\right)\right), \ j = 1, 2,$$

$$R_h^{ij} = \frac{\sigma^2}{2\nu\omega^2}\left(-\frac{\omega h}{2} - \frac{\omega^3 h^2}{2\nu} + O(h^2\nu) + O\left(\frac{h^3}{\nu^2}\right)\right), \ i \neq j,$$

where, for instance, $O\left(\frac{h^2}{\nu^2}\right)$ satisfies the inequality $\left|O\left(\frac{h^2}{\nu^2}\right)\right| \leqslant C\frac{h^2}{\nu^2}$ for all $\nu > 0$, $h > 0$ such that the ratio h/ν is sufficiently small, and C is a positive number.

Therefore, if one would like to approximate $\mu(x)$ by $\mu_h(x)$ quite accurately, then the step h must be essentially less than ν/ω^2, i.e. just the fulfillment of the stability condition (7.13) is not enough. Suppose that our aim is to evaluate

$$\int |x|^2 \, \mathrm{d}\mu(x) = \int |x|^2 \rho(x) \, \mathrm{d}x = \lim_{T\to\infty} E|X_x(T)|^2,$$

where $X_x(t)$ is the solution of (7.8) with $X_x(0) = x$.

We can approximate the limit by $E|X_x(T)|^2$ under a sufficiently large T. To evaluate $E|X_x(T)|^2$ by the explicit Euler method, we need to perform $N = T/h$ steps of (7.10). If the damping factor ν is small then the time T is rather large and the step h of the Euler method should be very small to satisfy the above condition $h \ll \nu/\omega^2$. Consequently, the number N is huge, and the Euler method is not appropriate for numerical solution of this problem under small ν.

Let us apply the implicit Euler method to system (7.8):

$$\begin{aligned} \bar{X}_{k+1}^1 &= \bar{X}_k^1 + \omega\bar{X}_{k+1}^2 h \\ \bar{X}_{k+1}^2 &= \bar{X}_k^2 - (\omega\bar{X}_{k+1}^1 + \nu\bar{X}_{k+1}^2)h + \frac{\sigma}{\omega}\Delta_k w. \end{aligned} \tag{7.14}$$

The eigenvalues of the homogeneous part of (7.14) are

$$\lambda_{1,2} = 1 - \frac{\nu h + 2\omega^2 h^2}{2(1 + \nu h + \omega^2 h^2)} \pm \frac{\sqrt{\nu^2 h^2 - 4\omega^2 h^2}}{2(1 + \nu h + \omega^2 h^2)}.$$

Under (7.12), the eigenvalues are again complex numbers and

$$|\lambda_{1,2}|^2 = 1 - \frac{\nu h + \omega^2 h^2}{1 + \nu h + \omega^2 h^2}.$$

Therefore, in contrast to the explicit Euler method, we do not need any restriction on h for asymptotic stability. This can give rise to the illusion about a possibility to choose a comparatively big step h in the implicit Euler scheme. However, the coming evaluations show that such an illusion is very dangerous. Indeed, the system (7.14) possesses a unique

invariant measure $\mu_h(x)$ corresponding to the normal law $\mathcal{N}(0, R_h)$ with zero mean and the covariance matrix R_h with the elements

$$R_h^{jj} = \frac{\sigma^2}{2\nu\omega^2}\left(1 - \frac{\omega^2 h}{\nu} + O(h\nu) + O\left(\frac{h^2}{\nu^2}\right)\right), \quad j = 1, 2,$$

$$R_h^{ij} = \frac{\sigma^2}{2\nu\omega^2}\left(\frac{\omega h}{2} - \frac{\omega^3 h^2}{2\nu} + O(h^2) + O\left(\frac{h^3}{\nu^2}\right)\right), \quad i \neq j,$$

and we are again forced to take a very small h to reach a satisfactory accuracy.

