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Numerical methods for Langevin type equations based on symplectic integrators

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ABSTRACT. 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 [17, 18] while symplectic methods in the weak sense are constructed in this paper. Special attention is paid to Hamiltonian systems with separable Hamiltonians, with additive noise, and with colored 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.

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. [21, 4] 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 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) [2] (see also [17]). For instance, systems of this type describe synchrotron oscillations of particles in storage rings under the influence of external fluctuating electromagnetic fields [23]. Another popular model from this class is the Kubo oscillator [8] which is used in the theory of magnetic resonance and laser physics. In [17, 18] mean-square symplectic methods for stochastic Hamiltonian systems were proposed. These methods have significant advantages over standard schemes for stochastic differential equations (SDEs) [12, 7].

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

(1.1)
$$dP = f(t,Q)dt - \nu f_{\nu}(t,P,Q)dt + \sum_{r=1}^{m} \sigma_{r}(t,Q)dw_{r}(t), \ P(t_{0}) = p,$$
$$dQ = g(P)dt, \ Q(t_{0}) = q,$$

where $P, Q, f, f_{\nu}, g, \sigma_r$ 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., [20] and references therein), for studying lattice dynamics in strongly anharmonic crystals [3], descriptions of noise-induced transport in stochastic ratchets [10], investigations of the dispersion of passive tracers in turbulent flows (see [31, 22] and references therein), etc.

In the present paper we construct special numerical methods (we call them as quasisymplectic) which preserve some specific properties of the Langevin type equations.

In Section 2, an auxiliary knowledge on numerical methods for SDEs is given to make the whole exposition self-contained.

In Section 3, 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), $f_{\nu}(t,p,q) = \Gamma p$, 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. [21, 25, 34]) and some ideas of [28], where methods for deterministic second-order differential equations with similar properties were obtained. In Section 4, we generalize mean-square methods of Section 3 to the Langevin type equations (1.1) and also to more general systems.

Mean-square methods are necessary for direct simulation of stochastic trajectories which, for instance, can be useful in studying qualitative behavior of stochastic models. Besides, they are the basis for construction of weak methods which are important for many practical applications. As is known (see, e.g. [12, 7, 19]), weak methods are relevant to calculate expectations of functionals of a solution to SDEs by 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

(1.2)
$$dP = f(t, P, Q)dt + \sum_{r=1}^{m} \sigma_r(t, P, Q) \circ dw_r(t), \ P(t_0) = p,$$
$$dQ = g(t, P, Q)dt + \sum_{r=1}^{m} \gamma_r(t, P, Q) \circ dw_r(t), \ Q(t_0) = q,$$

where $P, Q, f, g, \sigma_r, \gamma_r$ are *n*-dimensional column-vectors with the components $P^i, Q^i, f^i, g^i, \sigma^i_r, \gamma^i_r, i = 1, ..., n$, and $w_r(t), r = 1, ..., m$, are independent standard Wiener processes.

We denote by $X(t; t_0, x) = (P^{\mathsf{T}}(t; t_0, p, q), Q^{\mathsf{T}}(t; t_0, p, q))^{\mathsf{T}}, t_0 \leq t \leq t_0 + T$, 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, e.g. [2, 6]. If there are functions $H_r(t, p, q), r = 0, \ldots, m$, such that (see [2] and [17])

(1.3)
$$f^{i} = -\partial H_{0}/\partial q^{i}, \quad g^{i} = \partial H_{0}/\partial p^{i},$$
$$\sigma_{r}^{i} = -\partial H_{r}/\partial q^{i}, \quad \gamma_{r}^{i} = \partial H_{r}/\partial p^{i}, \quad i = 1, \dots, n, \quad r = 1, \dots, m,$$

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

$$(1.4) dP \wedge dQ = dp \wedge dq,$$

i.e., the sum of the oriented areas of projections onto the coordinate planes $(p^1, q^1), \ldots, (p^n, q^n)$ is an integral invariant [1]. 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, ..., 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

$$(1.5) dP \wedge dQ = dp \wedge dq \,.$$

In Section 5, weak symplectic methods for stochastic Hamiltonian systems with multiplicative noise are constructed. Section 6 and 7 are devoted to symplectic integrators for Hamiltonian systems with additive and colored noise respectively. 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 8, we derive quasi-symplectic methods in the weak sense for Langevin type equations using weak methods from Sections 5-7 together with the ideas of Sections 3-4. It is known [33, 24, 11] 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 is investigated first in [29] in the case of nondegenerate noise and globally Lipschitz coefficients. For Langevin equations, noise is degenerate and the coefficients may not be globally Lipschitz. In this case ergodicity of numerical schemes is considered in [11, 30]. 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 the present paper is proved under traditional conditions on the drift and diffusion coefficients which consist in 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 convergence of numerical methods for equations with locally Lipschitz coefficients are obtained in [5, 11].

An important instance of a stochastic system is given by a SDE with small noise, since often fluctuations, which affect a dynamical system are sufficiently small. It was shown in [15, 16] that numerical methods adapted to systems with small noise can be more efficient than general methods. The errors of these methods are estimated in terms of products $h^i \varepsilon^j$, where h is the step-size of discretization and ε is a small parameter at noise. Usually, their global errors have the form $O(h^j + \varepsilon^k h^l)$, where j > l, k > 0. Thanks to the fact that the accuracy order of such methods is equal to a comparatively small l, they are not too complicated, while due to the large j and the small factor ε^k at h^l , their errors are fairly low. This allows us to construct effective (high-exactness) methods with low time-step order but which nevertheless have small errors. Using these ideas, it is possible to construct special symplectic methods in the weak sense for Hamiltonian systems with small noise (see also [17, 18]) and special quasi-symplectic methods for Langevin equations with small noise. However, we do not consider this issue here.

In Section 9, we present numerical tests of both symplectic and quasi-symplectic methods. They clearly demonstrate superiority of the proposed methods over very long time intervals in comparison with standard methods.

2. AUXILIARY KNOWLEDGE ON NUMERICAL METHODS FOR SDES

In this section, we recall the main facts from the theory of numerical integration of SDEs both in the mean-square and weak sense. Further details are available in [12, 7]. Consider the system of SDEs in the Ito sense

(2.1)
$$dX = a(t, X)dt + \sum_{r=1}^{m} b_r(t, X)dw_r(t), \ X(t_0) = X_0$$

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. Note that X_0 may be a random variable which does not depend on the Wiener processes $w_r(t)$, $t \in [t_0, t_0 + T]$.

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

(2.2)
$$|a(t,x) - a(t,y)| + \sum_{r=1}^{m} |b_r(t,x) - b_r(t,y)| \le L |x-y|$$

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

$$t_{i+1} = t_i + h, \ i = 0, \dots, N-1, \ h = \frac{T-t_0}{N}$$

2.1. Mean-square methods for SDEs. A one-step mean-square approximation $\bar{X}(t + h; t, x)$, $t_0 \leq t < t + h \leq t_0 + T$, for (2.1) is constructed depending on t, x, h, and $\{w_1(\vartheta) - w_1(t), \ldots, w_m(\vartheta) - w_m(t); t \leq \vartheta \leq t + h\}$. We pay attention that the dependence on the Wiener processes is not reflected in the notation $\bar{X}(t + h; t, x)$. We note also that this notation is the same for both explicit and implicit approximations.

Using the one-step approximation, we recurrently obtain the approximation X_k , $k = 0, \ldots, N : X_0 = X(t_0), X_{k+1} = \overline{X}(t_{k+1}; t_k, X_k)$. Definition 1. If for some method

$$\left[E\left(X(t_k) - X_k\right)^2\right]^{1/2} \le Kh^l,$$

where l > 0 and K does not depend on k and h, then we say that the mean-square order of accuracy of the method is l.

The following general convergence theorem holds [12].

Theorem 2.1. Suppose the one-step approximation $\bar{X}(t+h;t,x)$ has order of accuracy l_1 for the expectation of the deviation and order of accuracy l_2 for the mean-square deviation; more precisely, for arbitrary $t_0 \leq t \leq t_0 + T - h$, $x \in \mathbb{R}^d$ the following inequalities hold:

(2.3)
$$\left| E\left(X(t+h;t,x) - \bar{X}(t+h;t,x)\right) \right| \leq K \cdot (1+|x|^2)^{1/2} h^{l_1},$$

(2.4)
$$\left[E\left|X(t+h;t,x)-\bar{X}(t+h;t,x)\right|^{2}\right]^{1/2} \leq K \cdot (1+|x|^{2})^{1/2} h^{l_{2}}.$$

Also, let

(2.5)
$$l_2 \ge \frac{1}{2}, \ l_1 \ge l_2 + \frac{1}{2}.$$

Then for any N and k = 0, ..., N the following inequality holds:

(2.6)
$$\left[E\left|X(t_k;t_0,X_0)-\bar{X}(t_k;t_0,X_0)\right|^2\right]^{1/2} \le K \cdot (1+E|X_0|^2)^{1/2} h^{l_2-1/2}$$

i.e., the mean-square order of accuracy of the method based on the one-step approximation $\overline{X}(t+h;t,x)$ is $l = l_2 - 1/2$.

2.2. Weak methods for SDEs.

Definition 2. If for some method we have

$$|EF(\bar{X}_k) - EF(X(t_k))| \le Kh^l$$

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 (2.1) in the weak sense with (weak) order of accuracy l (or $O(h^l)$).

Definition 3. A function F(x), $x \in \mathbb{R}^d$, is said to belong to the class \mathbf{F} , $F \in \mathbf{F}$, if there are constants K > 0 and $\varkappa \geq 0$ such that the inequality

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

holds for any $x \in \mathbb{R}^d$.

The following general convergence theorem is proved in [12] (see also [7]).

Theorem 2.2. Suppose that

(1) the coefficients of (2.1) are continuous, satisfy a Lipschitz condition (2.2) and together with their partial derivatives of order up to 2l + 2 belong to the class \mathbf{F} ;

(2) the following inequalities hold:

(2.7)
$$|E(\prod_{j=1}^{s} \Delta^{i_j} - \prod_{j=1}^{s} \bar{\Delta}^{i_j})| \le K(x)h^{l+1}, \ s = 1, \dots, 2l+1,$$

(2.8)
$$E \prod_{j=1}^{2l+2} |\bar{\Delta}^{i_j}| \le K(x)h^{l+1}, \ l > 0, \ K(x) \in \mathbf{F},$$

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 **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, ..., N.

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

In all the convergence theorems throughout the paper we suppose 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.

3. QUASI-SYMPLECTIC MEAN-SQUARE METHODS FOR LANGEVIN EQUATIONS

Consider the Langevin equation

(3.1)
$$dP = f(Q)dt - \nu \Gamma P dt + \sum_{r=1}^{m} \sigma_r dw_r(t), \quad P(t_0) = p,$$
$$dQ = M^{-1} P dt, \quad Q(t_0) = q,$$

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

(3.2)
$$f^i(q) = -\frac{\partial U_0}{\partial q^i}, \quad i = 1, \dots, n,$$

and if $\nu = 0$, then the system (3.1) is a Hamiltonian system with additive noise, i.e., its phase flow preserves symplectic structure (see [2, 17]).

The system (3.1) 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 $D_0 \in \mathbb{R}^d$, 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 (3.3)

$$V_t = \int_{D_t} dP^1 \dots dP^n dQ^1 \dots dQ^n = \int_{D_0} \left| \frac{D(P^1, \dots, P^n, Q^1, \dots, Q^n)}{D(p^1, \dots, p^n, q^1, \dots, q^n)} \right| dp^1 \dots dp^n dq^1 \dots dq^n.$$

In the case of the system (3.1) the Jacobian J is equal to [2, 9, 17]:

(3.4)
$$J = \frac{D(P^1, \dots, P^n, Q^1, \dots, Q^n)}{D(p^1, \dots, p^n, q^1, \dots, q^n)} = \exp\left(-\nu \, tr\Gamma \, \cdot (t - t_0)\right).$$

That is, the system (3.1) preserves phase volume for $\nu = 0$. If $\nu > 0$ and $tr\Gamma > 0$ 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 (3.1)-(3.2) degenerates to a symplectic method when $\nu = 0$, *i.e.*, for $\nu = 0$ and f from (3.2) $d\bar{P} \wedge d\bar{Q} = dp \wedge dq$;
- RL2. The Jacobian

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

does not depend on p, q.

As it is understood, a method is convergent and, consequently, \overline{J} is close to J at any rate. The requirement RL2 is natural since the Jacobian J of the original system (3.1) 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 more strong property consisting in the equality $\overline{J} = J$. However, such an requirement is too restrictive in general. In the context of deterministic equations the requirement RL2 was introduced in [28].

