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ACCURATE STATIONARY DENSITIES WITH PARTITIONED NUMERICAL METHODS FOR STOCHASTIC DIFFERENTIAL EQUATIONS*

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Abstract. We devise explicit partitioned numerical methods for second–order-in-time scalar stochastic differential equations, using one Gaussian random variable per timestep. The construction proceeds by analysis of the stationary density in the case of constant-coefficient linear equations, imposing exact stationary statistics in the position variable and absence of correlation between position and velocity; the remaining error is in the velocity variable. A new two-stage "reverse leapfrog" method has good properties in the position variable and is symplectic in the limit of zero damping. Explicit new "Runge–Kutta leapfrog" methods are constructed, sharing the property that $q_{n+1} = q_n + \frac{1}{2}(p_n + p_{n+1})\Delta t$, whose mean-square velocity order increases with the number of stages.

Key words. damped harmonic oscillators with noise, stationary distribution, stochastic Runge–Kutta methods, leapfrog methods

AMS subject classifications. 60-08, 65c30

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1. Introduction.

Long-term properties are the focus of much current research on numerical methods for differential equations that are second order in time. Separable Hamiltonian problems, for example, can be solved using explicit partitioned Runge–Kutta (PRK) methods that are symplectic [1], and the concept of symplectic structure can be extended to Hamiltonian dynamics, with a suitably-chosen noise term and the same stochastic realization for each trajectory [2]. In this work, however, we consider dynamics where an ensemble of different trajectories originates even from a single-point initial condition, corresponding to different realizations of the stochastic process. The most relevant long-term quantity is the stationary density [3, 4].

The stationary density of a numerical method differs from that of the continuous-time stochastic differential equation (SDE), assuming they both exist, by an amount that depends on the timestep Δt [5]. It can be studied by means of a modified action [6], reminiscent of modified equations used to understand finite-time convergence [7, 8]. Such techniques provide a procedure for devising numerical methods, as well as analyzing them, by matching terms in powers of Δt [9, 10, 11]. Here, by imposing conditions obtained from analysis of linear equations, we construct explicit PRK methods that approximate the stationary density with high-order accuracy.

The stationary densities of linear constant-coefficient SDEs have the simplicity of being Gaussian and, therefore, described by just the mean squares of the position and velocity variables, and the correlation between position and velocity, which is zero in the exact solution. Thus, as in the analysis of deterministic dynamics, linear

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constant-coefficient equations are a test bed for studies of stability and convergence. When comparing the (non-Gaussian) stationary densities that result from numerical methods applied to nonlinear equations with the exact stationary density, we shall use an integral quantity known as the Kullback–Leibler divergence, or relative entropy [12, 13].

Applied to linear equations, the simplest stochastic leapfrog method gives the exact stationary variance of the position variable and maintains the independence of position and velocity; the only error is in the variance of the velocity variable. Recently, Mannella introduced a modification of the stochastic leapfrog algorithm that reduces the mean-square velocity error [14, 15]. We show, by analysis of linear equations and numerical experiments on nonlinear equations, that this two-stage method is one of a family of s-stage explicit "Runge–Kutta leapfrog" methods whose accuracy approaches that of the implicit midpoint method as the number of stages is increased. The implicit midpoint method is the only Runge–Kutta method with a nonsingular tableau matrix that reproduces the exact stationary density, applied to linear SDEs with additive white noise, independent of the value of the damping [16, 17, 18]. In fact, all moments of the velocity are exactly integrated as $t \to \infty$, and there is no correlation between position and velocity for linear systems with additive noise in arbitrary dimensions [19, 9].

We shall consider second-order scalar SDEs of the following form:

$$\ddot{x} = f(x) - \eta\dot{x} + \epsilon\xi(t), \tag{1.1}$$

where $\xi(t)$ is a white noise process satisfying $\langle \xi(t)\xi(t') \rangle = \delta(t - t')$ and the damping parameter is denoted η. They describe the position of a particle in one dimension subject to deterministic forcing $f(x)$, related to the potential function $V(x)$ via $f(x) = -V'(x)$, and random forcing $\xi(t)$ whose amplitude ϵ is related to the temperature T and damping coefficient η by the fluctuation-dissipation relation $\epsilon^2 = 2\eta KT$. We can write (1.1) as a pair of first-order equations for $\mathbf{X}_t$ and $\mathbf{V}_t$, the position and velocity variables:

$$\begin{aligned} \mathrm{d}\mathbf{X}_t &= \mathbf{V}_t \mathrm{d}t, \\ \mathrm{d}\mathbf{V}_t &= -\eta \mathbf{V}_t \mathrm{d}t + f(\mathbf{X}_t)\mathrm{d}t + \epsilon \mathrm{d}\mathbf{W}_t, \end{aligned} \tag{1.2}$$

where $\mathbf{W}_t$ is a Wiener process satisfying $\langle \mathbf{W}_t \mathbf{W}_s \rangle = \min(t, s)$. Denote the probability density at time t by $\Pi(x, v; t)$:

$$\Pi(x, v; t) = \frac{\mathrm{d}}{\mathrm{d}x}\frac{\mathrm{d}}{\mathrm{d}v}\mathrm{Prob}\left(\mathbf{X}_t < x, \mathbf{V}_t < v\right). \tag{1.3}$$

The stationary density

$$\Pi_\infty(x, v) = \lim_{t\to\infty} \Pi(x, v; t) \tag{1.4}$$

has the analytical form: $\Pi_\infty(x, v) = N_0 \exp\left(-v^2/2KT - V(x)/KT\right)$, where the constant N_0 is determined by the condition $\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \Pi_\infty(x, v)\mathrm{d}x\mathrm{d}v = 1$. Thus the late-time statistics of the velocity are Gaussian and uncorrelated with the position.

Numerical methods produce approximate values for position q_n and for velocity p_n at discrete times $t_0, t_1, \ldots$, where $t_{n+1} - t_n = \Delta t$. We consider the evolution of q_n and p_n and compare their statistical properties as $t_n \to \infty$ with the exact form (1.4).

The exact density of the velocity variable is Gaussian, even when $f(x)$ is nonlinear, so that accuracy can be quantified in terms of σ_v^2 only. The position variable, however, requires further examination. In particular, we compare the density of q_n as $n \to \infty$ with the exact result

$$\rho(x) = \int_{-\infty}^{\infty} \Pi_\infty(x, v)\mathrm{d}v = \frac{\exp\left(-V(x)/KT\right)}{\int_{-\infty}^{\infty} \exp\left(-V(y)/KT\right)\mathrm{d}y}. \tag{1.5}$$

We have chosen to compare the late-time density of the position variable produced by the numerical method $\rho^*(x)$ with the exact density $\rho(x)$ (1.5), using the Kullback–Leibler divergence, or relative entropy [12]

$$D[\rho|\rho^*] = \int_{-\infty}^{\infty} \ln\left(\frac{\rho(x)}{\rho^*(x)}\right)\rho(x)\mathrm{d}x, \tag{1.6}$$

which integrates the log of the ratio $\frac{\rho(x)}{\rho^*(x)}$, weighted by $\rho(x)$ itself. It is zero if $\rho(x) = \rho^*(x)$ everywhere and positive otherwise.

In the remainder of this section, we outline the structure of PRK methods, extended to SDEs that are second order in time with damping and additive noise, and their implementation on a class of linear SDEs for which the stationary density is Gaussian. Certain matrix equalities are necessary in order for the stationary density of the discrete-time dynamical system defined by the numerical method to reproduce the exact stationary mean square of the position variable, the independence of position and velocity, and to approximate the stationary mean square of the velocity variable to high order in Δt. In section 2, we consider two-stage methods. In particular, we devise a new "reverse leapfrog" method. In section 3, we simplify the matrix conditions by introducing the concept of s-stage Runge–Kutta leapfrog methods, construct explicit methods, and perform numerical experiments to compare the performance of the methods, old and new, for both linear and nonlinear problems.