Now let us use the quasi-symplectic method based on the one-step approximation (2.7) with $\bar{P}_{\mathrm{I}}$, $\bar{Q}_{\mathrm{I}}$ from (2.12) with $\alpha = 0$. For simplicity we take $\bar{P}_{\mathrm{II}} = p - h\nu p$ instead of the exact P_{II}. As a result, we get

$$\begin{aligned} \bar{X}_{k+1}^1 &= \bar{X}_k^1 + \omega h(\bar{X}_k^2 - \omega h \bar{X}_k^1) \\ \bar{X}_{k+1}^2 &= \left(\bar{X}_k^2 - \omega h \bar{X}_k^1 + \frac{\sigma}{\omega}\Delta_k w\right)(1 - \nu h). \end{aligned} \tag{7.15}$$

In this case, if

$$\frac{\nu}{2} < \omega - \frac{\omega^2 h}{2},$$

the eigenvalues $\lambda_{1,2}$ are complex and

$$|\lambda_{1,2}|^2 = 1 - \nu h.$$

For all not too large h the system (7.15) is asymptotically stable and possesses a unique invariant measure with a Gaussian density. The corresponding normal law has zero mean and the covariance matrix with the elements

$$R_h^{11} = \frac{\sigma^2}{2\nu\omega^2}(1 - 2\nu h + O(h^2)), \quad R_h^{22} = \frac{\sigma^2}{2\nu\omega^2}\left(1 - \frac{3}{2}\nu h + O(h^2)\right),$$

$$R_h^{ij} = \frac{\sigma^2}{2\nu\omega^2}\left(\frac{\omega h}{2} - \frac{5}{4}\omega\nu h^2 + O(h^3)\right), \quad i \neq j.$$

We see that the implicit Euler method has advantages in comparison with the explicit Euler method due to its better stability properties. But both of them require too small a step to reach a sufficient accuracy, in particular if ν is small. At the same time, the quasi-symplectic method (7.15) gives very good results for very big steps. This is important, for instance, for the problem of computing a mean due to an invariant law which needs numerical integration on very long time intervals.

7.3 *An oscillator with cubic restoring force under external random excitation*

Consider the oscillator with cubic restoring force and additive noise (cf. (2.1) with $U_0(q) = \frac{1}{4}q^4 - \frac{1}{2}q^2$):

$$\ddot{Q} = Q - Q^3 - \nu\dot{Q} + \sigma\dot{w}. \tag{7.16}$$

The dynamical system (7.16) is ergodic (see e.g. Mattingly *et al.*, 2002) and its invariant measure has the density

$$\rho(p, q) = C \exp\left(-\frac{\nu}{\sigma^2}\left(p^2 + \frac{1}{2}q^4 - q^2\right)\right), \tag{7.17}$$

where C is defined by the normalization condition.

Here we compare an implicit quasi-symplectic method and the implicit Euler scheme. We use the implicit quasi-symplectic method based on the one-step approximation (2.7) and on the weak implicit symplectic method (4.5) with $\alpha = 1/2$. For simplicity we take $\bar{P}_{\rm II} = p - h\nu p$ instead of the exact $P_{\rm II}$. As a result, we get for (7.16):

$$\begin{gathered}\bar{P}_{\rm I} = P_k + h\left(\frac{\bar{Q}_{\rm I} + Q_k}{2} - \frac{\left(\bar{Q}_{\rm I} + Q_k\right)^3}{8}\right) + h^{1/2}\sigma\xi_k,\\ \bar{Q}_{\rm I} = Q_k + h(\bar{P}_{\rm I} + P_k)/2,\\ P_{k+1} = (1 - \nu h)\bar{P}_{\rm I}, \quad Q_{k+1} = \bar{Q}_{\rm I},\end{gathered} \tag{7.18}$$

where ξ_k are i.i.d. random variables with the law (4.6).