To construct methods satisfying RL1-RL2, we use ideas of splitting technique (see, e.g. [21, 25]). In connection with (3.1), introduce the systems

(3.5)
$$dP_{I} = f(Q_{I})dt + \sum_{r=1}^{m} \sigma_{r}dw_{r}(t), \quad P_{I}(t_{0}) = p$$
$$dQ_{I} = M^{-1}P_{I}dt, \quad Q_{I}(t_{0}) = q,$$

(3.6)
$$\frac{dP_{II}}{dt} = -\nu\Gamma P_{II}, \quad P_{II}(0) = p,$$

and denote their solutions as $P_I(t; t_0, p, q)$, $Q_I(t; t_0, p, q)$ and $P_{II}(t; p)$, respectively. The system (3.5) with f(q) from (3.2) is a Hamiltonian system with additive noise. The system (3.6) is a deterministic linear system with constant coefficients, and its solution $P_{II}(t; p)$ can be found explicitly.

3.1. First-order methods. Let $\bar{P}_I = \bar{P}_I(t_0 + h; t_0, p, q), \ \bar{Q}_I = \bar{Q}_I(t_0 + h; t_0, p, q)$ be a one-step approximation of a symplectic first-order mean-square method for (3.5), (3.2) (any explicit or implicit method from [17] can be used). Its Jacobian is equal to one, i.e.,

$$rac{D(P_I(t_0+h;t_0,p,q),Q_I(t_0+h;t_0,p,q))}{D(p,q)}=1.$$

We construct the one-step approximation \bar{P} , \bar{Q} for the solution of (3.1)-(3.2) as follows

$$(3.7) \qquad \qquad \bar{P} = \bar{P}(t_0 + h; t_0, p, q) := P_{II}(h; \bar{P}_I(t_0 + h; t_0, p, q)), \\ \bar{Q} = \bar{Q}(t_0 + h; t_0, p, q) := \bar{Q}_I(t_0 + h; t_0, p, q).$$

We have

(3.8)
$$\bar{J} = \frac{D(P,Q)}{D(p,q)} = \frac{D(P_{II},Q_I)}{D(\bar{P}_I,\bar{Q}_I)} \frac{D(P_I,Q_I)}{D(p,q)} = J.$$

Further, if $\nu = 0$, then $\bar{P} = \bar{P}_I$, $\bar{Q} = \bar{Q}_I$, i.e., the approximation (3.7) degenerates to the symplectic method for (3.1)-(3.2) with $\nu = 0$. Thus, the approximation \bar{P} , \bar{Q} satisfies both requirements RL1 and RL2.

Lemma 3.1. Let \bar{P}_I , \bar{Q}_I be a one-step approximation corresponding to any first-order mean-square method for the system (3.5). Then \bar{P} , \bar{Q} defined in (3.7) is a one-step approximation of the first-order mean-square method for the system (3.1).

Proof. Due to the assumption, we can write

(3.9)
$$\bar{P}_{I} = p + \sum_{r=1}^{m} \sigma_{r} \Delta w_{r} + hf(q) + r_{1},$$
$$\bar{Q}_{I} = q + hM^{-1}p + r_{2},$$

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

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

We have

(3.10)
$$P_{II}(h;p) = p - h\nu\Gamma p + \rho, \ \rho = O(h^2).$$

Using (3.9), (3.10), and (3.7), we get

(3.11)
$$\bar{P} = p + \sum_{r=1}^{m} \sigma_r \Delta w_r + h \left(f(q) - \nu \Gamma p \right) + R,$$

where

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

It is not difficult to see that

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

Denote by \tilde{P} , \tilde{Q} the Euler one-step approximation applied to (3.1). It follows from (3.9) and (3.11) that

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

Then, recalling that the Euler method has the first mean-square order of accuracy for systems with additive noise and using Theorem 2.1, we get the result. \Box

Thus, due to (3.8), we obtain the following convergence theorem.

Theorem 3.1. Let \bar{P}_I , \bar{Q}_I be a one-step approximation corresponding to a symplectic first-order mean-square method for the system (3.5), (3.2). Then \bar{P} , \bar{Q} defined in (3.7) 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 $\nu = 0$, (ii) its phase volume changes according to the same law as the phase volume of (3.1) 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}_I , \bar{Q}_I from [17]. The first one is explicit :

(3.12)
$$\mathcal{Q} = q + \alpha h M^{-1} p, \quad \mathcal{P} = p + h f(\mathcal{Q}),$$

 $\bar{Q}_I = \mathcal{Q} + (1 - \alpha) h M^{-1} \mathcal{P}, \quad \bar{P}_I = \mathcal{P} + \sum_{r=1}^m \sigma_r \Delta w_r,$

where α is a parameter. The second method:

(3.13)
$$\bar{P}_{I} = p + hf((1-\alpha)\bar{Q}_{I} + \alpha q) + \sum_{r=1}^{m} \sigma_{r}\Delta w_{r},$$
$$\bar{Q}_{I} = q + hM^{-1}(\alpha\bar{P}_{I} + (1-\alpha)p).$$

It is implicit for $0 < \alpha < 1$. Substitution of \bar{P}_I , \bar{Q}_I from (3.12) or (3.13) in (3.7) gives us the concrete one-step approximations for (3.1).

To use the method (3.13), (3.7), we need solvability of (3.13) with respect to \bar{P}_I , \bar{Q}_I . If f is globally Lipschitz, solvability is proved in [17]. But it can be proved in many other cases as well. As an illustration, consider the following example of system (3.1) with locally Lipschitz coefficients and n = 1:

(3.14)
$$dP = (Q - Q^3)dt - \nu Pdt + \sigma dw(t)$$
$$dQ = Pdt.$$

In the case of (3.14), substituting \bar{P}_I in the right-hand side of the second equation of (3.13), we obtain

(3.15)
$$\bar{Q}_I - q - hp - \alpha h^2 (\varphi(\bar{Q}_I) - \varphi^3(\bar{Q}_I)) - \alpha \sigma h \Delta w = 0,$$

where

$$\varphi(\bar{Q}_I) = (1 - \alpha)\bar{Q}_I + \alpha q.$$

We see that if

$$h < \frac{1}{\sqrt{\alpha(1-\alpha)}},$$

then the left-hand side of (3.15) is a strictly increasing cubic parabola in \bar{Q}_I and therefore there exists the only root of (3.15).

Of course, the convergence in locally Lipschitz cases has to be justified additionally. We recall that in all the proofs throughout this paper we assume existence and boundedness of certain derivatives of the coefficients, i.e., in particular, we assume the globally Lipschitz conditions to be fulfilled. Some results on convergence in cases of one-sided Lipschitz conditions are obtained in [5, 11]. One can be sure that the methods proposed are solvable (if implicit) and convergent in a broad fashion.

Remark 3.1. Theorem 3.1 also holds for the method based on the following one-step approximation:

Remark 3.2. In practice, it can be more convenient to use an approximation \bar{P}_{II} of the solution to (3.6) instead of the exact solution P_{II} in (3.7) (or (3.16)). Since (3.6) is a deterministic equation, we can exploit a high-order deterministic scheme in order to obtain \bar{P}_{II} . In this case the Jacobian \bar{J} approximates the original Jacobian J with the accuracy of the deterministic scheme. Due to the linearity of (3.6), this \bar{J} does not depend on the initial data p, q (it depends on $\nu\Gamma$ and h only).

There is another possibility to propose methods for (3.1) satisfying RL1-RL2. It consists in direct application of symplectic methods. For instance, the parametric first-order family of implicit methods from [17] in application to (3.1) takes the form

(3.17)
$$\bar{P} = p + hf((1-\alpha)\bar{Q} + \alpha q) - h\nu\Gamma \cdot (\alpha\bar{P} + (1-\alpha)p) + \sum_{r=1}^{m} \sigma_r \Delta w_r,$$
$$\bar{Q} = q + hM^{-1}(\alpha\bar{P} + (1-\alpha)p).$$

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 (3.12)) can be directly applied to the Langevin equation (3.1) itself. Thus, on the way of the direct application of symplectic methods to (3.1) we have rather restrictive opportunities. Nevertheless, we can obtain on this way some new methods.

3.2. Second-order methods. In order to construct second-order methods for the Langevin equation (3.1) with the properties RL1 and RL2, we use ideas of the method of fractional steps [34, 21, 25]. In the deterministic case (i.e., when $\sigma_r = 0, r = 1, ..., m$) a second-order method satisfying RL1 and RL2 can be based on the following one-step approximation

(3.18)
$$\bar{P} = \bar{P}(t_0 + h; t_0, p, q) := P_{II}(\frac{h}{2}; \bar{P}_I(t_0 + h; t_0, P_{II}(\frac{h}{2}; p), q)),$$
$$\bar{Q} = \bar{Q}(t_0 + h; t_0, p, q) := \bar{Q}_I(t_0 + h; t_0, P_{II}(\frac{h}{2}; p), q),$$

where \bar{P}_I , \bar{Q}_I corresponds to a one-step approximation of a symplectic method for (3.5), (3.2) with $\sigma_r = 0$.

In the stochastic case the interconnection between terms in (3.1) is more complicated and a correction to (3.18) is needed. Consider the following approximation for solution of (3.1):

$$ar{P} = ar{P}(t_0 + h; t_0, p, q) := P_{II}(rac{h}{2}; ar{P}_I(t_0 + h; t_0, P_{II}(rac{h}{2}; p), q)) -
u \sum_{r=1}^m \Gamma \sigma_r(I_{r0} - rac{h}{2}\Delta w_r), \ ar{Q} = ar{Q}(t_0 + h; t_0, p, q) := ar{Q}_I(t_0 + h; t_0, P_{II}(rac{h}{2}; p), q),$$

where \bar{P}_I , \bar{Q}_I is a one-step approximation corresponding to a symplectic (explicit or implicit) second-order mean-square method for (3.5), (3.2) (such methods are available in [17]),

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

Lemma 3.2. Let \bar{P}_I , \bar{Q}_I be a one-step approximation corresponding to any second-order mean-square method for the system (3.5). Then \bar{P} , \bar{Q} defined in (3.19) is a one-step approximation of the second-order mean-square method for the system (3.1).

Proof. Due to the assumption, we can write

$$(3.20) \quad \bar{P}_{I}(t_{0}+h;t_{0},p,q) = p + \sum_{r=1}^{m} \sigma_{r} \Delta w_{r} + hf(q) + \frac{h^{2}}{2} \sum_{i=1}^{n} \left(M^{-1}p\right)^{i} \frac{\partial f}{\partial q^{i}} + r_{1},$$

$$\bar{Q}_{I}(t_{0}+h;t_{0},p,q) = q + hM^{-1}p + \sum_{r=1}^{m} M^{-1}\sigma_{r}I_{r0} + \frac{h^{2}}{2}M^{-1}f(q) + r_{2},$$

where the remainders r_1 and r_2 are such that

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

We also have

(3.21)
$$P_{II}(h;p) = p - h\nu\Gamma p + \frac{h^2}{2}\nu^2\Gamma^2 p + \rho, \ \rho = O(h^3).$$

We obtain from (3.19)-(3.21) that

(3.22)
$$\bar{P} = p + \sum_{r=1}^{m} \sigma_r \Delta w_r + h \left(f(q) - \nu \Gamma p \right) - \nu \sum_{r=1}^{m} \Gamma \sigma_r I_{r0} + \frac{h^2}{2} \left[\sum_{i=1}^{n} \left(M^{-1} p \right)^i \frac{\partial f}{\partial q^i} + \nu^2 \Gamma^2 p - \nu \Gamma f(q) \right] + R_1,$$
$$\bar{Q} = q + h M^{-1} p + \sum_{r=1}^{m} M^{-1} \sigma_r I_{r0} + \frac{h^2}{2} M^{-1} \left[f(q) - \nu \Gamma p \right] + R_2,$$

where R_1 and R_2 are such that

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

It is not difficult to show that the standard Taylor-type mean-square method of order 3/2 for systems with additive noise [12, p. 37] has the second order of accuracy when it is

applied to (3.1). Comparing the one-step approximation of this standard method with (3.22), we obtain that the method based on (3.19) is of mean-square order 2. \Box

One can easily check that the approximation (3.19) satisfies our requirements RL1 and RL2. The following theorem summarizes the result.

Theorem 3.2. Let P_I , Q_I be a one-step approximation corresponding to a symplectic second-order mean-square method for the system (3.5), (3.2). Then \overline{P} , \overline{Q} defined in (3.7) is a one-step approximation of the second-order mean-square method for the system (3.1)-(3.2) such that (i) it is symplectic when applied to (3.1)-(3.2) with $\nu = 0$, (ii) its phase volume changes according to the same law as the phase volume of (3.1)-(3.2) does.