1.1. Partitioned Runge–Kutta methods. When solving (1.1) under a PRK method with s stages, q_{n+1} and p_{n+1} are obtained from q_n and p_n as a weighted sum of s evaluations of f at intermediate values Y_i:

$$\begin{aligned} p_{n+1} &= p_n + \sum_{j=1}^{s} b_j(-\eta Z_j + f(Y_j))\Delta t + \epsilon \Delta W_n, \\ q_{n+1} &= q_n + \sum_{j=1}^{s} \hat{b}_j Z_j \Delta t, \end{aligned} \tag{1.7}$$

where each ΔW_n is drawn independently from a Gaussian distribution with mean zero and variance Δt. The intermediate values satisfy

$$\begin{aligned} Z_i &= p_n + \sum_{j=1}^{s} a_{ij}(-\eta Z_j + f(Y_j))\Delta t + \epsilon c_i \Delta W_n, \\ Y_i &= q_n + \sum_{j=1}^{s} \hat{a}_{ij} Z_j \Delta t. \end{aligned} \tag{1.8}$$

Note that only one random variable is required per timestep. Let

$$k_1 = \eta \Delta t,$$

and define column vectors by $Z = (Z_1, Z_2, \ldots, Z_s)^{\mathrm{T}}$, $Y = (Y_1, Y_2, \ldots, Y_s)^{\mathrm{T}}$, and $f(Y) = (f(Y_1), f(Y_2), \ldots, f(Y_s))^{\mathrm{T}}$. Then we can write (1.8) as

$$\begin{aligned} Z &= (I + k_1 A)^{-1}(p_n e + \Delta t A f(Y) + \epsilon \Delta W_n c), \\ Y &= q_n e + \Delta t \hat{A} Z. \end{aligned} \tag{1.9}$$

We also use the notation $e = (1, 1, \ldots, 1)^{\mathrm{T}}$, $b = (b_1, b_2, \ldots, b_s)^{\mathrm{T}}$, $\hat{b} = (\hat{b}_1, \hat{b}_2, \ldots, \hat{b}_s)^{\mathrm{T}}$, $c = (c_1, c_2, \ldots, c_s)^{\mathrm{T}}$, and let A and $\hat{A}$ be the $s \times s$ matrices whose entries are the a_{ij} and $\hat{a}_{ij}$ in (1.8). We can represent PRK methods by pairs of Butcher tableaux:

$$\begin{array}{c|c} c & A \\ \hline & b^{\top} \end{array} \qquad \begin{array}{c|c} & \hat{A} \\ \hline & \hat{b}^{\top} \end{array}.$$

In this paper, we assume

$$b^{\mathrm{T}} e = 1, \qquad \hat{b}^{\mathrm{T}} e = 1, \qquad Ae = c, \tag{1.10}$$

and denote $\hat{c} = \hat{A}e$ [20]. In explicit methods, A and $\hat{A}$ are lower triangular and the matrix $\hat{A}(I + k_1 A)^{-1} A$ is strictly lower triangular. Let $B = \mathrm{diag}(b_1, \ldots, b_s)$ and [21, 22]

$$M = B\hat{A} + A^{\mathrm{T}} B - bb^{\mathrm{T}}. \tag{1.11}$$

In a deterministic setting, a PRK method is said to be symplectic [1] if $b = \hat{b}$ and all elements of M are zero.

1.2. Linear equations. If $f(x) = -gx$, then (1.4) is

$$P_\infty(x, v) = N \exp\left(-g\, x^2/2KT - v^2/2KT\right).$$

In other words, the stationary density is Gaussian and completely characterized by three quantities: The mean squares of the position and velocity variables and the (absence of) correlation between the position and velocity. We refer to this as the linear system. In the exact solution, these three quantities are $\lim_{t\to\infty} \langle \mathbf{X}_t{}^2 \rangle = \frac{1}{g} KT$, $\lim_{t\to\infty} \langle \mathbf{V}_t^2 \rangle = KT$, and $\lim_{t\to\infty} \langle \mathbf{X}_t \mathbf{V}_t \rangle = 0$. The linear system is actually a class of SDEs parametrized by the damping η. The exact stationary density is independent of η, but the stationary density obtained from a numerical method will, in general, depend on η.

Let

$$k_2 = g\Delta t^2.$$

If a PRK method is applied to the linear system, then (1.9) simplifies to

$$\begin{aligned} Z &= P^{-1}\left(p_n e - g q_n c \Delta t + \epsilon c \Delta W_n\right), \\ Y &= q_n e + \hat{A} Z \Delta t, \end{aligned} \tag{1.12}$$

where

$$P = I + Ak_1 + A\hat{A}k_2. \tag{1.13}$$

Since the numerical evolution is linear, $P^*_\infty(x,v)$ is a Gaussian density. Let

$$\sigma_x^2 = \lim_{t_n\to\infty}\langle p_n^2\rangle, \qquad \sigma_v^2 = \lim_{t_n\to\infty}\langle q_n^2\rangle, \quad \mu = \lim_{t_n\to\infty}\langle q_n p_n\rangle, \quad \text{and} \qquad \Sigma = \begin{pmatrix}\sigma_x^2 & \mu\\ \mu & \sigma_v^2\end{pmatrix}.$$

We shall search for methods for which

$$\Sigma = KT\begin{pmatrix}1/g & 0\\ 0 & \alpha(k_1,k_2)\end{pmatrix}. \tag{1.14}$$

That is, the mean square of the position variable is exact, and there is no correlation between position and velocity variables. (This severely restricts the allowed choices of A, $\hat{A}$, b, and $\hat{b}$.) The mean square of the velocity variable is the function $\alpha(k_1,k_2)$ of the dimensionless combinations $k_1 = \eta\Delta t$ and $k_2 = g\Delta t^2$; for clarity in what follows, we shall omit these arguments. In the exact solution $\alpha = 1$, so the departure from unity is the the error in the mean-square velocity.

We will say that a PRK method has mean-square velocity order p if $\alpha = 1 + C\Delta t^p$, where C is independent of Δt. The advantage of this approach is that, while the stationary mean-square velocity is not exact, the error can be made arbitrarily small, and furthermore, the implementation is explicit, unlike the implicit midpoint method. Hence, issues associated with solving a nonlinear system at each step are avoided. Explicit Runge–Kutta leapfrog methods are efficient in terms of computer memory use because only the most recent intermediate velocity value need be retained.

A Runge–Kutta method for the linear stochastic system can be written as

$$\begin{pmatrix}q_{n+1}\\ p_{n+1}\end{pmatrix} = R(\Delta t)\begin{pmatrix}q_n\\ p_n\end{pmatrix} + \epsilon r\Delta W \tag{1.15}$$

for some

$$R(\Delta t) = \begin{pmatrix}r_{11} & r_{12}\\ r_{21} & r_{22}\end{pmatrix} \qquad \text{and} \qquad r = \begin{pmatrix}r_1\\ r_2\end{pmatrix}.$$

Comparing (1.12) with (1.15), we find

$$\begin{aligned} r_{11} &= 1 - \hat{b}^{\mathrm{T}}P^{-1}ck_2,\\ r_{12} &= \hat{b}^{\mathrm{T}}P^{-1}e\Delta t,\\ r_{21} &= -g\left(1 - b^{\mathrm{T}}P^{-1}ck_1 - b^{\mathrm{T}}\hat{A}P^{-1}ck_2\right)\Delta t,\\ r_{22} &= 1 - b^{\mathrm{T}}P^{-1}ek_1 - b^{\mathrm{T}}\hat{A}P^{-1}ek_2, \end{aligned} \tag{1.16}$$

$$r_1 = -\frac{1}{g\Delta t}(r_{11}-1), \qquad \text{and} \qquad r_2 = -\frac{1}{g\Delta t}r_{21}. \tag{1.17}$$

The condition (1.14) can be written using the notation of (1.15) as $S = 0$, where

$$S = \begin{pmatrix}r_{11} & r_{12}\\ r_{21} & r_{22}\end{pmatrix}\begin{pmatrix}1/g & 0\\ 0 & \alpha\end{pmatrix}\begin{pmatrix}r_{11} & r_{21}\\ r_{12} & r_{22}\end{pmatrix} - \begin{pmatrix}1/g & 0\\ 0 & \alpha\end{pmatrix} + 2\eta\Delta t r r^{\mathrm{T}}.$$