In application to (7.16) the weak implicit Euler scheme has the form

$$\begin{gathered}P_{k+1} = P_k + h\left(Q_{k+1} - Q_{k+1}^3 - \nu P_{k+1}\right) + h^{1/2}\sigma\xi_k\\ Q_{k+1} = Q_k + hP_{k+1},\end{gathered} \tag{7.19}$$

where ξ_k are i.i.d. random variables with the law (4.6).

Figure 1 gives results of evaluation of $E\,(Q(T))^2$ for a large T by these two methods. We see that even for such a small step as $h = 0{\cdot}01$ the implicit Euler method tends to a wrong limit with increasing T, while the quasi-symplectic method gives quite accurate results, e.g. for $h = 0{\cdot}25$.

Now consider the *explicit* quasi-symplectic method based on the one-step approximation (2.7) and on the weak explicit symplectic method (4.15)–(4.16) with $\alpha = 0$. We take $\bar{P}_{\rm II} = p - h\nu p$ instead of the exact $P_{\rm II}$ again. This method for (7.16) is written as

$$\begin{gathered}P_{k+1} = (1 - \nu h)\left(P_k + h\left(Q_k - Q_k^3\right) + h^{1/2}\sigma\xi_k\right)\\ Q_{k+1} = Q_k + h\left(P_k + h\left(Q_k - Q_k^3\right)\right).\end{gathered} \tag{7.20}$$

Since this quasi-symplectic method is explicit, it is much simpler than (7.18). However, for comparatively large h the difference system (7.20) has unstable behaviour (e.g. for ν, σ as in Fig. 1 and $h = 0{\cdot}2$). Most likely, for all sufficiently small h the system (7.20) acquires

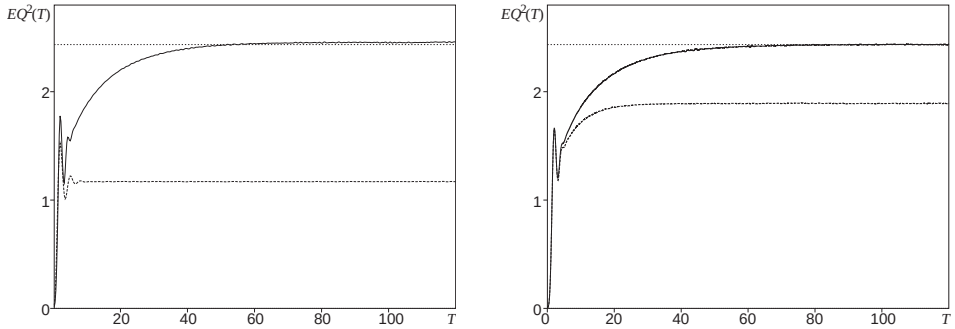

FIG. 1. The oscillator with cubic restoring force (7.16). Behaviour of $E(Q(T))^2$ with $P(0) = 0$, $Q(0) = 0$, $\nu = 0{\cdot}05$, $\sigma = 1$, $h = 0{\cdot}25$ (left) and $h = 0{\cdot}01$ (right) on the time interval $t \leqslant 120$ in the case of the weak implicit Euler method (7.19) (dashed line) and the weak quasi-symplectic method (7.18) (solid line). The Monte Carlo error is not greater than 0·005 with probability 0·95. The dotted line presents the limit value of $E(Q(T))^2$ as $T \to \infty$ evaluated due to $\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} q^2\rho(p,q)\,\mathrm{d}p\,\mathrm{d}q$ with the invariant measure $\rho(p,q)$ from (7.17). This value is equal to 2·435.

stable behaviour (of course, this assertion requires further investigation). For instance, $E\bar{Q}^2(T)$ obtained by (7.20) for ν, σ as in Fig. 1 and $h = 0{\cdot}1$ visually coincides with the results obtained by the implicit quasi-symplectic method (7.18). Thus, even an explicit quasi-symplectic method can effectively be used for solution of Langevin equations on long time intervals, in contrast to the implicit Euler method which is more complicated than (7.20).

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