Let us give a concrete example of a method based on (3.19) (to this end, we use one of explicit symplectic second-order partitioned Runge-Kutta (PRK) methods from [17]):

(3.23)
$$\mathcal{P}_1 = P_{II}(\frac{h}{2}; P_k), \quad \mathcal{Q}_1 = Q_k + \frac{h}{2}M^{-1}\mathcal{P}_1,$$

$$\mathcal{P}_{2} = \mathcal{P}_{1} + \sum_{r=1}^{m} \sigma_{r} \Delta_{k} w_{r} + hf(\mathcal{Q}_{1}), \quad \mathcal{Q}_{2} = \mathcal{Q}_{1} + \sum_{r=1}^{m} M^{-1} \sigma_{r} (I_{r0})_{k} + \frac{h^{2}}{2} M^{-1} f(\mathcal{Q}_{1}),$$
$$P_{k+1} = P_{II} (\frac{h}{2}; \mathcal{P}_{2}) - \nu \sum_{r=1}^{m} \Gamma \sigma_{r} (I_{r0} - \frac{h}{2} \Delta w_{r}), \quad Q_{k+1} = \mathcal{Q}_{2}, \quad k = 0, \dots, N-1.$$

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 N(0, 1)-distributed random variables ξ_{rk} and η_{rk} , $r = 0, \ldots, m$:

(3.24)
$$\Delta_k w_r = h^{1/2} \xi_{rk}, \ (I_{r0})_k = h^{3/2} (\xi_{rk} + \eta_{rk}/\sqrt{3})/2$$

Note that Remark 3.2 is applicable here if one will approximate $P_{II}(t)$ using a deterministic method of one-step order not less than 3.

3.3. Third-order methods. Using ideas of the method of fractional steps, as we did in the previous subsections, it is possible to construct a third-order method for (3.1) which satisfies the requirements RL1 and RL2. But such a method contains two fractional steps at which we have to approximate the Hamiltonian system (3.5), (3.1) using a third-order symplectic method. This makes a method of this kind too complicated, and we will use another approach. In [28] a similar problem for deterministic second-order differential equations was solved by a modification of symplectic Runge-Kutta-Nyström (RKN) methods from [26]. Here we modify the symplectic RKN method from [17] using ideas of [28].

As a result, we obtain the method

(3.25)
$$Q_1 = Q_k + \frac{7}{24} h M^{-1} P_k, \quad \mathcal{P}_1 = P_k + \frac{7}{24} h \left[f(Q_1) - \nu \Gamma \mathcal{P}_1 \right],$$

$$Q_{2} = Q_{k} + \frac{25}{24}hM^{-1}P_{k} + \frac{h^{2}}{2}M^{-1}\left[f(Q_{1}) - \nu\Gamma\mathcal{P}_{1}\right],$$

$$\mathcal{P}_{2} = P_{k} + \frac{2}{3}h\left[f(Q_{1}) - \nu\Gamma\mathcal{P}_{1}\right] + \frac{3}{8}h\left[f(Q_{2}) - \nu\Gamma\mathcal{P}_{2}\right]$$

$$Q_{3} = Q_{k} + hM^{-1}P_{k} + \frac{17}{36}h^{2}M^{-1}\left[f(Q_{1}) - \nu\Gamma\mathcal{P}_{1}\right] + \frac{1}{36}h^{2}M^{-1}\left[f(Q_{2}) - \nu\Gamma\mathcal{P}_{2}\right],$$

$$\mathcal{P}_{3} = P_{k} + \frac{2}{3}h\left[f(Q_{1}) - \nu\Gamma\mathcal{P}_{1}\right] - \frac{2}{3}h\left[f(Q_{2}) - \nu\Gamma\mathcal{P}_{2}\right] + h\left[f(Q_{3}) - \nu\Gamma\mathcal{P}_{3}\right],$$
(3.26)

$$P_{k+1} = \mathcal{P}_3 + \sum_{r=1}^m \sigma_r \Delta_k w_r - \nu \sum_{r=1}^m \Gamma \sigma_r \cdot (I_{r0})_k + \sum_{r=1}^m \left[\sum_{i=1}^n (M^{-1} \sigma_r)^i \frac{\partial f}{\partial q^i}(\mathcal{Q}_3) + \nu^2 \Gamma^2 \sigma_r \right] (I_{r00})_k,$$
$$Q_{k+1} = \mathcal{Q}_3 + \sum_{r=1}^m M^{-1} \sigma_r \cdot (I_{r0})_k - \nu \sum_{r=1}^m M^{-1} \Gamma \sigma_r (I_{r00})_k, \quad k = 0, \dots, N-1,$$

where

$$(I_{r00})_k:=\int\limits_{t_k}^{t_k+h}\int\limits_{t_k}^{artheta_1}(w_r(artheta_2)-w_r(t_k))\;dartheta_2dartheta_1$$

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 N(0, 1)-distributed random variables ξ_{rk} , η_{rk} , and ζ_{rk} , $r = 0, \ldots, m$:

(3.27)
$$\Delta_k w_r = h^{1/2} \xi_{rk}, \quad (I_{r0})_k = h^{3/2} (\xi_{rk} + \eta_{rk}/\sqrt{3})/2, (I_{r00})_k = h^{5/2} (\xi_{rk} + \sqrt{3}\eta_{rk}/2 - \zeta_{rk}/(2\sqrt{5}))/6.$$

Using (3.27), the method (3.25)-(3.26) can be written in the constructive form. It 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 (3.25)-(3.26) coincides with the third-order symplectic method from [17] and so it satisfies the requirement RL1. For $\sigma_r = 0, r = 1, \ldots, m$, (deterministic case), the RKN method (3.25)-(3.26) satisfies conditions set up in [28, Section 5]. These conditions ensure that the Jacobian of the deterministic RKN method depend on $\nu\Gamma$ and h only, more precisely [28, 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 \overline{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 [17] and prove that the method (3.25)-(3.26) is of mean-square order 3. Thus, we obtain the theorem.

Theorem 3.3. The method (3.25)-(3.26) for the system (3.1) is of mean-square order 3 and it is such that (i) it is symplectic when applied to (3.1)-(3.2) with $\nu = 0$, (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 3.3. A method of mean-square order 7/2 for (3.1) contains complicated Ito integrals, and it is not efficient with respect to simulation of the used random variables.

Remark 3.4. All the methods of this section can be carried over to nonautonomous Langevin equations.

4. QUASI-SYMPLECTIC MEAN-SQUARE METHODS FOR GENERAL LANGEVIN TYPE EQUATIONS

Here we generalize methods of Section 3 to the Langevin type system

(4.1)
$$dP = f(t,Q)dt - \nu f_{\nu}(t,P,Q)dt + \sum_{r=1}^{m} \sigma_{r}(t,Q)dw_{r}(t), \ P(t_{0}) = p,$$
$$dQ = g(P)dt, \ Q(t_{0}) = q,$$

where $P, Q, f, f_{\nu}, g, \sigma_r$ are *n*-dimensional column-vectors, ν is a parameter, and $w_r(t)$, $r = 1, \ldots, m$, 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, ..., m, such that

(4.2)
$$f^i = -\partial H_0 / \partial q^i, \quad g^i = \partial H_0 / \partial p^i, \quad \sigma^i_r = -\partial H_r / \partial q^i, \quad i = 1, \dots, n,$$

and if $\nu = 0$, then (4.1) is a Hamiltonian system with multiplicative noise [2, 17, 18]. Note that the system (4.1) has the same form in the sense of Stratonovich.

Our aim is to construct methods for (4.1) such that they inherit the properties RL1-RL2 of the specific methods for the Langevin equation (3.1), more precisely we require

RLT1. The methods become symplectic when the system degenerate to Hamiltonian; **RLT2.** The methods degenerate to those satisfying the requirement RL2 from Section 3 when the system degenerates to the Langevin equation (3.1).

We recall that the Euler method for general systems with multiplicative noise is of order 1/2. But due to specific features of system (4.1), the Euler method (and other usual methods of order 1/2) applied to (4.1) is of order 1. Therefore, we start with methods of order 1.

4.1. First-order methods based on splitting. In connection with (4.1) introduce the systems (cf. (3.5)-(3.6)):

(4.3)
$$dP_{I} = f(t,Q_{I})dt + \sum_{r=1}^{m} \sigma_{r}(t,Q_{I})dw_{r}(t), P_{I}(t_{0}) = p,$$
$$dQ_{I} = g(P_{I})dt, Q_{I}(t_{0}) = q,$$

(4.4)
$$\frac{dP_{II}}{dt} = -\nu f_{\nu}(t, P_{II}, q), \quad P_{II}(t_0) = p_{II}($$

and denote their solutions as $P_I(t; t_0, p, q)$, $Q_I(t; t_0, p, q)$ and $P_{II}(t; t_0, p, q)$ correspondingly. The system (4.3), (4.2) is a Hamiltonian system with separable Hamiltonians. Symplectic integrators for such systems are proposed in [18]. The system (4.4) is deterministic.

Let \bar{P}_I , \bar{Q}_I be a one-step approximation corresponding to a symplectic method for (4.3), (4.2) and \bar{P}_{II} be a one-step approximation of a deterministic method for (4.4). Introduce the approximation for (4.1) as follows

$$(4.5) \qquad \bar{P} = \bar{P}(t_0 + h; t_0, p, q) := \bar{P}_{II}(t_0 + h; t_0, \bar{P}_I(t_0 + h; t_0, p, q), \bar{Q}_I(t_0 + h; t_0, p, q)), \bar{Q} = \bar{Q}(t_0 + h; t_0, p, q) := \bar{Q}_I(t_0 + h; t_0, p, q).$$

Clearly, the approximation (4.5) satisfies the requirements RLT1 and RLT2. Further, using arguments similar to those in the proof of Lemma 3.1, we prove that if \bar{P}_I , \bar{Q}_I is a one-step approximation corresponding to any first-order mean-square method for (4.3) and \bar{P}_{II} is a one-step approximation corresponding to any first-order deterministic method for (4.4), then \bar{P} , \bar{Q} defined in (4.5) is a one-step approximation of the first-order mean-square method for the system (4.1). Therefore, the following theorem holds.

Theorem 4.1. Let \bar{P}_I , \bar{Q}_I be a one-step approximation corresponding to a symplectic firstorder mean-square method for the system (4.3), (4.2) and \bar{P}_{II} be a one-step approximation corresponding to a first-order deterministic method for the system (4.4). Then \bar{P} , \bar{Q} defined in (4.5) is a one-step approximation of the first-order mean-square method for the system (4.1) such that (i) it is symplectic when applied to (4.1)-(4.2) with $\nu = 0$, (ii) it satisfies the requirement RL2 from Section 3 when (4.1) degenerates to the Langevin equation (3.1).

Let us give a concrete example of a first-order splitting method (to this end we use a PRK method from [18]):

(4.6)

$$Q_{1} = Q_{k} + \alpha h g(P_{k}), \quad \mathcal{P}_{1} = P_{k} + h f(t_{k} + \alpha h, Q_{1}),$$

$$Q_{2} = Q_{1} + (1 - \alpha) h g(\mathcal{P}_{1}), \quad \mathcal{P}_{2} = P_{k} + h f(t_{k} + \alpha h, Q_{1}) + \sum_{r=1}^{m} \sigma_{r}(t_{k}, Q_{2}) \Delta_{k} w_{r},$$

$$Q_{k+1} = Q_{2}, \quad P_{k+1} = \mathcal{P}_{2} - h \nu f_{\nu}(t_{k}, \mathcal{P}_{2}, Q_{2}).$$

Remark 4.1. If we take \bar{P}_{II} in (4.5) such that it corresponds to a high-order deterministic method for (4.4), this will ensure better phase-volume contractivity properties of (4.5) (i.e., in this case the approximate volume contractivity law is closer to the exact one than in the case of first-order deterministic method).

Remark 4.2. Theorem 4.1 also holds for the method based on the one-step approximation

(4.7)

$$\bar{P} := \bar{P}_I(t_0 + h; t_0, \bar{P}_{II}(t_0 + h; t_0, p, q), q), \\
\bar{Q} := \bar{Q}_I(t_0 + h; t_0, \bar{P}_{II}(t_0 + h; t_0, p, q), q).$$

Remark 4.3. The discussion in the end of Section 3.1 is also valid here: there are first-order implicit symplectic methods which directly applied to (4.1) give the methods satisfying the requirements RLT1-RLT2.

The particular case of system (4.1), when $f_{\nu}(t, p, q) = \Gamma(q)p$, 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. [20] and references therein). In this case the system (4.4) becomes deterministic linear system with constant coefficients, which can be solved exactly. If in addition to $f_{\nu}(t, p, q) = \Gamma(q)p$ the system (4.1) 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 (4.9) (see Subsection 4.2) 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

$$(4.8) \quad dP = (f(t, P, Q) - \nu f_{\nu}(t, P, Q)) dt + \sum_{r=1}^{m} \sigma_{r}(t, P, Q) \circ dw_{r}(t), \ P(t_{0}) = p,$$

$$dQ = (g(t, P, Q) - \nu g_{\nu}(t, P, Q)) dt + \sum_{r=1}^{m} \gamma_{r}(t, P, Q) \circ dw_{r}(t), \ Q(t_{0}) = q,$$

where $\nu \ge 0$ 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 (4.8) in two parts: in the Hamiltonian system (1.2) and the deterministic system, and then use a relation like (4.5) or (4.7) to approximate (4.8). In such an approximation we have \bar{P}_I, \bar{Q}_I corresponding to a full implicit symplectic method from [18]. As a result, we obtain the approximation \bar{P}, \bar{Q} for (4.8) which satisfies the requirements RLT1-RLT2. The method for (4.8) based on this approximation is of order 1/2.