This is equivalent to (2.6) in [18]. With (1.17), we require

$$\begin{aligned} r_{22} &= r_{11}(1+2k) - 2k,\\ r_{21}^2 &= g\alpha(1-r_{11})(1-2k+r_{11}(1+2k)),\\ r_{12} &= -(g\alpha)^{-1}r_{21}, \end{aligned}$$

where $k = k_1/k_2$. Thus, using (1.16) and simplifying, we find that the following two conditions must hold for all k_1 and k_2, if Σ is to take the form (1.14):

$$
\begin{aligned}
&k_1\left(b^{\mathrm{T}}P^{-1}e - 2\hat{b}^{\mathrm{T}}P^{-1}c\right) + k_2\left(b^{\mathrm{T}}\hat{A}P^{-1}e - \hat{b}^{\mathrm{T}}P^{-1}c\right) = 0,\\
&\hat{b}^{\mathrm{T}}P^{-1}e - 2\hat{b}^{\mathrm{T}}P^{-1}c + k_1\left(2(\hat{b}^{\mathrm{T}}P^{-1}c)^2 - b^{\mathrm{T}}P^{-1}c\hat{b}^{\mathrm{T}}P^{-1}e\right)\\
&\qquad + k_2\left((\hat{b}^{\mathrm{T}}P^{-1}c)^2 - b^{\mathrm{T}}\hat{A}P^{-1}c\hat{b}^{\mathrm{T}}P^{-1}e\right) = 0,
\end{aligned}
\tag{1.18}
$$

and we can write

$$
\alpha = \frac{2\hat{b}^{\mathrm{T}}P^{-1}c}{(\hat{b}^{\mathrm{T}}P^{-1}e)^2}\left(1 - \left(k_1 + \frac{1}{2}k_2\right)\hat{b}^{\mathrm{T}}P^{-1}c\right). \tag{1.19}
$$

Expanding P^{-1} in the first few powers of k_1 and k_2, and substituting in (1.18) using (1.10), we find the following necessary conditions:

$$
\begin{aligned}
&\hat{b}^{\mathrm{T}}c = \frac{1}{2} \qquad b^{\mathrm{T}}\hat{c} = \frac{1}{2}, \hat{b}^{\mathrm{T}}Ac = \frac{1}{2}b^{\mathrm{T}}c, \qquad b^{\mathrm{T}}\hat{A}A\hat{c} = b^{\mathrm{T}}A\hat{A}c,\\
&\qquad \text{and} \qquad \hat{b}^{\mathrm{T}}A\hat{c} - \frac{1}{4} = -\frac{1}{2}b^{\mathrm{T}}c + b^{\mathrm{T}}A\hat{c} = 2\hat{b}^{\mathrm{T}}A\hat{A}c - b^{\mathrm{T}}\hat{A}c.
\end{aligned}
\tag{1.20}
$$

Expanding (1.19) similarly yields

$$
\begin{aligned}
\alpha &= 1 + k_1\left(\frac{1}{2} - b^{\mathrm{T}}c\right) + k_2\left(2\hat{b}^{\mathrm{T}}A\hat{c} - b^{\mathrm{T}}A\hat{c} - b^{\mathrm{T}}\hat{A}c + \frac{1}{2}b^{\mathrm{T}}c - \frac{1}{4}\right) + \cdots\\
&= 1 + k_1\left(\frac{1}{2} - b^{\mathrm{T}}c\right) + k_2\left(b^{\mathrm{T}}A\hat{c} - b^{\mathrm{T}}\hat{A}c + \frac{1}{4} - \frac{1}{2}b^{\mathrm{T}}c\right) + \cdots.
\end{aligned}
\tag{1.21}
$$

Using the requirement $S = 0$, we develop numerical methods with $\alpha = 1 + \mathcal{O}(\Delta t^{j+2})$. That is, the stationary mean square of the position variable obtained when solving linear SDEs is exact, and the independence of position and velocity is exactly preserved, while the error in the mean square of the velocity is $\mathcal{O}(\Delta t^{j+2})$, i.e., the mean-square velocity order is $j + 2$. The task is to find explicit methods that satisfy (1.18).

2. Two-stage methods. In this section, we consider two-stage PRK methods that satisfy (1.18). Recall that explicit PRK methods have the property that $\hat{A}(I + k_1A)^{-1}A$ is strictly lower triangular. If $s = 2$, then it is only possible to satisfy (1.20) if either $A\hat{A} = 0$ or $\hat{A}A = 0$.

We first describe three methods which share the property that $\hat{A}A = 0$. The leapfrog method is represented in Butcher tableaux as

$$
\begin{array}{c|cc} 0 & 0 & 0\\ 1 & 1 & 0\\ \hline & 1 & 0 \end{array} \qquad \begin{array}{c|cc} & 1/2 & 0\\ & 1/2 & 0\\ \hline & 1/2 & 1/2 \end{array}.
$$

This gives $\alpha = (1 - \frac{1}{2}k_1 - \frac{1}{4}k_2)^{-1}$ [18]. Mannella's modification of the leapfrog method is represented as

$$
\begin{array}{c|cc} 0 & 0 & 0\\ 1 & 1/2 & 1/2\\ \hline & 1/2 & 1/2 \end{array} \qquad \begin{array}{c|cc} & 1/2 & 0\\ & 1/2 & 0\\ \hline & 1/2 & 1/2 \end{array};
$$

it has $\alpha = (1 - \frac{1}{4}k_2)^{-1}$ [18]. The implicit midpoint method has

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 1/2 & 0 & 1/2 \\ \hline & 0 & 1 \end{array} \qquad \begin{array}{|cc} 0 & 0 \\ 0 & 1/2 \\ \hline 0 & 1 \end{array},$$

which gives the exact value $\alpha = 1$ [16, 17, 18].

2.1. The "reverse leapfrog" method. To devise a new method, now we suppose that $\hat{b} = b$ and $A\hat{A} = 0$. The method is characterized by

$$\begin{array}{c|cc} 1/2 & 1/2 & 0 \\ 1/2 & 1/2 & 0 \\ \hline & 1/2 & 1/2 \end{array} \qquad \begin{array}{|cc} 0 & 0 \\ 1/2 & 1/2 \\ \hline 1/2 & 1/2 \end{array}$$

and has $\alpha = 1 - \frac{1}{4}k_2 = 1 - \frac{1}{4}g\Delta t^2$. This "reverse leapfrog" method can be written as

$$\begin{aligned} Z_1 &= \frac{1}{1 + \frac{1}{2}k_1}\left(p_n + \frac{1}{2}\Delta t f(q_n) + \frac{1}{2}\epsilon\Delta W_n\right), \\ q_{n+1} &= q_n + \Delta t Z_1, \\ p_{n+1} &= p_n - Z_1 k_1 + \frac{1}{2}\Delta t(f(q_n) + f(q_{n+1})) + \epsilon\Delta W_n. \end{aligned} \tag{2.1}$$

We note that both the reverse leapfrog and the Mannella method are symplectic in a deterministic setting. That is, they satisfy $M = 0$, where M is given by (1.11).

In numerical experiments on nonlinear systems, we have found that the reverse leapfrog method outperforms all other two-stage Runge–Kutta methods in terms of the position variable. On the other hand, the implicit midpoint rule is the most accurate in the velocity variable and most closely respects the independence of position and velocity [18]. In Figure 1, we display mean-square results for the double-well system when $f(x) = x - x^3$. The numerical experiments were carried out by evolving 10000 realizations for a time of order 10^6.

In Figure 2, we plot $\rho^*(x)/\rho(x)$ for two-stage methods, with $KT = 0.1$ and $\Delta t = 0.2$. Leapfrog-type methods overestimate the density close to the maximum of the potential; the implicit midpoint method underestimates it in the same region. In Figure 3, we plot the Kullback–Leibler divergence (1.6) as a function of Δt for two-stage methods. Under this measure of accuracy, the reverse leapfrog method performs best of the two-stage methods in the position variable.

A characteristic feature of the reverse leapfrog method (2.1) is that the quantity p_{n+1} is the last one produced in each step, from a combination of q_n and q_{n+1}. In contrast, the final operation in all the other methods discussed in this paper is

$$q_{n+1} = q_n + \frac{1}{2}(p_n + p_{n+1})\Delta t.$$

We explore such schemes further in section 3.

2.2. Error conditions. Let us return to (1.21) and to the quest for explicit methods that give α as close as possible to unity, whilst being exact in the position variable and respecting the independence of position and velocity. In order to eliminate the error term proportional to k_1, we need $b^{\mathrm{T}}c = \frac{1}{2}$. Then

$$\begin{aligned} \alpha &= 1 + k_2(b^{\mathrm{T}}A\hat{c} - b^{\mathrm{T}}\hat{A}c) + \cdots \\ &= 1 + k_2(b^{\mathrm{T}}A\hat{A}e - b^{\mathrm{T}}\hat{A}Ae) + \cdots . \end{aligned}$$

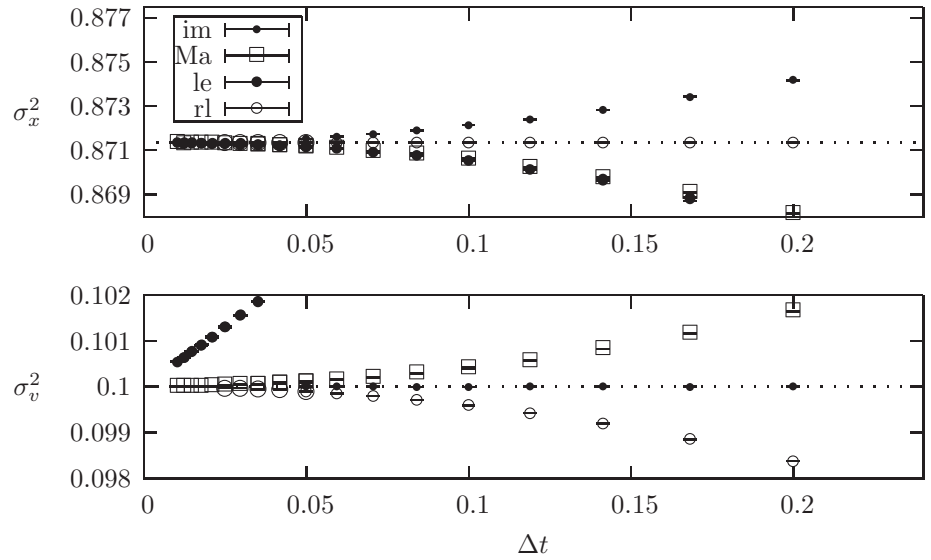

FIG. 1. *Double-well system with $KT = 0.1$ and $\eta = 1$. Upper graph: Mean-squared position versus Δt for the implicit midpoint, Mannella, leapfrog, and reverse leapfrog methods. Lower graph: Mean-squared velocity versus Δt. The dotted lines are the exact results.*

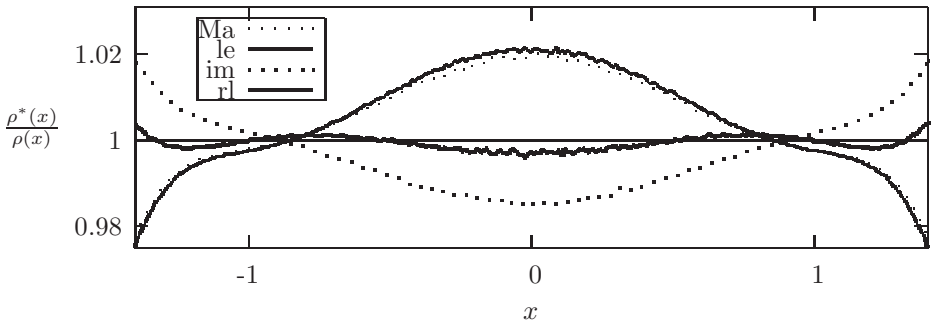

FIG. 2. *The ratio of the stationary density in the position variable produced by numerical methods, and the exact stationary density $\rho(x)$ is plotted, as a function of x, for the implicit midpoint, Mannella, leapfrog, and reverse leapfrog methods. In each case, $\Delta t = 0.2$. Double-well system with $KT = 0.1$ and $\eta = 1$.*

Because explicit two-stage PRK methods have either $A\hat{A} = 0$ or $\hat{A}A = 0$, but not both, we cannot eliminate the error term proportional to k_2. That is, we can at best obtain $\alpha = 1 + \mathcal{O}(\Delta t^2)$, corresponding to mean-square velocity order 2. Inspection of (1.21) and (1.20) reveals that the following conditions are necessary in order to obtain $\alpha = 1 + \mathcal{O}(\Delta t^3)$ or better:

$$b^{\mathrm{T}}c = \hat{b}^{\mathrm{T}}c = b^{\mathrm{T}}\hat{c} = \frac{1}{2}, \qquad \hat{b}^{\mathrm{T}}A\hat{c} = b^{\mathrm{T}}A\hat{c} = b^{\mathrm{T}}\hat{A}c,$$
$$\hat{b}^{\mathrm{T}}Ac = \frac{1}{4}, \qquad \hat{b}^{\mathrm{T}}A\hat{A}c = b^{\mathrm{T}}\hat{A}A\hat{c} = b^{\mathrm{T}}A\hat{c} - \frac{1}{8}. \tag{2.2}$$

In the next section, we devise explicit PRK methods, with $s \geq 3$, satisfying (2.2).

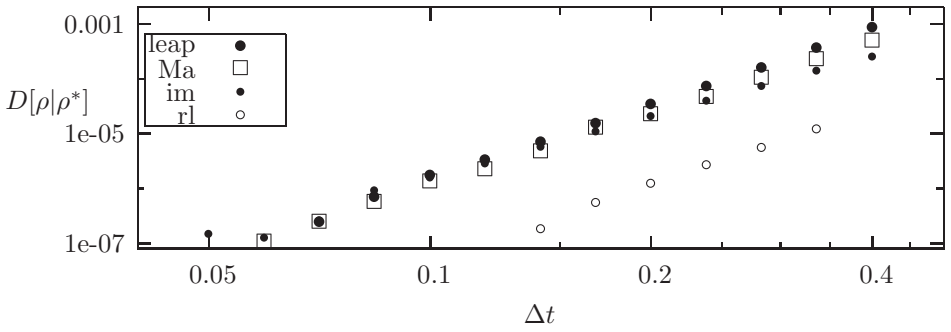

FIG. 3. *The Kullback–Leibler divergence, or relative entropy, between the numerical and exact stationary densities is plotted, as a function of Δt, for the implicit midpoint, Mannella, leapfrog, and reverse leapfrog methods. Double-well system with $KT = 0.1$ and $\eta = 1$. The two-stage method with the best performance in the position variable is the "reverse leapfrog" method.*

3. Runge–Kutta leapfrog methods. We consider a class of methods that we shall call Runge–Kutta leapfrog methods, defined via conditions on the entries in the Butcher tableaux.

THEOREM 3.1. *If, in addition to* (1.10),

$$b = \hat{b} \qquad \text{and} \qquad b^{\mathrm{T}} A = \frac{1}{2} b^{\mathrm{T}},$$

then a PRK method has an update of the form

$$\begin{aligned} p_{n+1} &= \frac{1}{1+\frac{1}{2}\eta\Delta t}\left(\left(1-\frac{1}{2}\eta\Delta t\right)p_n + \Delta t\sum_{j=1}^{s} b_j f(Y_j) + \epsilon\Delta W_n\right), \\ q_{n+1} &= q_n + \frac{1}{2}\Delta t(p_n + p_{n+1}). \end{aligned} \tag{3.1}$$

Proof. If $b = \hat{b}$, then (1.7) can be written

$$\begin{aligned} q_{n+1} &= q_n + \Delta t b^{\mathrm{T}} Z, \\ p_{n+1} &= p_n - k_1 b^{\mathrm{T}} Z + \Delta t b^{\mathrm{T}} f(Y) + \epsilon\Delta W_n. \end{aligned}$$

If $b^{\mathrm{T}}(A - \frac{1}{2}I) = 0$, then, by a power series expansion, $b^{\mathrm{T}}(I + k_1 A)^{-1} = b^{\mathrm{T}}(1 + \frac{1}{2}k_1)^{-1}$. With (1.9) we find

$$\begin{aligned} b^{\mathrm{T}} Z &= b^{\mathrm{T}}\left(I + \frac{1}{2}k_1\right)^{-1}(p_n e + \Delta t A f(Y) + \epsilon\Delta W_n c) \\ &= \left(1 + \frac{1}{2}k_1\right)^{-1}\left(p_n + \frac{1}{2}\Delta t b^{\mathrm{T}} f(Y) + \frac{1}{2}\epsilon\Delta W_n\right) \\ &= \frac{1}{2}(p_n + p_{n+1}). \qquad \square \end{aligned}$$

The implicit midpoint method, too, satisfies the conditions of Theorem 3.1 and can be written in the form (3.1). It is, of course, not explicit, but the implicit part of each timestep can be performed as a finite number of fixed-point iterations [18].