4.2. Methods of order 3/2. Using the fractional step method, we propose the following approximation for (4.1)

$$(4.9) \qquad \bar{P}(t_{0}+h;t_{0},p,q) \\ := \bar{P}_{II}(t_{0}+\frac{h}{2};t_{0},\bar{P}_{I}(t_{0}+h;t_{0},\bar{P}_{II}(t_{0}+\frac{h}{2};t_{0},p,q),q),\bar{Q}_{I}(t_{0}+h;t_{0},\bar{P}_{II}(t_{0}+\frac{h}{2};t_{0},p,q),q)) \\ -\nu\sum_{r=1}^{m}\sum_{i=1}^{n}\sigma_{r}^{i}\frac{\partial f_{\nu}}{\partial p^{i}}(t_{0},p,q)\left[I_{r0}-\frac{h}{2}\Delta w_{r}\right] -\frac{h^{2}}{4}\nu\frac{\partial f_{\nu}}{\partial t}(t_{0},p,q), \\ \bar{Q}(t_{0}+h;t_{0},p,q):=\bar{Q}_{I}(t_{0}+h;t_{0},\bar{P}_{II}(t_{0}+\frac{h}{2};t_{0},p,q),q), \end{cases}$$

where \bar{P}_I , \bar{Q}_I is a one-step approximation corresponding to a symplectic method of order 3/2 for (4.3), (4.2) (such methods are available in [18]) and \bar{P}_{II} is a one-step approximation of a second-order deterministic method for (4.4).

By argument similar to those exploited in previous sections, we prove the following theorem. **Theorem 4.2.** Let \bar{P}_I , \bar{Q}_I be a one-step approximation corresponding to a symplectic mean-square method of order 3/2 for the system (4.3), (4.2), and \bar{P}_{II} be a one-step approximation corresponding to a second-order deterministic method for the system (4.4). Then \bar{P} , \bar{Q} defined in (4.9) is the one-step approximation of mean-square method of order 3/2 for the system (4.1) which satisfies the requirements RLT1-RLT2.

A remark analogous to Remark 4.1 is valid here. As it is also noted in Section 4.1, if $f_{\nu}(t, p, q) = \Gamma(q)p$, then $P_{II}(t)$ can be found explicitly. Consequently, in this important case we can use an approximation of the form (3.19). The corresponding mean-square method is again of order 3/2.

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

5.1. Implicit first-order methods for general stochastic Hamiltonian systems. In this subsection weak symplectic methods for the stochastic Hamiltonian system (1.2), (1.3) are constructed. All the methods in this subsection 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 [21]. The standard implicit methods for SDEs with multiplicative noise (see [12, 7]) contain implicitness in deterministic terms only. Meanwhile to construct symplectic methods for general stochastic Hamiltonian systems, full implicit methods are needed. Such mean-square methods are proposed in [18]. Increments of Wiener processes in these implicit schemes are substituted by some truncated random variables. As a result, general mean-square symplectic 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 [18], we propose the weak method:

(5.1)
$$P_{k+1} = P_k + hf(t_k + \beta h, \alpha P_{k+1} + (1 - \alpha)P_k, (1 - \alpha)Q_{k+1} + \alpha Q_k) + h(\frac{1}{2} - \alpha) \sum_{r=1}^m \sum_{j=1}^n (\frac{\partial \sigma_r}{\partial p^j} \sigma_r^j - \frac{\partial \sigma_r}{\partial q^j} \gamma_r^j) + h^{1/2} \sum_{r=1}^m \sigma_r \xi_{rk}, Q_{k+1} = Q_k + hg(t_k + \beta h, \alpha P_{k+1} + (1 - \alpha)P_k, (1 - \alpha)Q_{k+1} + \alpha Q_k) + h(\frac{1}{2} - \alpha) \sum_{r=1}^m \sum_{j=1}^n (\frac{\partial \gamma_r}{\partial p^j} \sigma_r^j - \frac{\partial \gamma_r}{\partial q^j} \gamma_r^j) + h^{1/2} \sum_{r=1}^m \gamma_r \xi_{rk},$$

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

(5.2)
$$P(\xi = \pm 1) = 1/2$$

Note that if $\alpha = \beta = 1/2$ the method (5.1) 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 5.1. The implicit method (5.1) for the system (1.2), (1.3) is symplectic and of the first weak order.

Proof. The symplecticness is proved as in Theorem 3.2 from [18]. Let us prove convergence of the method. Denote by $\bar{X} = \bar{X}(t+h;t,x) = (\bar{P}^{\intercal}, \bar{Q}^{\intercal})^{\intercal}$ the one-step approximation corresponding to the method (5.1):

(5.3)

$$\bar{P} = p + hf(t + \beta h, \alpha \bar{P} + (1 - \alpha)p, (1 - \alpha)\bar{Q} + \alpha q) \\
+ h(\frac{1}{2} - \alpha) \sum_{r=1}^{m} \sum_{j=1}^{n} (\frac{\partial \sigma_{r}}{\partial p^{j}} \sigma_{r}^{j} - \frac{\partial \sigma_{r}}{\partial q^{j}} \gamma_{r}^{j}) + h^{1/2} \sum_{r=1}^{m} \sigma_{r} \xi_{r}, \\
\bar{Q} = q + hg(t + \beta h, \alpha \bar{P} + (1 - \alpha)p, (1 - \alpha)\bar{Q} + \alpha q) \\
+ h(\frac{1}{2} - \alpha) \sum_{r=1}^{m} \sum_{j=1}^{n} (\frac{\partial \gamma_{r}}{\partial p^{j}} \sigma_{r}^{j} - \frac{\partial \gamma_{r}}{\partial q^{j}} \gamma_{r}^{j}) + h^{1/2} \sum_{r=1}^{m} \gamma_{r} \xi_{r},$$

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

Using the Lipschitz condition (2.2), one can prove (cf. Lemma 2.3 in [18]) that there are constants K > 0 and $h_0 > 0$ such that for any $h \le h_0$, $t_0 \le t \le t_0 + T$, $x = (p^{\intercal}, q^{\intercal})^{\intercal} \in \mathbb{R}^d$, d = 2n, the equation (5.3) has a unique solution \overline{X} which satisfies the inequality

(5.4)
$$|\bar{X} - x| \le K(1 + |x|)\sqrt{h},$$

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

The condition (2.8) with l = 1 of Theorem 2.2 holds for the approximation (5.3) due to (5.4). Let us check the fulfillment of condition (2.7) with l = 1. To this end, introduce the weak Euler approximation $\hat{X} = (\hat{P}^{\intercal}, \hat{Q}^{\intercal})^{\intercal}$ for the Stratonovich system (1.2), (1.3):

(5.5)
$$\hat{P} = p + hf + \frac{h}{2} \sum_{r=1}^{m} \sum_{j=1}^{n} \left(\frac{\partial \sigma_r}{\partial p^j} \sigma_r^j + \frac{\partial \sigma_r}{\partial q^j} \gamma_r^j\right) + h^{1/2} \sum_{r=1}^{m} \sigma_r \xi_r,$$
$$\hat{Q} = q + hg + \frac{h}{2} \sum_{r=1}^{m} \sum_{j=1}^{n} \left(\frac{\partial \gamma_r}{\partial p^j} \sigma_r^j + \frac{\partial \gamma_r}{\partial q^j} \gamma_r^j\right) + h^{1/2} \sum_{r=1}^{m} \gamma_r \xi_r,$$

where f, g and σ_r , γ_r , r = 1, ..., m, and their derivatives are calculated at (t, p, q). Expanding the terms in the right-hand side of (5.3) around (t, p, q) and using (5.4) and the corresponding conditions on smoothness and boundedness of the coefficients, it is not

the corresponding conditions on smoothness and boundedness of difficult to obtain that s s

(5.6)
$$|E(\prod_{j=1}^{n} \hat{\Delta}^{i_{j}} - \prod_{j=1}^{n} \bar{\Delta}^{i_{j}})| \le K(x)h^{2}, \ s = 1, 2, 3, \ i_{j} = 1, \dots, 2n, \ K(x) \in \mathbf{F},$$

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

Taking into account (5.6) and the fact that the Euler approximation (5.5) satisfies (2.7) with l = 1 [12, 7], we get that the approximation (5.3) satisfies (2.7) with l = 1 as well.

Finally, to check the fourth condition of Theorem 2.2, we use Lemma 9.1 from [12, p. 114] which ensures existence and uniform boundedness of the moments $E|\bar{X}_k|^{\bar{m}}$ under the conditions: (i) $|E\bar{\Delta}| \leq K(1+|x|)h$ and (ii) $|\bar{\Delta}| \leq M(\xi)(1+|x|)\sqrt{h}$ with $M(\xi)$ having moments of all orders. The inequalities (5.6) and $|E\hat{\Delta}| \leq K(1+|x|)h$ imply fulfillment of the condition (i), while the condition (ii) holds here due to (5.4). \Box

Remark 5.1. 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, ..., m, the method (5.1) with $\alpha = 1$, $\beta = 0$ acquires the form

(5.7)
$$P_{k+1} = P_k + f(t_k, P_{k+1}, Q_k)h + \frac{h}{2} \sum_{r=1}^m \sum_{j=1}^n \frac{\partial \sigma_r}{\partial q^j}(t_k, Q_k) \cdot \gamma_r^j(t_k, P_{k+1}) + h^{1/2} \sum_{r=1}^m \sigma_r(t_k, Q_k)\xi_{rk},$$

$$Q_{k+1} = Q_k + g(t_k, P_{k+1}, Q_k)h - \frac{h}{2} \sum_{r=1}^m \sum_{j=1}^n \frac{\partial \gamma_r}{\partial p^j}(t_k, P_{k+1}) \cdot \sigma_r^j(t_k, Q_k) + h^{1/2} \sum_{r=1}^m \gamma_r(t_k, P_{k+1})\xi_{rk}$$

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 $H_r(t, p, q) = \Gamma_r^{\top}(t)p + U_r(t, q)$, $r = 1, \ldots m$, $\Gamma_r(t)$ are *n*-dimensional vectors, one obtains full explicit symplectic methods.

Remark 5.2. As is known [12, 7], 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 investigations. In the next subsection a symplectic method of weak order 2 is proposed for a particular case of (1.2), (1.3).

5.2. Explicit first-order methods in the case of separable Hamiltonians. In this and in the next subsections we consider a special case of the Hamiltonian system (1.2), (1.3) such that

(5.8)
$$H_0(t,p,q) = V_0(p) + U_0(t,q), \ H_r(t,p,q) = U_r(t,q), \ r = 1, \dots m.$$

In this case we get the following system

(5.9)
$$dP = f(t,Q)dt + \sum_{r=1}^{m} \sigma_r(t,Q)dw_r(t), \ P(t_0) = p,$$
$$dQ = g(P)dt, \ Q(t_0) = q,$$

with

(5.10)
$$f^{i} = -\partial U_{0}/\partial q^{i}, \ g^{i} = \partial V_{0}/\partial p^{i}, \ \sigma_{r}^{i} = -\partial U_{r}/\partial q^{i}, \ r = 1, \dots, m, \ i = 1, \dots, n.$$

Recall that the system (5.9) has the same form in the sense of Stratonovich. Due to specific features of the system (5.9), (5.10) 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 [18] we obtain the weak PRK method for (5.9):

(5.11)
$$Q_1 = Q_k + \alpha h g(P_k), \quad \mathcal{P}_1 = P_k + h f(t_k + \alpha h, Q_1),$$
$$Q_2 = Q_1 + (1 - \alpha) h g(\mathcal{P}_1),$$

(5.12)
$$P_{k+1} = \mathcal{P}_1 + h^{1/2} \sum_{r=1}^m \sigma_r(t_k, \mathcal{Q}_2) \xi_{rk}, \quad Q_{k+1} = \mathcal{Q}_2, \quad k = 0, \dots, N-1,$$

where $0 \le \alpha \le 1$ is a parameter and ξ_{rk} are i.i.d. random variables with the law (5.2). **Theorem 5.2.** The explicit method (5.11)-(5.12) for the system (5.9), (5.10) is symplectic and of the first weak order.