In the remainder of this section, we develop a procedure to produce the PRK methods with $s = 3, 4, 5$. Applied to linear systems, they are exact in the position variable and respect the independence of position and velocity, while the error in the σ_v^2 is proportional to $\Delta t^s \eta^{s-2}$. We begin by introducing a set of conditions on the matrices A and $\hat{A}$ and the column vectors b and $\hat{b}$, which ensure that (1.18) are satisfied and simplify the expression for α.

LEMMA 3.2. *If, in addition to* (1.10) *and* (1.18),

$$b = \hat{b}, \qquad b^{\mathrm{T}} c = \frac{1}{2}, \qquad \text{and} \qquad A\hat{c} = \frac{1}{2}c,$$

then

$$b^{\mathrm{T}} P^{-1} e = 1 - \left(k_1 + \frac{1}{2}k_2\right) b^{\mathrm{T}} P^{-1} c$$

and

$$\alpha = \frac{2 b^{\mathrm{T}} P^{-1} c}{1 - (k_1 + \frac{1}{2}k_2) b^{\mathrm{T}} P^{-1} c}. \tag{3.2}$$

Proof. Using (1.13),

$$\begin{aligned}
1 - \left(k_1 + \frac{1}{2}k_2\right) b^{\mathrm{T}} P^{-1} c - b^{\mathrm{T}} P^{-1} e &= -\sum_{i=1}^{\infty} (-1)^i b^{\mathrm{T}} (k_1 A + k_2 A\hat{A})^i e \\
&\quad - \left(k_1 + \frac{1}{2}k_2\right) \sum_{i=0}^{\infty} (-1)^i b^{\mathrm{T}} (k_1 A + k_2 A\hat{A})^i c \\
&= \sum_{i=1}^{\infty} (-1)^i b^{\mathrm{T}} (k_1 A + k_2 A\hat{A})^i \\
&\qquad \left(-k_1 c - k_2 A\hat{c} + \left(k_1 + \frac{1}{2}k_2\right) c\right) \\
&= \sum_{i=1}^{\infty} (-1)^{j-1} (k_1 A - k_2 A\hat{A})^i k_2 \left(A\hat{c} - \frac{1}{2}c\right)^i \\
&= 0.
\end{aligned}$$

The relation (3.2) now follows from (1.19). ∎

3.1. Properties A and B. We now introduce conditions on the parameters of the method that simplify the order conditions in α, allowing us to construct high-order methods.

Property A. Let the conditions (1.10) plus

$$b = \hat{b}, \qquad b^{\mathrm{T}} A = \frac{1}{2} b^{\mathrm{T}}, \qquad A\hat{c} = \frac{1}{2}c,$$

be known as Property A.

COROLLARY 3.3. *Let*

$$\kappa = \frac{1}{2}k_1 + \frac{1}{4}k_2 = \frac{1}{2}\eta\Delta t + \frac{1}{4}g\Delta t^2.$$

Suppose Property A holds. Let $j \geq 0$ be the largest integer such that

$$b^{\mathrm{T}}(k_1 A + k_2 A\hat{A})^i c = \frac{1}{2}\kappa^i, \qquad i = 0, \ldots, j. \tag{3.3}$$

Then $\alpha = 1 + \mathcal{O}(\Delta t^{j+2})$. The $\mathcal{O}(\Delta t^{j+2})$ term is proportional to $k_1^j k_2$.

Proof. Using the definition (1.13),

$$b^{\mathrm{T}} P^{-1} c = \sum_{i=0}^{\infty} (-1)^i b^{\mathrm{T}}(k_1 A + k_2 A\hat{A})^i c.$$

If (3.3) holds, then $b^{\mathrm{T}}P^{-1}c = \frac{1}{2}\sum_{i=0}^{j}(-1)^i\kappa^i + R_j$, where $R_j = \sum_{i=j+1}^{\infty}(-1)^i b^{\mathrm{T}}(k_1 A + k_2 A\hat{A})^i c$. Consequently,

$$\begin{aligned}
\alpha &= 2b^{\mathrm{T}}P^{-1}c\left(1 - 2\kappa b^{\mathrm{T}}P^{-1}c\right)^{-1} \\
&= \left(1 + \sum_{i=1}^{j}(-1)^i\kappa^i + 2R_j\right)\left(1 - \sum_{i=1}^{j+1}(-1)^{i-1}\kappa^i - 2\kappa R_j\right)^{-1} \\
&= \left(1 + \sum_{i=1}^{j}(-1)^i\kappa^i + 2R_j\right)\left(1 + \sum_{i=1}^{j+1}(-1)^i\kappa^i - 2\kappa R_j\right)^{-1} \\
&= 1 + (-1)^j(\kappa^{j+1} + \kappa^{j+2}) + 2(1+\kappa)R_j + \mathcal{O}(\Delta t^{j+3}).
\end{aligned}$$

Now, using Property A,

$$b^{\mathrm{T}}A^i c = \left(\frac{1}{2}\right)^{i+1}$$

for any integer $i \geq 0$, and

$$\begin{aligned}
R_j &= (-1)^{j+1} b^{\mathrm{T}}(k_1 A + k_2 A\hat{A})^{j+1} c + (-1)^{j+2} b^{\mathrm{T}}(k_1 A + k_2 A\hat{A})^{j+2} c + \cdots \\
&= (-1)^{j+1}\frac{1}{2}\left(\frac{1}{2}k_1\right)^{j+1} + (-1)^{j+1}k_1^j k_2 \sum_{i=0}^{j} b^{\mathrm{T}} A^{j+1-i}\hat{A}A^i c \\
&\quad + (-1)^{j+2}\frac{1}{2}\left(\frac{1}{2}k_1\right)^{j+2} + \mathcal{O}(\Delta t^{j+3}).
\end{aligned}$$

Using

$$\kappa^{j+1} = \left(\frac{1}{2}k_1\right)^{j+1} + \frac{j+1}{4}k_2\left(\frac{1}{2}k_1\right)^j + \mathcal{O}(\Delta t^{j+3}),$$

we find

$$\alpha = 1 + (-1)^j k_1^j k_2 \left(\frac{1}{2}\right)^j \left(\frac{j+1}{4} - 2\sum_{i=0}^{j} b^{\mathrm{T}} A^{j+1-i}\hat{A}A^i c\right) + \mathcal{O}(\Delta t^{j+3}). \qquad \square$$

Hence $\alpha - 1 = C\Delta t^{j+2} + \mathcal{O}(\Delta t^{j+3})$, corresponding to mean-square velocity error of order $j+2$, with constant

$$C = (-1)^j g\left(\frac{\eta}{2}\right)^j \left(\frac{j+1}{4} - 2\sum_{i=0}^{j} b^{\mathrm{T}} A^{j+1-i}\hat{A}A^i c\right).$$

A summary of the conditions (3.3) under Property A is given in Table 3.1.

TABLE 3.1
Conditions for $\alpha = 1 + \mathcal{O}(\Delta t^{j+2})$ under Property A.

j	Conditions
1	$b^{\mathrm{T}}\hat{A}c = \frac{1}{4}$
2	$b^{\mathrm{T}}\hat{A}c = \frac{1}{4}$, $b^{\mathrm{T}}\hat{A}Ac = \frac{1}{8}$, $b^{\mathrm{T}}\hat{A}A\hat{A}c = \frac{1}{16}$

TABLE 3.2
Conditions for $\alpha = 1 + \mathcal{O}(\Delta t^{j+2})$ under Property B.

j	Conditions
2	$b^{\mathrm{T}}\hat{A}Ac = \frac{1}{8}$
3	$b^{\mathrm{T}}\hat{A}c = \frac{1}{4}$, $b^{\mathrm{T}}\hat{A}A^2c = \frac{1}{16}$, $b^{\mathrm{T}}\hat{A}A\hat{A}Ac = \frac{1}{32}$

TABLE 3.3
Conditions for $\alpha = 1 + \mathcal{O}(k_1^j k_2)$ under (3.5).

j	Conditions
1	$v^{\mathrm{T}}e = 0$, $v^{\mathrm{T}}c = 0$
2	$v^{\mathrm{T}}e = 0$, $v^{\mathrm{T}}c = 0$, $v^{\mathrm{T}}Ac = 0$
3	$v^{\mathrm{T}}e = 0$, $v^{\mathrm{T}}c = 0$, $v^{\mathrm{T}}Ac = 0$, $v^{\mathrm{T}}A^2c = 0$, $v^{\mathrm{T}}A\hat{A}Ac = 0$

Runge–Kutta leapfrog methods thus have mean-square velocity error proportional to $\eta^j \Delta t^{j+2}$. Note that the two-stage Runge–Kutta leapfrog method is Mannella's "symplectic low order (SLO)" method [14, 15], which satisfies Property A and (3.3) with $j = 0$; the error is independent of η.