Proof. Due to (5.10), $\partial \sigma_r^i / \partial q^j = \partial \sigma_r^j / \partial q^i$. Using this, we obtain $dP_{k+1} \wedge dQ_{k+1} = d\mathcal{P}_1 \wedge d\mathcal{Q}_2$. It is easy to prove that $d\mathcal{P}_1 \wedge d\mathcal{Q}_2 = d\mathcal{P}_1 \wedge d\mathcal{Q}_1 = dP_k \wedge dQ_k$. Therefore the method (5.11)-(5.12) is symplectic. The order of convergence is proved as in Theorem 5.1 (even simpler). \Box

Remark 5.3. By swapping the roles of p and q, we can propose another symplectic method of the first weak order for the system (5.9), (5.10). Namely, instead of (5.11)-(5.12) one can propose

(5.13)
$$\mathcal{P}_1 = P_k + \alpha h f(t_k, Q_k), \ \mathcal{Q}_1 = Q_k + h g(\mathcal{P}_1), \mathcal{P}_2 = \mathcal{P}_1 + (1 - \alpha) h f(t_k + h, \mathcal{Q}_1),$$

(5.14)
$$P_{k+1} = \mathcal{P}_2 + h^{1/2} \sum_{r=1}^m \sigma_r(t_k, \mathcal{Q}_1) \xi_{rk}, \quad Q_{k+1} = \mathcal{Q}_1, \ k = 0, \dots, N-1.$$

5.3. Explicit second-order method in the case of separable Hamiltonians. Introduce the explicit PRK method for the system (5.9), (5.10):

(5.15)
$$Q_1 = Q_k + \frac{h}{2}g(P_k), \quad \mathcal{P}_1 = P_k + hf(t_k + \frac{h}{2}, Q_1) + h^{1/2}\sum_{r=1}^m \sigma_r(t_k + \frac{h}{2}, Q_1)\xi_{rk},$$

$$P_{k+1} = \mathcal{P}_1, \quad Q_{k+1} = \mathcal{Q}_1 + \frac{h}{2}g(\mathcal{P}_1), \quad k = 0, \dots, N-1,$$

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

(5.16)
$$P(\xi = 0) = 2/3, \ P(\xi = \pm\sqrt{3}) = 1/6.$$

It follows from Lemma 4.1 from [18] that this method is symplectic. Comparing (5.15) with the standard Taylor type second-order weak method from [12, p. 115] applied to (5.9), we prove that the method (5.15) is of weak order 2.

Theorem 5.3. The explicit method (5.15) for the system (5.9), (5.10) is symplectic and of the second weak order.

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

Consider Hamiltonian systems with additive noise

(6.1)
$$dP = f(t, P, Q)dt + \sum_{r=1}^{m} \sigma_r(t)dw_r(t), \ P(t_0) = p,$$
$$dQ = g(t, P, Q)dt + \sum_{r=1}^{m} \gamma_r(t)dw_r(t), \ Q(t_0) = q,$$

where f and g satisfy (1.3).

The first order method for (6.1) follows from the method (5.1).

6.1. 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 [17], we construct the weak method:

(6.2)
$$\mathcal{P}_{1} = P_{k} + \frac{\alpha}{2} h f(t_{k} + \frac{\alpha}{2}h, \mathcal{P}_{1}, \mathcal{Q}_{1}) + \lambda_{1} h^{1/2} \sum_{r=1}^{m} \sigma_{r}(t_{k} + \frac{h}{2}) \xi_{rk},$$
$$\mathcal{Q}_{1} = Q_{k} + \frac{\alpha}{2} h g(t_{k} + \frac{\alpha}{2}h, \mathcal{P}_{1}, \mathcal{Q}_{1}) + \lambda_{1} h^{1/2} \sum_{r=1}^{m} \gamma_{r}(t_{k} + \frac{h}{2}) \xi_{rk},$$

$$egin{aligned} \mathcal{P}_2 &= P_k + lpha hf(t_k + rac{lpha}{2}h, \mathcal{P}_1, \mathcal{Q}_1) + rac{1-lpha}{2}hf(t_k + rac{1+lpha}{2}h, \mathcal{P}_2, \mathcal{Q}_2) \ &+ \lambda_2 h^{1/2}\sum_{r=1}^m \sigma_r(t_k + rac{h}{2})\xi_{rk}, \ \mathcal{Q}_2 &= Q_k + lpha hg(t_k + rac{lpha}{2}h, \mathcal{P}_1, \mathcal{Q}_1) + rac{1-lpha}{2}hg(t_k + rac{1+lpha}{2}h, \mathcal{P}_2, \mathcal{Q}_2) \ &+ \lambda_2 h^{1/2}\sum_{r=1}^m \gamma_r(t_k + rac{h}{2})\xi_{rk}, \end{aligned}$$

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

where the parameters α , λ_1 , λ_2 are such that

(6.3)
$$\alpha \lambda_1 + (1-\alpha)\lambda_2 = \frac{1}{2}, \ \alpha \lambda_1^2 + (1-\alpha)\lambda_2^2 = \frac{1}{2},$$

and ξ_{rk} are i.i.d. random variables with the law (5.16).

For example, the following set of parameters satisfies (6.3):

(6.4)
$$\alpha = \frac{1}{2}, \ \lambda_1 = 0, \ \lambda_2 = 1.$$

The symplecticness follows from Lemma 3.5 of [17]. The order of convergence is proved similarly to the proof of Theorem 5.1 comparing (6.2) with the standard Taylor type second-order weak method from [12, p. 115] applied to (6.1).

Theorem 6.1. The implicit method (6.2), (6.3) for the system (6.1) is symplectic and of the second weak order.

6.2. A third-order method in a particular case of Hamiltonian system. In this subsection we propose a symplectic weak method of order 3 for the system with additive noise:

(6.5)
$$dP = f(t,Q)dt + \sum_{r=1}^{m} \sigma_r(t)dw_r(t), \ f^i(t,Q) = -\frac{\partial U_0}{\partial q^i}, \ P(t_0) = p,$$
$$dQ = M^{-1}Pdt, \ Q(t_0) = q.$$

On the basis of a symplectic mean-square method of order 3 from [17], we construct the weak method:

$$Q_{k+1} = Q_3 + h^{3/2} \sum_{r=1}^m M^{-1} \sigma_r(t_k) (\xi_r/2 + \eta_r)_k + h^{5/2} \sum_{r=1}^m M^{-1} \sigma_r'(t_k) \xi_{rk}/6,$$

$$k = 0, \dots, N-1,$$

where ξ_{rk} , η_{rk} are mutually independent random variables distributed by the laws (6.8) $P(\xi = 0) = \frac{1}{3}, P(\xi = \pm 1) = \frac{3}{10}, P(\xi = \pm \sqrt{6}) = \frac{1}{30},$

$$P(\eta = \pm 1/\sqrt{12}) = \frac{1}{2}.$$

The symplecticness of this method follows from Theorem 5.3 of [17]. The order of convergence can be proved by standard arguments [12, Section 10] using the fact that the corresponding mean-square method from [17] has the third order of convergence or by comparing the method (6.6)-(6.7) with the weak method of order 3 from [12, p. 126] applied to (6.5).

Theorem 6.2. The explicit method (6.6) - (6.7) for the system (6.5) is symplectic and of the third weak order.

7. METHODS IN THE WEAK SENSE FOR HAMILTONIAN SYSTEMS WITH COLORED NOISE

Consider the system with colored noise

(7.1)
$$dP = f(t, P, Q)dt + \sum_{r=1}^{m} \sigma_{r}(t, P, Q)Y^{r}dt, \ P(t_{0}) = p,$$
$$dQ = g(t, P, Q)dt + \sum_{r=1}^{m} \gamma_{r}(t, P, Q)Y^{r}dt, \ Q(t_{0}) = q,$$
$$dY = \Gamma(t)Ydt + \sum_{r=1}^{l} \delta_{r}(t)dw_{r}(t), \ Y(t_{0}) = y,$$

where $P, Q, f, g, \sigma_r, \gamma_r$ are *n*-dimensional column vectors, Y and δ_r are *m*-dimensional column vectors, $\Gamma(t)$ is an $m \times m$ matrix, and

(7.2)
$$\begin{aligned} f^i &= -\partial H_0 / \partial q^i, \quad g^i = \partial H_0 / \partial p^i, \\ \sigma^i_r &= -\partial H_r / \partial q^i, \quad \gamma^i_r = \partial H_r / \partial p^i, \quad i = 1, \dots, n, \quad r = 1, \dots, m. \end{aligned}$$

It can be proved that the transformation $(p,q) \mapsto (P,Q)$ defined by (7.1) preserves symplectic structure if the coefficients f, g, σ_r, γ_r satisfy (7.2). In particular, when all the coefficients σ_r, γ_r at the colored noise do not depend on p and q, the phase flow of (7.1) preserves symplectic structure if $f^i = -\partial H_0/\partial q^i, g^i = \partial H_0/\partial p^i, i = 1, \ldots, n$.

Using specific features of a general system with colored noise, high-order mean-square and weak methods were constructed in [13] (see also references therein). Here we propose symplectic weak methods for the Hamiltonian system with colored noise (7.1), (7.2).

7.1. First-order methods. Consider the weak implicit method for (7.1), (7.2):

(7.3)
$$P_{k+1} = P_k + hf + h\sum_{r=1}^m \sigma_r Y_k^r, \quad Q_{k+1} = Q_k + hg + h\sum_{r=1}^m \gamma_r Y_k^r,$$
$$Y_{k+1} = Y_k + h\Gamma(t_k)Y_k + h^{1/2}\sum_{r=1}^l \delta_r(t_k)\xi_{rk},$$

where f, g, σ_r, γ_r are calculated at $(t_k + \beta h, \alpha P_{k+1} + (1 - \alpha)P_k, (1 - \alpha)Q_{k+1} + \alpha Q_k)$, the parameters $\alpha, \beta \in [0, 1]$, and ξ_{rk} are i.i.d. random variables with the law (5.2).

It is not difficult to prove the following theorem.

Theorem 7.1. The implicit method (7.3) for the system (7.1), (7.2) is symplectic and of the first weak order.

7.2. Second-order methods. Introduce the method for (7.1), (7.2):

(7.4)
$$\mathcal{Y} = Y_k + \frac{h}{2}\Gamma(t_k)Y_k + \frac{1}{2}h^{1/2}\sum_{r=1}^l \delta_r(t_k)\xi_{rk},$$

(7.5)
$$P_{k+1} = P_k + hf + h\sum_{r=1}^m \sigma_r \mathcal{Y}^r, \quad Q_{k+1} = Q_k + hg + h\sum_{r=1}^m \gamma_r \mathcal{Y}^r,$$

$$Y_{k+1} = Y_k + h\Gamma(t_k + h/2)\mathcal{Y} + h^{1/2}\sum_{r=1}^{i} \delta_r(t_k + h/2)\xi_{rk}$$

where f, g, σ_r, γ_r are calculated at $(t_k + h/2, (P_{k+1} + P_k)/2, (Q_{k+1} + Q_k)/2)$ and ξ_{rk} are i.i.d. random variables with the law (5.16).

The symplecticness of this method follows from the symplecticness of the midpoint scheme for deterministic Hamiltonian systems [21, 27]. Using the standard arguments [12] (see also [13]), we prove that this method is of weak order 2.

Theorem 7.2. The implicit method (7.4) - (7.5) for the system (7.1), (7.2) is symplectic and of the second weak order.

Remark 7.1. The method (7.4) - (7.5) is based on the implicit midpoint rule for deterministic Hamiltonian systems. Using other deterministic symplectic integrators of order 2 (see e.g. [21, 27]), it is possible to obtain the other symplectic methods for (7.1), (7.2).

7.3. Third-order method. Introduce the notation

$$egin{aligned} \mathbf{f}(t,p,q,y) &:= f(t,p,q) + \sum_{r=1}^m \sigma_r(t,p,q) y^r, \ \mathbf{g}(t,p,q,y) &:= g(t,p,q) + \sum_{r=1}^m \gamma_r(t,p,q) y^r, \end{aligned}$$

Consider the implicit method for (7.1), (7.2):

(7.6)
$$\mathcal{Y}_0 = Y_k + \frac{h^{1/2}}{3} \sum_{r=1}^l \delta_r(t_k) \xi_{rk} + \frac{h}{3} \Gamma(t_k) Y_k,$$

$$\begin{aligned} \mathcal{Y}_1 &= Y_k + \varkappa h^{1/2} \sum_{r=1}^l \delta_r (t_k + \frac{h}{3}) (\xi_{rk}/2 + \eta_{rk}) + \frac{\varkappa}{2} h \Gamma (t_k + \frac{h}{3}) \mathcal{Y}_0, \\ \mathcal{P}_1 &= P_k + h \frac{\varkappa}{2} \mathbf{f}(t_k + \frac{\varkappa}{2} h, \mathcal{P}_1, \mathcal{Q}_1, \mathcal{Y}_1), \quad \mathcal{Q}_1 = Q_k + h \frac{\varkappa}{2} \mathbf{g}(t_k + \frac{\varkappa}{2} h, \mathcal{P}_1, \mathcal{Q}_1, \mathcal{Y}_1), \end{aligned}$$

$$\begin{aligned} \mathcal{Y}_{2} &= Y_{k} + h^{1/2} \sum_{r=1}^{l} \delta_{r} (t_{k} + \frac{h}{3}) (\xi_{rk}/2 + \eta_{rk}) + \frac{h}{2} \Gamma(t_{k} + \frac{h}{3}) \mathcal{Y}_{0}, \\ \mathcal{P}_{2} &= P_{k} + h[\varkappa \mathbf{f}(t_{k} + \frac{\varkappa}{2}h, \mathcal{P}_{1}, \mathcal{Q}_{1}, \mathcal{Y}_{1}) + \frac{1 - 2\varkappa}{2} \mathbf{f}(t_{k} + \frac{h}{2}, \mathcal{P}_{2}, \mathcal{Q}_{2}, \mathcal{Y}_{2})], \\ \mathcal{Q}_{2} &= Q_{k} + h[\varkappa \mathbf{g}(t_{k} + \frac{\varkappa}{2}h, \mathcal{P}_{1}, \mathcal{Q}_{1}, \mathcal{Y}_{1}) + \frac{1 - 2\varkappa}{2} \mathbf{g}(t_{k} + \frac{h}{2}, \mathcal{P}_{2}, \mathcal{Q}_{2}, \mathcal{Y}_{2})], \\ \mathcal{Y}_{3} &= Y_{k} + (2 - \varkappa)h^{1/2} \sum_{r=1}^{l} \delta_{r} (t_{k} + \frac{h}{3}) (\xi_{rk}/2 + \eta_{rk}) + \frac{(2 - \varkappa)}{2} h \Gamma(t_{k} + \frac{h}{3}) \mathcal{Y}_{0}, \\ \mathcal{P}_{3} &= P_{k} + h[\varkappa \mathbf{f}(t_{k} + \frac{\varkappa}{2}h, \mathcal{P}_{1}, \mathcal{Q}_{1}, \mathcal{Y}_{1}) + (1 - 2\varkappa)\mathbf{f}(t_{k} + \frac{h}{2}, \mathcal{P}_{2}, \mathcal{Q}_{2}, \mathcal{Y}_{2}) \\ &\quad + \frac{\varkappa}{2} \mathbf{f}(t_{k} + \frac{2 - \varkappa}{2}h, \mathcal{P}_{3}, \mathcal{Q}_{3}, \mathcal{Y}_{3})], \\ \mathcal{Q}_{3} &= Q_{k} + h[\varkappa \mathbf{g}(t_{k} + \frac{\varkappa}{2}h, \mathcal{P}_{1}, \mathcal{Q}_{1}, \mathcal{Y}_{1}) + (1 - 2\varkappa)\mathbf{g}(t_{k} + \frac{h}{2}, \mathcal{P}_{2}, \mathcal{Q}_{2}, \mathcal{Y}_{2}) \\ &\quad + \frac{\varkappa}{2}\mathbf{g}(t_{k} + \frac{2 - \varkappa}{2}h, \mathcal{P}_{3}, \mathcal{Q}_{3}, \mathcal{Y}_{3})], \end{aligned}$$

(7.7)
$$P_{k+1} = P_k + h[\varkappa \mathbf{f}(t_k + \frac{\varkappa}{2}h, \mathcal{P}_1, \mathcal{Q}_1, \mathcal{Y}_1) + (1 - 2\varkappa)\mathbf{f}(t_k + \frac{h}{2}, \mathcal{P}_2, \mathcal{Q}_2, \mathcal{Y}_2) + \varkappa \mathbf{f}(t_k + \frac{2 - \varkappa}{2}h, \mathcal{P}_3, \mathcal{Q}_3, \mathcal{Y}_3)],$$

$$Q_{k+1} = Q_k + h[\varkappa \mathbf{g}(t_k + \frac{\varkappa}{2}h, \mathcal{P}_1, \mathcal{Q}_1, \mathcal{Y}_1) + (1 - 2\varkappa)\mathbf{g}(t_k + \frac{h}{2}, \mathcal{P}_2, \mathcal{Q}_2, \mathcal{Y}_2) \\ + \varkappa \mathbf{g}(t_k + \frac{2 - \varkappa}{2}h, \mathcal{P}_3, \mathcal{Q}_3, \mathcal{Y}_3)], \\ Y_{k+1} = Y_k + \frac{1}{6}(\Phi_1 + 4\Phi_2 + \Phi_3),$$

where

$$\Phi_{1} = h^{1/2} \sum_{r=1}^{l} \delta_{r}(t_{k})(\xi_{rk} + 6\eta_{rk}) + h\Gamma(t_{k})Y_{k},$$

$$\Phi_{2} = h^{1/2} \sum_{r=1}^{l} \delta_{r}(t_{k} + \frac{h}{2})\xi_{rk} + h\Gamma(t_{k} + \frac{h}{2})(Y_{k} + \frac{1}{2}\Phi_{1}),$$

$$\Phi_{3} = h^{1/2} \sum_{r=1}^{l} \delta_{r}(t_{k+1})(\xi_{rk} - 6\eta_{rk}) + h\Gamma(t_{k+1})(Y_{k} - \Phi_{1} + 2\Phi_{2}),$$

 ξ_{rk} , η_{rk} are mutually independent random variables distributed by the laws (6.8), and the number \varkappa is equal to

$$\varkappa = rac{1}{3}(2+2^{1/3}+2^{-1/3}).$$

This method is based on the well-known deterministic symplectic method of order 4 [21] and it is not difficult to check that (7.6)-(7.7) is symplectic. We prove that this weak method is of order 3 using the standard arguments [12, 13] (of course, the corresponding calculations require much routine work).

Theorem 7.3. The implicit method (7.6) - (7.7) for the system (7.1), (7.2) is symplectic and of the third weak order.

Remark 7.2. A Taylor type weak method of order 3 for a general system with colored noise was proposed in [13] and an explicit Runge-Kutta weak method of order 3 for such a system was constructed in [14]. These methods are not symplectic in application to the Hamiltonian system (7.1), (7.2).

7.4. Explicit methods in the case of second-order differential equations with colored noise. Here we consider the important particular case of the system with colored noise (7.1), (7.2):

(7.8)
$$dP = f(t,Q)dt + \sum_{r=1}^{m} \sigma_r(t,Q)Y^r dt, \ P(t_0) = p,$$
$$dQ = M^{-1}Pdt, \ Q(t_0) = q,$$
$$dY = \Gamma(t)Ydt + \sum_{r=1}^{l} \delta_r(t)dw_r(t), \ Y(t_0) = y,$$

with

(

(7.9)
$$f^{i} = -\partial H_{0}/\partial q^{i}, \quad \sigma^{i}_{r} = -\partial H_{r}/\partial q^{i}, \quad i = 1, \dots, n$$

and M is a constant positive definite matrix. This system can be written as a secondorder differential equation with colored noise. Some physical applications of such systems are discussed in [23]. Since in this case we have the system with separable Hamiltonians, we can construct both *implicit* and *explicit* symplectic methods.

The method (7.3) with $\alpha = 1$ applied to (7.8)-(7.9) gives us the explicit symplectic method of weak order 1 for the system (7.8)-(7.9).

7.4.1. Second-order method. Introduce the explicit PRK method for the system (7.8)-(7.9) (cf. (5.15)):

(7.10)
$$\mathcal{Y} = Y_k + \frac{h}{2}\Gamma(t_k)Y_k + \frac{h^{1/2}}{2}\sum_{r=1}^l \delta_r(t_k)\xi_{rk},$$

$$\mathcal{Q}_1=Q_k+rac{h}{2}M^{-1}P_k, \ \ \mathcal{P}_1=P_k+hf(t_k+rac{h}{2},\mathcal{Q}_1)+h\sum_{r=1}^m\sigma_r(t_k+rac{h}{2},\mathcal{Q}_1)\mathcal{Y}^r,$$

7.12)
$$P_{k+1} = \mathcal{P}_1, \quad Q_{k+1} = \mathcal{Q}_1 + \frac{h}{2}M^{-1}\mathcal{P}_1,$$
$$Y_{k+1} = Y_k + h\Gamma(t_k + h/2)\mathcal{Y} + h^{1/2}\sum_{r=1}^l \delta_r(t_k + h/2)\xi_{rk},$$

where ξ_{rk} are i.i.d. random variables with the law (5.16).

It is not difficult to prove the following theorem (cf. Theorem 5.3).

Theorem 7.4. The explicit method (7.10)-(7.12) for the system (7.8)-(7.9) is symplectic and of the second weak order.

7.4.2. Third-order method. Introduce the notation

$$\mathbf{f}(t,q,y):=f(t,q)+\sum_{r=1}^m\sigma_r(t,q)y^r.$$

On the basis of deterministic third-order RKN method [21, 4] (cf. (6.6)-(6.7)), we propose the explicit method for (7.8)-(7.9):

(7.13)
$$\Phi_{1} = h^{1/2} \sum_{r=1}^{l} \delta_{r}(t_{k})(\xi_{rk} + 6\eta_{rk}) + h\Gamma(t_{k})Y_{k},$$
$$\Phi_{2} = h^{1/2} \sum_{r=1}^{l} \delta_{r}(t_{k} + \frac{h}{2})\xi_{rk} + h\Gamma(t_{k} + \frac{h}{2})(Y_{k} + \frac{1}{2}\Phi_{1}),$$
$$\Phi_{3} = h^{1/2} \sum_{r=1}^{l} \delta_{r}(t_{k+1})(\xi_{rk} - 6\eta_{rk}) + h\Gamma(t_{k+1})(Y_{k} - \Phi_{1} + 2\Phi_{2}),$$
$$Q_{1} = Q_{k} + \frac{7}{24}hM^{-1}P_{k}, \quad \mathcal{P}_{1} = P_{k} + \frac{2}{3}h\mathbf{f}(t_{k} + \frac{7h}{24}, Q_{1}, Y_{k} + \frac{1}{3}\Phi_{1}),$$
$$Q_{2} = Q_{1} + \frac{3}{4}hM^{-1}\mathcal{P}_{1}, \quad \mathcal{P}_{2} = \mathcal{P}_{1} - \frac{2}{3}h\mathbf{f}(t_{k} + \frac{25h}{24}, Q_{2}, Y_{k} + \frac{5}{6}\Phi_{1} - \frac{1}{2}\Phi_{2}),$$

(7.14)
$$Q_{k+1} = Q_2 - \frac{1}{24}hM^{-1}\mathcal{P}_2, \quad P_{k+1} = \mathcal{P}_2 + h\mathbf{f}(t_k + h, \mathcal{Q}_{k+1}, Y_k + \frac{1}{2}\Phi_1),$$
$$Y_{k+1} = Y_k + \frac{1}{6}(\Phi_1 + 4\Phi_2 + \Phi_3), \quad k = 0, \dots, N-1,$$

where ξ_{rk} , η_{rk} are mutually independent random variables distributed by the laws (6.8). It is not difficult to check that this method is symplectic. Further, we prove that this weak method is of order 3 using the standard arguments [12, 13] (of course, the corresponding calculations require much routine work).

Theorem 7.5. The explicit method (7.13)-(7.14) for the system (7.8)-(7.9) is symplectic and of the third weak order.

8. WEAK METHODS FOR LANGEVIN TYPE EQUATIONS

Symplectic methods in the weak sense proposed in Section 5-7 together with the ideas of Sections 3-4 allow us to derive efficient weak methods for Langevin type equations.

8.1. Langevin equation: linear damping and additive noise. In this subsection we propose weak methods for the Langevin equation (3.1), which satisfy the requirements RL1-RL2 from Section 3.

Using splitting ideas presented in Section 3, we obtain the first-order method.

Theorem 8.1. Let \bar{P}_I , \bar{Q}_I be a one-step approximation corresponding to a symplectic method of first weak order for the system (3.5), (3.2). Then \bar{P} , \bar{Q} defined in (3.7) or in (3.16) is a one-step approximation of the method of first weak order for the system (3.1) which satisfies the requirements RL1-RL2.

As for \bar{P}_I , \bar{Q}_I appearing in the above theorem, one can take the approximation corresponding to the symplectic implicit method (5.1) or to the explicit one (5.11)-(5.12).

Remark 8.1. The implicit method (5.1) can directly be applied to the Langevin equation (3.1). Of course, it satisfies the requirement RL1. The method (5.1) satisfies the requirement RL2 for $\alpha = 0$ and $\alpha = 1$ only (see also the discussion in the end of Section 3.1).

Now we construct a method of weak order 2. To this end, consider the following approximation for (3.1) (cf. (3.19))

(8.1)
$$\bar{P} = \bar{P}(t_0 + h; t_0, p, q) := P_{II}(\frac{h}{2}; \bar{P}_I(t_0 + h; t_0, P_{II}(\frac{h}{2}; p), q)),$$

 $\bar{Q} = \bar{Q}(t_0 + h; t_0, p, q) := \bar{Q}_I(t_0 + h; t_0, P_{II}(\frac{h}{2}; p), q),$

where \bar{P}_I , \bar{Q}_I is a one-step approximation corresponding to any symplectic weak secondorder method for (3.5), (3.2) (for instance, one can use the implicit method (6.2) or the explicit method (5.15)), and $P_{II}(t)$ is the exact solution of (3.6).

Theorem 8.2. Let \bar{P}_I , \bar{Q}_I be a one-step approximation corresponding to a symplectic method of second weak order for the system (3.5), (3.2). Then \bar{P} , \bar{Q} defined in (8.1) is a one-step approximation of the method of second weak order for the system (3.1) which satisfies the requirements RL1-RL2.

Note that Remark 3.2 is applicable for both first and second order methods.