Property B. Let the conditions of Property A plus

$$\hat{A}c = \frac{1}{2}c \tag{3.4}$$

be known as Property B. (No explicit two-stage method can have Property B because it must have either $A\hat{A} = 0$ or $\hat{A}A = 0$.) A summary of the conditions (3.3) that hold under Property B is given in Table 3.2.

3.2. Construction of Runge–Kutta leapfrog methods. The condition (3.4) can be satisfied if $\hat{c} = \frac{1}{2}e$. In fact, a considerable simplification in the order conditions takes place if

$$\hat{A} = \frac{1}{2}I - e_s v^{\mathrm{T}}, \tag{3.5}$$

where $v^{\mathrm{T}} = (v_1, v_2, \ldots, \frac{1}{2})$ and $e_s^{\mathrm{T}} = (0, \ldots, 0, 1)$. Comparison with Table 3.2 yields the conditions in Table 3.3.

Further analysis reveals that the last condition of Table 3.3 is, in fact, unnecessary. If (3.5) holds and $v^{\mathrm{T}}Ac = 0$, $v^{\mathrm{T}}A^2c = 0$, then

$$\begin{aligned} v^{\mathrm{T}}A\hat{A}Ac &= v^{\mathrm{T}}A\left(\frac{1}{2}I - e_s v^{\mathrm{T}}\right)Ac \\ &= \frac{1}{2}v^{\mathrm{T}}A^2c - (v^{\mathrm{T}}Ae_s)(v^{\mathrm{T}}Ac) \\ &= 0. \end{aligned}$$

THEOREM 3.4. *If*

$$Ae = c, \qquad b^{\mathrm{T}} = \hat{b}^{\mathrm{T}}, \qquad b^{\mathrm{T}}e = 1, \qquad b^{\mathrm{T}}A = \frac{1}{2}b^{\mathrm{T}}, \qquad \textit{and} \qquad \hat{A} = \frac{1}{2}I - e_s v^{\mathrm{T}},$$

then $\alpha = 1 + \mathcal{O}(\Delta t^{j+2})$ *if and only if*

$$v^{\mathrm{T}}e = 0 \qquad \textit{and} \qquad v^{\mathrm{T}}A^i c = 0, \quad i = 1, \ldots, j-1.$$

Proof. We verify Property B as follows:

$$A\hat{c} = A\hat{A}e = A\left(\frac{1}{2}I - e_s v^{\mathrm{T}}\right)e = \frac{1}{2}c,$$
$$\hat{A}c = \frac{1}{2}ce_s v^{\mathrm{T}}e = \frac{1}{2}c.$$

Thus

$$b^{\mathrm{T}}(k_1 A + k_2 A\hat{A})^i c = \frac{1}{2}\kappa^i, \qquad i = 1, \ldots, j.$$

By Corollary 3.3, $\alpha = 1 + \mathcal{O}(\Delta t^{j+2})$. ∎

We now turn to a constructive procedure for producing PRK methods. The requirement that the method be explicit imposes the condition that $\hat{A}(1+k_1A)^{-1}A$ be strictly lower triangular, which will be satisfied if the products of the diagonal elements of A and $\hat{A}$ are zero. In other words, whenever there is a nonzero diagonal element of $\hat{A}$, there must be a corresponding zero element of A. A systematic construction of v^{T} and A so that the conditions of theorem 3.4 hold is as follows.

1. Take

$$c_i = \frac{i-1}{s-1}, \quad i = 1, \ldots, s, \qquad b_i = \begin{cases} \dfrac{1}{2}\dfrac{1}{s-1} & i = 1, \\ \dfrac{1}{s-1} & i = 2, \ldots, s-1, \\ \dfrac{1}{2}\dfrac{1}{s-1} & i = s, \end{cases}$$

and

$$A = \begin{pmatrix} 0 & 0 & \cdots & 0 & 0 & 0 \\ 1/(s-1) & 0 & \cdots & 0 & 0 & 0 \\ 0 & 2/(s-1) & \cdots & 0 & 0 & 0 \\ & & \vdots & & & \\ 0 & 0 & \cdots & (s-2)/(s-1) & 0 & 0 \\ a_1 & a_2 & \cdots & a_{s-2} & a_{s-1} & 1/2 \end{pmatrix}. \tag{3.6}$$

2. Choose the entries in the last row of A such that $b^{\mathrm{T}}A = \frac{1}{2}b^{\mathrm{T}}$:

$$a_1 = \frac{1}{2} - \frac{2}{s-1},$$
$$a_i = 1 - \frac{2i}{s-1}, \qquad i = 2, \ldots, s-2,$$
$$a_{s-1} = 1.$$

3. Find v such that $v^{\mathrm{T}}e = 0$ and

$$v^{\mathrm{T}}A^i c = 0, \qquad i = 0, \ldots, s-3. \tag{3.7}$$

Let $a^T = (a_1, \ldots, a_{s-1}, \frac{1}{2})$. With A as given in (3.6), the entries of Ac are

$$(Ac)_l = \begin{cases} 0, & l = 1, 2, \\ (l-1)(l-2)/(s-1)^2, & l = 3, \ldots, s-1, \\ a^{\mathrm{T}}c, & l = s. \end{cases}$$

For any $i = 1, \ldots, s-3$, the entries of $A^i c$ are

$$(A^i c)_l = \begin{cases} 0, & l = 1, \ldots, i+1, \\ \dfrac{(l-1)(l-2)\cdots(l-i-1)}{(s-1)^{i+1}}, & l = i+2, \ldots, s-1, \\ a^T A^{i-1} c, & l = s. \end{cases}$$

We can solve (3.7) recursively for $v_{s-1}, \ldots, v_1$ by back substitution of an upper triangular system. The first relation, giving v_{s-1}, is

$$v_{s-1}\frac{(s-2)!}{(s-1)^{s-2}} + \frac{1}{2}a^T A^{s-4}c = 0.$$

We followed this procedure to produce the following PRK methods with $s = 3, 4, 5$ and

$$\alpha = 1 + \frac{(-1)^s}{2^s} g\eta^{s-2}\Delta t^s + \mathcal{O}(\Delta t^{s+1}). \tag{3.8}$$

3.3. Three-stage Runge–Kutta leapfrog method. With $s = 3$, we can satisfy (3.3) up to $j = 1$ so that $\alpha = 1 + \mathcal{O}(\Delta t^3)$. The resulting tableaux are

$$\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ 1/2 & 1/2 & 0 & 0 \\ 1 & -1/2 & 1 & 1/2 \\ \hline & 1/4 & 1/2 & 1/4 \end{array} \qquad \begin{array}{c|ccc} 1/2 & 0 & 0 \\ 0 & 1/2 & 0 \\ -1/2 & 1 & 0 \\ \hline 1/4 & 1/2 & 1/4 \end{array}.$$