To get a method of weak order 3 for (3.1), we modify the symplectic RKN method (6.6)-(6.7) as we did in Section 3.3 in the case of mean-square methods. On this way we obtain the following method

(8.3)
$$P_{k+1} = \mathcal{P}_3 + h^{1/2} \sum_{r=1}^m \sigma_r \xi_{rk} - \nu h^{3/2} \sum_{r=1}^m \Gamma \sigma_r \cdot (\xi_r/2 + \eta_r)_k$$

$$+h^{5/2}\sum_{r=1}^{m}\left[\sum_{i=1}^{n}(M^{-1}\sigma_{r})^{i}\frac{\partial f}{\partial q^{i}}(\mathcal{Q}_{3})+\nu^{2}\Gamma^{2}\sigma_{r}\right]\xi_{rk}/6,$$

$$Q_{k+1} = \mathcal{Q}_3 + h^{3/2} \sum_{r=1}^m M^{-1} \sigma_r \cdot (\xi_r/2 + \eta_r)_k - \nu h^{5/2} \sum_{r=1}^m M^{-1} \Gamma \sigma_r \xi_{rk}/6, \quad k = 0, \dots, N-1,$$

where ξ_{rk} , η_{rk} are mutually independent random variables distributed by the laws (6.8).

The weak order of this method can be proved by standard arguments [12] and its phase-volume contractivity properties are proved by the same arguments as those before Theorem 3.3.

Theorem 8.3. The method (8.2)-(8.3) for the system (3.1) has third weak order and satisfies the requirements RL1-RL2.

Remark 8.2. The methods given in this subsection can be carried over to nonautonomous Langevin equations. It is also possible to apply the presented approach to Langevin equations with colored noise using symplectic methods from Section 7.

8.2. Langevin type equation: nonlinear damping and multiplicative noise. In this subsection we propose weak methods for the Langevin type equation (4.1) which satisfy the requirements RLT1-RLT2 from Section 4. As for first-order methods, we have the theorem.

Theorem 8.4. Let \bar{P}_I , \bar{Q}_I be a one-step approximation corresponding to a symplectic method of first weak order for the system (4.3), (4.2), and \bar{P}_{II} be a one-step approximation corresponding to a first-order deterministic method for the system (4.4). Then \bar{P} , \bar{Q} defined in (4.5) or (4.7) is a one-step approximation of the method of first weak order for the system (4.1) which satisfies the requirements RLT1-RLT2.

Remark 4.1 is applicable here. A concrete method based on \overline{P} , \overline{Q} from the above theorem can be written using the implicit symplectic method (5.1) or the explicit one (5.11)-(5.12) for \overline{P}_I , \overline{Q}_I . Further, as in the case of mean-square methods, the proposed approach can be generalized to a more general system of the form (4.8) (see the comment in the end of Section 4.1).

By the method of fractional steps (as in Sections 3.2 and 4.2) we construct the second order weak method for (4.1) on the basis of the symplectic method (5.15). The method has the form

$$(8.4)\mathcal{P}_{1} = \bar{P}_{II}(t_{k} + \frac{h}{2}; t_{k}, P_{k}, Q_{k}), \ \mathcal{Q}_{1} = Q_{k} + \frac{h}{2}g(\mathcal{P}_{1}),$$

$$\mathcal{P}_{2} = \mathcal{P}_{1} + hf(t_{k} + \frac{h}{2}, Q_{1}) + h^{1/2}\sum_{r=1}^{m}\sigma_{r}(t_{k} + \frac{h}{2}, Q_{1})\xi_{rk}, \ \mathcal{Q}_{2} = \mathcal{Q}_{1} + \frac{h}{2}g(\mathcal{P}_{1}),$$

$$P_{k+1} = \bar{P}_{II}(t_{k} + \frac{h}{2}; t_{k}, \mathcal{P}_{2}, Q_{2}) - \frac{h^{2}}{4}\nu\frac{\partial f_{\nu}}{\partial t}(t_{k}, P_{k}, Q_{k}), \ Q_{k+1} = \mathcal{Q}_{2}, \ k = 0, \dots, N-1,$$

where ξ_{rk} are i.i.d. random variables with the law (5.16) and \bar{P}_{II} is a one-step approximation of any second-order deterministic method for system (4.4).

Using a specific approximation instead of \bar{P}_{II} , it is possible to modify the method (8.4) in such a way that it will become a derivative-free method (i.e., the correction with the derivative $\partial f_{\nu}/\partial t$ can be incorporated in \bar{P}_{II}) but we do not consider this here.

The following theorem holds for the method (8.4).

Theorem 8.5. The method (8.4) has the second weak order and satisfies the requirements RLT1-RLT2.

A remark analogous to Remark 4.1 is valid here. We also note that for $f_{\nu}(t, p, q) = \Gamma(q)p$, $\Gamma - m \times m$ dimensional matrix, $P_{II}(t)$ can be found explicitly. Consequently, we can put P_{II} instead of \bar{P}_{II} in (8.4) (see also the discussion after Remark 4.3).

9. NUMERICAL TESTS

9.1. Kubo oscillator. The system of SDEs in the sense of Stratonovich (Kubo oscillator [8])

(9.1)
$$dX^{1} = -aX^{2}dt - \sigma X^{2} \circ dw(t), \quad X^{1}(0) = x^{1},$$
$$dX^{2} = aX^{1}dt + \sigma X^{1} \circ dw(t), \quad X^{2}(0) = x^{2},$$

is often used for testing numerical methods (see, e.g., [32, 18]). Here a and σ are constants and w(t) is a one-dimensional standard Wiener process.

The phase flow of this system preserves symplectic structure. Moreover, the quantity $\mathcal{H}(x^1, x^2) = (x^1)^2 + (x^2)^2$ is conservative for this system, i.e.

$$\mathcal{H}(X^1(t), X^2(t)) = \mathcal{H}(x^1, x^2) \text{ for } t \ge 0.$$

Here we test three specific methods of weak order 1. The weak Euler method in application to (9.1) takes the form:

(9.2)
$$X_{k+1}^{1} = X_{k}^{1} - haX_{k}^{2} - h\frac{\sigma^{2}}{2}X_{k}^{1} - h^{1/2}\sigma X_{k}^{2}\xi_{k},$$
$$X_{k+1}^{2} = X_{k}^{2} + haX_{k}^{1} - h\frac{\sigma^{2}}{2}X_{k}^{2} + h^{1/2}\sigma X_{k}^{1}\xi_{k},$$

where ξ_k are i.i.d random variables with the law (5.2). This method is, of course, not symplectic.

The weak midpoint method (the symplectic method (5.1) with $\alpha = 1/2$) is written for the autonomous system (9.1) as

(9.3)
$$X_{k+1}^{1} = X_{k}^{1} - ha \frac{X_{k}^{2} + X_{k+1}^{2}}{2} - h^{1/2} \sigma \frac{X_{k}^{2} + X_{k+1}^{2}}{2} \xi_{k},$$
$$X_{k+1}^{2} = X_{k}^{2} + ha \frac{X_{k}^{1} + X_{k+1}^{1}}{2} + h^{1/2} \sigma \frac{X_{k}^{1} + X_{k+1}^{1}}{2} \xi_{k}.$$

This is an implicit method in both deterministic and stochastic terms.



FIGURE 1. The Kubo oscillator (9.1). Behavior of $E\mathcal{H}(X_k^1(t), X_k^2(t))$ with $X^1(0) = 1$, $X^2(0) = 0$, a = 1, $\sigma = 1$, h = 0.05 on the time interval $t \leq 200$ in the case of the Euler method (9.2) (left, computed due to (9.5)), symplectic method (9.4) (dashed line on the right, computed by the Monte Carlo technique, the Monte Carlo error is not greater than 0.0035 with probability 0.95), and the midpoint method (9.3) (solid line on the right, coincides with the exact value).

When applied to (9.1), the PRK method (5.7) has the form:

(9.4)
$$X_{k+1}^{1} = X_{k}^{1} - haX_{k}^{2} - h\frac{\sigma^{2}}{2}X_{k+1}^{1} - h^{1/2}\sigma X_{k}^{2}\xi_{k},$$
$$X_{k+1}^{2} = X_{k}^{2} + haX_{k+1}^{1} + h\frac{\sigma^{2}}{2}X_{k}^{2} + h^{1/2}\sigma X_{k+1}^{1}\xi_{k}.$$

This method is symplectic and of the first weak order. It is implicit in the deterministic part only.

Let us analyze how accurately these methods approximate $E\mathcal{H}(X^1(t), X^2(t))$. In the case of the Euler method we obtain

$$(9.5) \quad E\mathcal{H}(X_k^1, X_k^2) = (1 + h^2(a^2 + \frac{\sigma^4}{4}))^k \cdot \mathcal{H}(x^1, x^2) \ge \exp(\frac{1}{2}(a^2 + \frac{\sigma^4}{4})ht_k) \cdot \mathcal{H}(x^1, x^2),$$

i.e., the quantity grows exponentially fast as t increases.

It is not difficult to check that $\mathcal{H}(x^1, x^2)$ is conserved by the midpoint method (9.3). But the PRK method (9.4) does not preserve the quantity $\mathcal{H}(x^1, x^2)$. This is similar to the deterministic case. Indeed, it is known [21] that symplectic deterministic RK methods (e.g., the implicit midpoint rule) conserve all quadratic functions that are conserved by the Hamiltonian system being integrated, while symplectic deterministic PRK methods do not possess this property (see also a similar discussion concerning the mean-square midpoint method in [18]).

Figure 1 illustrates behavior of $E\mathcal{H}(X_k^1(t), X_k^2(t))$ in the case of the first order methods (9.2), (9.3), and (9.4).



FIGURE 2. The Kubo oscillator (9.1). Simulation of $EX^{1}(t)$ with $X^{1}(0) = 1$, $X^{2}(0) = 0$, a = 1, $\sigma = 0.2$, h = 0.05 on the time interval $t \leq 60$. The results obtained by the Euler method (9.2) – dashed line. The results obtained by the midpoint method (9.3) and the symplectic method (9.4) visually coincide with the exact solution (9.6) (solid line). The Monte Carlo error is not greater than 0.03 with probability 0.95.

Further, it is not difficult to find the following exact expressions for the Kubo oscillator (9.1):

(9.6)
$$EX_{0,x}^{1}(t) = e^{-\sigma^{2}t/2}(x^{1}\cos at - x^{2}\sin at),$$
$$EX_{0,x}^{2}(t) = e^{-\sigma^{2}t/2}(x^{2}\cos at + x^{1}\sin at).$$

Figure 2 gives results of Monte Carlo simulation of $EX_{0,x}^1(t)$ by the methods (9.2), (9.3), and (9.4). We see that the Euler method is not appropriate for simulation of the oscillator (9.1) on long time intervals while the symplectic methods produce quite accurate results. The Kubo oscillator is also considered with colored noise (see e.g. [13] and references therein). Symplectic methods from Section 7 can be used for simulation of the Kubo oscillator with colored noise.

9.2. A model for synchrotron oscillations of particles in storage rings. In [23] 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

$$(9.7) dP = -\omega^2 \sin(Q) dt - \sigma_1 \cos(Q) dw_1 - \sigma_2 \sin(Q) dw_2,$$

dQ = Pdt.

P and Q are scalars here. The system (9.7) is of the form (5.9) and therefore its phase flow preserves symplectic structure.

Let us mention that a certain weak numerical method for the system (5.9) with $g(p) = M^{-1}p$ was proposed in [23]. In the absence of noise this method coincides with a deterministic symplectic method but in the stochastic case the method of [23] is not symplectic (also see similar methods in [32]). 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 (5.11)-(5.12)) and two second-order methods (a standard second-order weak method [12, 7] and the symplectic method (5.15)).

The weak Euler method for (9.7) takes the form

(9.8)
$$P_{k+1} = P_k - h\omega^2 \sin(Q_k) - h^{1/2} (\sigma_1 \cos(Q_k) \xi_{1k} + \sigma_2 \sin(Q_k) \xi_{2k}),$$
$$Q_{k+1} = Q_k + hP_k,$$

where ξ_{1k} , ξ_{2k} are i.i.d random variables with the law (5.2).

In application to (9.7) the first-order symplectic method (5.11)-(5.12) with $\alpha = 1$ is written as

(9.9)
$$\mathcal{Q} = Q_k + hP_k,$$
$$P_{k+1} = P_k - h\omega^2 \sin(\mathcal{Q}) - h^{1/2} (\sigma_1 \cos(\mathcal{Q})\xi_{1k} + \sigma_2 \sin(\mathcal{Q})\xi_{2k}), \quad Q_{k+1} = \mathcal{Q},$$

where ξ_{1k} , ξ_{2k} are i.i.d random variables with the law (5.2). The standard second-order method from [12, 7] applied to (9.7) has the form

$$(9.10) P_{k+1} = P_k - h^{1/2} (\sigma_1 \cos(Q_k)\xi_{1k} + \sigma_2 \sin(Q_k)\xi_{2k}) - h\omega^2 \sin(Q_k) + \frac{h^{3/2}}{2} (\sigma_1 \sin(Q_k)\xi_{1k} - \sigma_2 \cos(Q_k)\xi_{2k}) P_k - \frac{h^2}{2} \omega^2 \cos(Q_k) P_k, Q_{k+1} = Q_k + hP_k - \frac{h^{3/2}}{2} (\sigma_1 \cos(Q_k)\xi_{1k} + \sigma_2 \sin(Q_k)\xi_{2k}) - \frac{h^2}{2} \omega^2 \sin(Q_k),$$

where ξ_{1k} , ξ_{2k} are i.i.d. random variables with the law (5.16).