The method can be written as

$$\begin{aligned} &Z_1 = p_n, \\ &Z_2 = (1 - \tfrac{1}{2}k_1)p_n + \tfrac{1}{2}(f(Y_1)\Delta t + \epsilon\Delta W_n), \end{aligned} \qquad \begin{aligned} Y_1 &= q_n + \tfrac{1}{2}\Delta t Z_1, \\ Y_2 &= q_n + \tfrac{1}{2}\Delta t Z_2, \\ Y_3 &= 2Y_2 - Y_1, \end{aligned}$$

$$p_{n+1} = \frac{1}{1 + \frac{1}{2}k_1}\left(\left(1 - \frac{1}{2}k_1\right)p_n + \frac{1}{4}\Delta t(f(Y_1) + 2f(Y_2) + f(Y_3)) + \epsilon\Delta W\right),$$

$$q_{n+1} = q_n + \frac{1}{2}\Delta t(p_n + p_{n+1}).$$

This method, applied to the linear system $f(x) = -gx$, gives

$$\begin{aligned} \alpha - 1 &= \frac{1}{8}k_1 k_2 - \frac{1}{16}k_2^2 - \frac{1}{32}k_1 k_2^2 + \cdots \\ &= \frac{1}{8}g\eta\Delta t^3 - \frac{1}{16}g^2\Delta t^4 - \frac{1}{32}g^2\eta\Delta t^4 + \cdots. \end{aligned} \tag{3.9}$$

3.4. Four-stage Runge–Kutta leapfrog method. With $s = 4$, we can satisfy (3.3) up to $j = 2$ so that $\alpha = 1 + \mathcal{O}(\Delta t^4)$. The solution is represented as

0	0	0	0	0
1/3	1/3	0	0	0
2/3	0	2/3	0	0
1	−1/6	−1/3	1	1/2
	1/6	1/3	1/3	1/6

1/2	0	0	0
0	1/2	0	0
0	0	1/2	0
$\frac{11}{8}$	$-\frac{26}{8}$	$\frac{19}{8}$	0
1/6	1/3	1/3	1/6

.

The method can be written as

$$\begin{aligned} Z_1 &= p_n, \\ Z_2 &= (1 - \tfrac{1}{3}k_1)p_n + \tfrac{1}{3}(f(Y_1)\Delta t + \epsilon \Delta W_n), \\ Z_3 &= p_n - \tfrac{2}{3}k_1 Z_2 + \tfrac{2}{3}(f(Y_2)\Delta t + \epsilon \Delta W_n), \end{aligned} \qquad \begin{aligned} Y_1 &= q_n + \tfrac{1}{2}\Delta t Z_1, \\ Y_2 &= q_n + \tfrac{1}{2}\Delta t Z_2, \\ Y_3 &= q_n + \tfrac{1}{2}\Delta t Z_3, \\ Y_4 &= \tfrac{1}{4}(11Y_1 - 26Y_2 + 19Y_3), \end{aligned}$$

$$p_{n+1} = \frac{1}{1 + \frac{1}{2}k_1}\left(\left(1 - \frac{1}{2}k_1\right)p_n + \frac{1}{6}\Delta t(f(Y_1) + 2f(Y_2) + 2f(Y_3) + f(Y_4)) + \epsilon \Delta W\right),$$

$$q_{n+1} = q_n + \frac{1}{2}\Delta t(p_n + p_{n+1}).$$

In this case,

$$\alpha - 1 = \frac{1}{16}g\eta^2\Delta t^4 + \frac{1}{16}g^2\eta\Delta t^5 + \cdots. \tag{3.10}$$

3.5. Five-stage Runge–Kutta leapfrog method. With $s = 5$, we can satisfy (3.3) up to $j = 3$ so that $\alpha = 1 + \mathcal{O}(\Delta t^5)$. The solution is represented as

0	0	0	0	0	0
1/4	1/4	0	0	0	0
1/2	0	1/2	0	0	0
3/4	0	0	3/4	0	0
1	0	0	−1/2	1	1/2
	1/8	1/4	1/4	1/4	1/8

1/2	0	0	0	0
0	1/2	0	0	0
0	0	1/2	0	0
0	0	0	1/2	0
$-\frac{11}{6}$	7	−9	$\frac{13}{3}$	0
1/8	1/4	1/4	1/4	1/8

and can be written as

$$\begin{aligned} Z_1 &= p_n, \\ Z_2 &= (1 - \tfrac{1}{4}k_1)p_n + \tfrac{1}{4}(f(Y_1)\Delta t + \epsilon \Delta W_n), \\ Z_3 &= p_n - \tfrac{1}{2}k_1 Z_2 + \tfrac{1}{2}(f(Y_2)\Delta t + \epsilon \Delta W_n), \\ Z_4 &= p_n - \tfrac{3}{4}k_1 Z_3 + \tfrac{3}{4}(f(Y_3)\Delta t + \epsilon \Delta W_n), \end{aligned} \qquad \begin{aligned} Y_1 &= q_n + \tfrac{1}{2}\Delta t Z_1, \\ Y_2 &= q_n + \tfrac{1}{2}\Delta t Z_2, \\ Y_3 &= q_n + \tfrac{1}{2}\Delta t Z_3, \\ Y_4 &= q_n + \tfrac{1}{2}\Delta t Z_4, \\ Y_5 &= \frac{1}{3}(-11Y_1 + 42Y_2 - 54Y_3 + 26Y_4), \end{aligned}$$

$$p_{n+1} = \frac{1}{1 + \frac{1}{2}k_1}\left(\left(1 - \frac{1}{2}k_1\right)p_n + \frac{1}{8}\Delta t(f(Y_1) + 2f(Y_2) + 2f(Y_3) + 2f(Y_4) + f(Y_5)) + \epsilon \Delta W\right),$$

$$q_{n+1} = q_n + \frac{1}{2}\Delta t(p_n + p_{n+1}).$$

For this five-stage method,

$$\alpha - 1 = -\frac{1}{32}g\eta^3\Delta t^5 - \frac{3}{64}g^2\eta^4\Delta t^6 + \cdots. \tag{3.11}$$

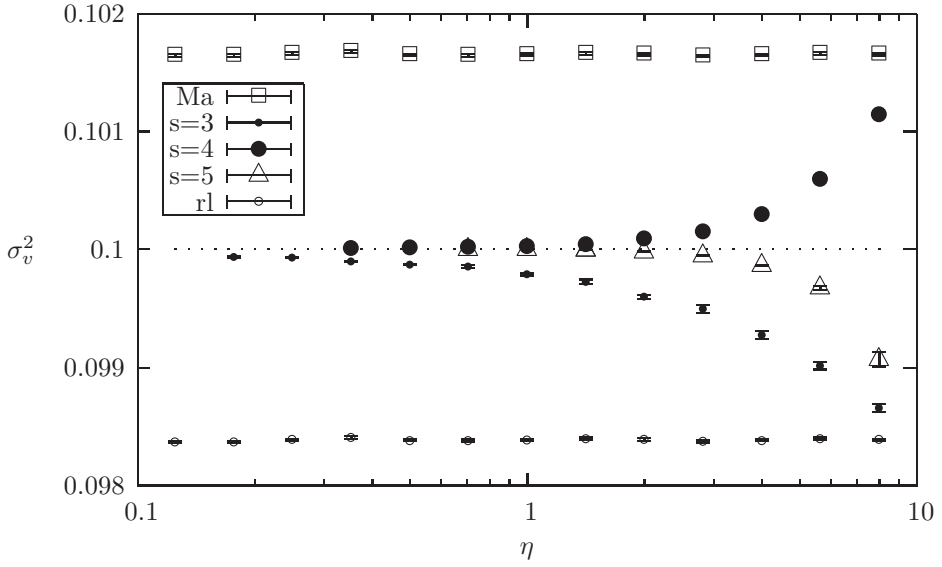

FIG. 4. *Double-well system with* $KT = 0.1$, $g = 1$, *and* $\Delta t = 0.2$. *Mean-squared velocity is plotted versus* η *for Mannella's leapfrog method (squares), the reverse leapfrog method (small empty circles), and the PRK methods with* 3, 4, *and* 5 *stages. The dotted line is the exact result.*

3.6. Double-well system. We have compared the performance of the reverse leapfrog and PRK methods with some existing methods on the double-well system $f(x) = x - x^3$. As the number of stages is increased, or as $\eta \to 0$, the explicit PRK methods approach the accuracy of the implicit midpoint method, which is exact in all variables for the linear system and exact in the velocity variable for double-well systems [18].

In Figure 4, we plot the mean square of the velocity variable versus η. Mannella's modified leapfrog method and the reverse leapfrog method, although less accurate than the PRK methods in the velocity variable, have the virtue of giving an error independent of damping.