The second-order symplectic method (5.15) is written for the system (9.7) as

(9.11)
$$Q_1 = Q_k + \frac{h}{2}P_k, \quad \mathcal{P}_1 = P_k - h\omega^2 \sin(Q_1) - h^{1/2}(\sigma_1 \cos(Q_1)\xi_{1k} + \sigma_2 \sin(Q_1)\xi_{2k}),$$

 $P_{k+1} = \mathcal{P}_1, \quad Q_{k+1} = \mathcal{Q}_1 + \frac{h}{2}\mathcal{P}_1,$

where ξ_{1k} , ξ_{2k} are i.i.d. random variables with the law (5.16). Consider the quantity

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



FIGURE 3. The model (9.7). Simulation of $E\mathcal{E}(P(t), Q(t))$ with P(0) = 1, Q(0) = 0, $\omega = 2$, $\sigma_1 = \sigma_2 = 0.5$, h = 0.05 on the time interval $t \leq 200$: the Euler method (9.8) - dashed line; the results obtained by the symplectic method (9.9) visually coincide with the exact solution (9.12) (solid line). The Monte Carlo error is not greater than 0.43 for (9.8) and 0.2 for (9.9) with probability 0.95.

TABLE 1. The model (9.7). Simulation of $E\mathcal{E}(P(t), Q(t))$ with P(0) = 1, Q(0) = 0, $\omega = 4$, $\sigma_1 = \sigma_2 = 0.3$, t = 200 for various time steps h by the Euler method (9.8), the first-order symplectic method (9.9), the standard second-order method (9.10), and the second-order symplectic method (9.11). The exact solution is -6.5. M is a number of independent realizations in the Monte Carlo simulation. Note that the " \pm " reflects the Monte Carlo error only (cf. (9.13)), it does not reflect the error of a method.

h	M	(9.8)	(9.9)	(9.10)	(9.11)
0.1	10^{5}	493.3 ± 0.3	-6.268 ± 0.059	462.2 ± 0.6	-6.316 ± 0.059
0.05	10^{5}	966.1 ± 0.7	-6.397 ± 0.059	0.896 ± 0.094	-6.421 ± 0.058
0.01	$4 \cdot 10^{6}$	234.5 ± 0.06	-6.503 ± 0.009	-6.456 ± 0.009	-6.502 ± 0.009

Its mean value $E\mathcal{E}(P(t), Q(t))$ is treated in physical literature (see e.g. [23] and references therein) as a mean energy of the system. Under the assumption $\sigma_1 = \sigma_2 = \sigma$ one can obtain that

(9.12)
$$E\mathcal{E}(P_{0,p,q}(t),Q_{0,p,q}(t)) = \mathcal{E}(p,q) + \frac{\sigma^2}{2}t.$$

Figure 3 illustrates Monte Carlo simulation of $E\mathcal{E}(P(t), Q(t))$ by the first order methods (9.8) and (9.9). 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

(9.13)
$$E\mathcal{E}(\bar{P}(t),\bar{Q}(t)) \doteq \frac{1}{M} \sum_{m=1}^{M} \mathcal{E}(\bar{P}^{(m)}(t),\bar{Q}^{(m)}(t)) \pm 2\sqrt{\frac{\bar{D}_{M}}{M}},$$

where

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

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 "± " reflects the Monte Carlo error only, it does not reflect the error of a method.

The above experiments with the model (9.7) demonstrate once again superiority of symplectic methods in comparison with nonsymplectic ones. In [23] the system (9.7) is also considered with colored noise. In this case symplectic methods from Section 7.4 can be exploited. We note that the authors of [23] are interested in systems with small noise. Effective symplectic methods in the weak sense for Hamiltonian systems with small noise can be obtained attracting ideas from [16] (see also [17, 18] where mean-square symplectic methods for Hamiltonian systems with small noise were obtained).

9.3. Linear oscillator with linear damping under external random excitation. Let us consider the linear oscillator with linear damping term and additive noise

$$(9.14) dX^1 = \omega X^2 dt$$

$$dX^2 = (-\omega X^1 - \nu X^2)dt + rac{\sigma}{\omega}dw(t),$$

where W(t) is a standard Wiener process, ω , ν , σ are positive constants. The system (9.14) is dissipative, its invariant measure μ is gaussian $\mathcal{N}(0, R)$ with the density

(9.15)
$$\rho(x) = (2\pi)^{-1} (\det R)^{-1/2} \exp\{-\frac{1}{2}(R^{-1}x, x)\},\$$

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 unity matrix.

The discretized system by the explicit Euler scheme is

(9.16)
$$\bar{X}_{k+1}^1 = \bar{X}_k^1 + \omega \bar{X}_k^2 h$$

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

The eigenvalues of the homogeneous part of (9.16) are

(9.17)
$$\lambda_{1,2} = 1 - \frac{\nu h}{2} \pm h \sqrt{\frac{\nu^2}{4} - \omega^2}.$$

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

$$(9.18) \qquad \qquad \frac{\nu}{2} < \omega.$$

If (9.18) is fulfilled, then $|\lambda_{1,2}|^2 = 1 - \nu h + \omega^2 h^2$, and consequently (9.16) is asymptotically stable if and only if

$$(9.19) h < \frac{\nu}{\omega^2}$$

In this case, the system (9.16) 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

$$R_h = rac{\sigma^2}{\omega^2 \varkappa} \left[egin{array}{cc} 1 -
u h/2 + \omega^2 h^2/2 & -\omega h/2 \ -\omega h/2 & 1 \end{array}
ight],$$

where

$$arkappa := 2
u - 2\omega^2 h -
u^2 h + rac{3
u\omega^2 h^2}{2} - rac{\omega^4 h^3}{2}$$

Due to (9.18) and (9.19), it is possible to prove that $\varkappa > 0$. The elements of R_h can be represented as

$$R_{h}^{jj} = \frac{\sigma^{2}}{2\nu\omega^{2}} \left(1 + \frac{\omega^{2}h}{\nu} + O(h\nu) + O(\frac{h^{2}}{\nu^{2}})\right), \ j = 1, 2,$$
$$R_{h}^{ij} = \frac{\sigma^{2}}{2\nu\omega^{2}} \left(-\frac{\omega h}{2} - \frac{\omega^{3}h^{2}}{2\nu} + O(h^{2}\nu) + O(\frac{h^{3}}{\nu^{2}})\right), \ i \neq j,$$

where, for instance, $O(\frac{h^2}{\nu^2})$ satisfies the inequality $|O(\frac{h^2}{\nu^2})| \leq C\frac{h^2}{\nu^2}$ for all $\nu > 0$, h > 0 such that the ratio h/ν is sufficiently small, 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 (9.19) is not enough. Suppose our aim is to evaluate

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

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 (9.16). 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 (9.14):

(9.20)
$$\bar{X}_{k+1}^1 = \bar{X}_k^1 + \omega \bar{X}_{k+1}^2 h$$

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

The eigenvalues of the homogeneous part of (9.20) are

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

Under (9.18), the eigenvalues are again complex numbers and

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

Therefore, in contrast to the explicit Euler method, we need not 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 up evaluations show that such an illusion is very dangerous. Indeed, the system (9.20) 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

$$\begin{aligned} R_h^{jj} &= \frac{\sigma^2}{2\nu\omega^2} \left(1 - \frac{\omega^2 h}{\nu} + O(h\nu) + O(\frac{h^2}{\nu^2})\right), \ j = 1, 2, \\ R_h^{ij} &= \frac{\sigma^2}{2\nu\omega^2} \left(\frac{\omega h}{2} - \frac{\omega^3 h^2}{2\nu} + O(h^2) + O(\frac{h^3}{\nu^2})\right), \ i \neq j, \end{aligned}$$

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 (3.7) with \bar{P}_I , \bar{Q}_I from (3.12) with $\alpha = 0$. For simplicity we take $\bar{P}_{II} = p - h\nu p$ instead of the exact P_{II} (see Remark 3.2). As a result, we get

(9.21)
$$\bar{X}_{k+1}^{1} = \bar{X}_{k}^{1} + \omega h (\bar{X}_{k}^{2} - \omega h \bar{X}_{k}^{1})$$
$$\bar{X}_{k+1}^{2} = (\bar{X}_{k}^{2} - \omega h \bar{X}_{k}^{1} + \frac{\sigma}{\omega} \Delta_{k} w) (1 - \nu h)$$

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 (9.21) 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

$$\begin{aligned} R_h^{11} &= \frac{\sigma^2}{2\nu\omega^2} (1 - 2\nu h + O(h^2)), \\ R_h^{22} &= \frac{\sigma^2}{2\nu\omega^2} (1 - \frac{3}{2}\nu h + O(h^2)), \\ R_h^{ij} &= \frac{\sigma^2}{2\nu\omega^2} (\frac{\omega h}{2} - \frac{5}{4}\omega\nu h^2 + O(h^3)), \ i \neq j. \end{aligned}$$



FIGURE 4. The linear oscillator with linear damping (9.14). Behavior of $E(X^1(T))^2$ with $X^1(0) = 0$, $X^2(0) = 0$, $\omega = 3$, $\nu = 0.1$, $\sigma = 1$, h = 0.1 (left) and h = 0.01 (right) on the time interval $t \leq 100$ in the case of the weak implicit Euler method (dashed line) and the weak quasi-symplectic method (solid line, which visually coincides with the exact dependence $E(X^1(T))^2$). The Monte Carlo error is not greater than 0.00005 (left) and 0.0003 (right) for the Euler method and 0.0005 for the quasi-symplectic method with probability 0.95.

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 step to reach a sufficient accuracy, in particular, if ν is small. At the same time, the quasi-symplectic method (9.21) gives very good results for highly 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.

As an example, we evaluate $E(X^1(T))^2$ for a large T by weak analogues of the implicit Euler method (9.20) and the quasi-symplectic method (9.21) (i.e., we replace $\Delta_k w$ in this methods by $h^{1/2}\xi_k$, ξ_k are i.i.d. random variables with the law (5.2)). Notice that the moments $E(X^i(t)X^j(t))$, i, j = 1, 2, satisfy a system of linear differential equations and $E(X^1(T))^2$ can be found exactly. The results of simulation are presented on Figure 4. We see that even for the small step h = 0.01 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 = 0.1. The explicit Euler method is unstable for h = 0.1 (see (9.19)).

9.4. An oscillator with cubic restoring force under external random excitation. Consider the oscillator with cubic restoring force and additive noise

$$(9.22) \qquad \qquad \ddot{Q} = Q - Q^3 - \nu \dot{Q} + \sigma \dot{w} \; .$$

Another form of this Langevin two-dimensional equation is (3.14) (see also (3.1) with $U_0(q) = \frac{1}{4}q^4 - \frac{1}{2}q^2$). The dynamical system (9.22) is ergodic (see, e.g. [11]) and its



FIGURE 5. The oscillator with cubic restoring force (9.22). Behavior of $E(Q(T))^2$ with P(0) = 0, Q(0) = 0, $\nu = 0.05$, $\sigma = 1$, h = 0.1 (left) and h = 0.01 (right) on the time interval $t \leq 120$ in the case of the weak implicit Euler method (9.25) (dashed line) and the weak quasi-symplectic method (9.24) (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 $\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} q^2 \rho(p, q) dp dq$ with the invariant measure $\rho(p, q)$ from (9.23). This value is equal to 2.435.

invariant measure has the density

(9.23)
$$\rho(p,q) = C \exp(-\frac{\nu}{\sigma^2}(p^2 + \frac{1}{2}q^4 - q^2))$$

where C is defined by the normalization condition.

Here we compare a quasi-symplectic method and the implicit Euler scheme. We use the quasi-symplectic method based on the one-step approximation (3.7) and on the weak symplectic method (5.11)-(5.12) with $\alpha = 0$. For simplicity we take $\bar{P}_{II} = p - h\nu p$ instead of the exact P_{II} (see Remark 3.2). As a result, we get for (9.22):

(9.24)
$$P_{k+1} = (1 - \nu h) \left(P_k + h \left(Q_k - Q_k^3 \right) + h^{1/2} \sigma \xi_k \right)$$
$$Q_{k+1} = Q_k + h \left(P_k + h \left(Q_k - Q_k^3 \right) \right),$$

where ξ_k are i.i.d. random variables with the law (5.2).

In application to (9.22) the weak implicit Euler scheme has the form

(9.25)
$$P_{k+1} = P_k + h \left(Q_{k+1} - Q_{k+1}^3 - \nu P_{k+1} \right) + h^{1/2} \sigma \xi_k$$
$$Q_{k+1} = Q_k + h P_{k+1},$$

where ξ_k are i.i.d. random variables with the law (5.2).

Figure 5 gives results of evaluation of $E(Q(T))^2$ for a large T by these two methods. We see again that even for the small step h = 0.01 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 = 0.1.

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