In the linear system, the mean-square velocity order of the explicit Runge-Kutta leapfrog methods is equal to the number of stages. The error constant, proportional to η^{s-2}, for $s \geq 3$, is given in (3.8). See the left panel of Figure 5. In the right panel Figure 5, log-log plots of the mean-square error in the in the (nonlinear) double-well system show similar scalings, but the constants are fits to the data. Recall that the implicit midpoint method is exact in the mean-square velocity in both the linear and nonlinear cases but involves an iterative evaluation at each step.

4. Discussion. Analysis of linear test equations is a convenient way to determine the properties of numerical methods. In this respect, numerical analysis of SDEs has much in common with that of deterministic equations. Instead of the classical method of imposing finite-time convergence by matching Taylor series [23, 2], in this work we seek accurate reproduction of stationary densities, which can be thought of as the analogues of steady states.

We have introduced new classes of explicit methods, using only one, Gaussian, random variable per timestep. The methods are devised based on analysis of linear

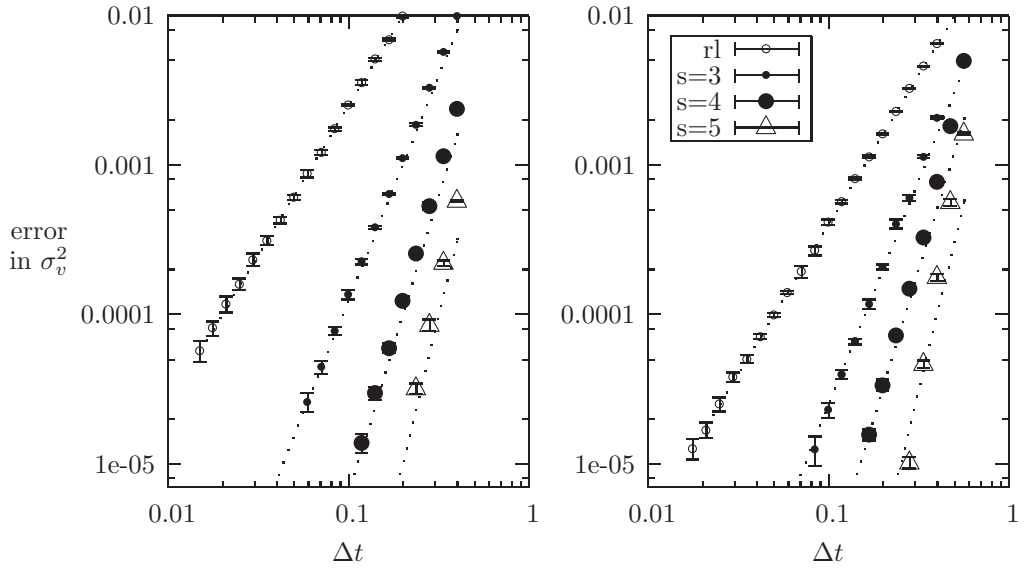

FIG. 5. *Left panel: Numerical results for the linear system with* $KT = 1$, $g = 1$, *and* $\eta = 1$. *The error in the mean square of the velocity variable under the reverse leapfrog method is compared with that using the* 3*-stage,* 4*-stage, and* 5*-stage methods. The dotted lines are error=*$\frac{1}{4}\Delta t^2$, $\frac{1}{8}\Delta t^3$, $\frac{1}{16}\Delta t^4$, *and* $\frac{1}{32}\Delta t^5$. *Right panel: Numerical results for the double-well system with* $KT = 0.1$, $g = 1$, *and* $\eta = 1$. *The dotted lines are error=*$\frac{1}{25}\Delta t^2$, $\frac{1}{40}\Delta t^3$, $\frac{1}{50}\Delta t^4$, *and* $\frac{1}{100}\Delta t^5$.

systems and tested on the (nonlinear) double-well system. In our numerical experiments, these new methods have similar behavior to that seen in linear systems when the errors are calculated analytically. In nonlinear systems, where the error in the mean square does not fully describe the difference between the probability density of the position variable and its exact form, we have used the Kullback–Leibler divergence to quantify how close two probability densities are. We adopt this quantity as a measure of accuracy and we compute it, for a number of numerical methods, in the double-well system.

The implicit midpoint method remains optimal in the velocity variable. The (explicit) Runge–Kutta leapfrog methods that we have devised in the work approach the accuracy of the implicit midpoint method as the number of stages is increased. On the other hand, the reverse leapfrog method outperforms the implicit midpoint method in the position variable.

Partitioned methods have the advantages of being fully explicit and not requiring the evaluation of derivatives. The "reverse leapfrog" method, for example, is a two-stage method with very good properties in the position variable for scalar equations second order in time and with the virtue of being symplectic at zero damping. We have also constructed new explicit PRK methods that require s function evaluations per timestep. Extending these methods and the methodology of analysis to multi-dimensional systems is expected to be straightforward. In the case of multiplicative noise, the stationary density is unchanged [18] if the damping coefficient is multiplied by a suitable nonlinear function. However, there are many ways to extend a given additive-noise method to multiplicative noise, corresponding to evaluating the noise amplitude at different combinations of intermediate values.

REFERENCES

[1] E. Hairer, C. Lubich, and G. Wanner, *Geometric Numerical Integration: Structure-Preserving Algorithms for Ordinary Differential Equations*, Springer, New York, 2002.

[2] G.N. Milstein and M.V. Tretyakov, *Stochastic Numerics for Mathematical Physics*, Springer, New York, 2004.

[3] C.W. Gardiner, *Handbook of Stochastic Methods for Physics, Chemistry and the Natural Sciences*, 3rd ed., Springer, New York, 2004.

[4] J.C. Mattingley, A.M. Stuart, and D.J. Higham, *Ergodicity for SDEs and approximations: Locally Lipschitz vector fields and degenrate noise*, Stochastic Process. Appl., 101 (2002), pp. 185–232.

[5] D. Talay, *Simulation of stochastic differential syatems*, in Probabilistic Methods in Applied Physics, Vol. 451, P. Kree and W. Wedig, eds., Springer, New York, 1995, pp. 63–106.

[6] G.G. Batrouni, G.R. Katz, A.S. Kronfeld, G.P. Lepage, B. Svetitsky, and K.G. Wilson, *Langevin simulations of lattice field theories*, Phys. Rev. D, 32 (1985), pp. 2736–2747.

[7] T. Shardlow, *Modified equations for stochastic differential equations*, BIT, 46 (2006), pp. 111–125.

[8] W. Wang and R.D. Skeel, *Analysis of a few numerical integration methods for the Langevin equation*, Mol. Phys., 101 (2003), pp. 2149–2156.

[9] H. Schurz, *Numerical analysis of SDEs without tears*, in Handbook of Stochastic Analysis and Applications, D. Kannan and V. Lakshmikantham, eds., Marcel Dekker, New York, 2002, pp. 237–359.

[10] A. Tocino and J. Vigo-Aguiar, *Weak second order conditions for stochastic Runge–Kutta methods*, SIAM J. Sci. Comput., 24 (2002), pp. 507–523.

[11] A. Rössler, *Runge–Kutta methods for Itô stochastic differential equations with scalar noise*, BIT, 46 (2006), pp. 97–110.

[12] S. Kullback and R.A. Leibler, *On information and sufficiency*, Ann. of Math. Statist., 22 (1951), pp. 79–86.

[13] R.Y. Rubinstein and D.P. Kroese, *Simulation and the Monte Carlo Method*, 2nd ed., Wiley, New York, 2008.

[14] R. Mannella, *Quasisymplectic integrators for stochastic differential equations*, Phys. Rev. E, 69 (2004), p. 041107.

[15] R. Mannella, *Numerical stochastic integration for quasi-symplectic flows*, SIAM J. Sci. Comput., 27 (2006), pp. 2121–2139.

[16] B. Mishra and T. Schlick, *The notion of error in Langevin dynamics.* I. *Linear analysis*, J. Chem. Phys., 105 (1996), pp. 299–318.

[17] H. Schurz, *The invariance of asymptotic laws of linear stochastic systems under discretization*, Z. Angew. Math. Mech., 6 (1999), pp. 375–382.

[18] K. Burrage, I. Lenane, and G. Lythe, *Numerical methods for second-order stochastic differential equations*, SIAM J. Sci. Comput., 29 (2007), pp. 245–264.

[19] H. Schurz, *Preservation of probabilistic laws through Euler methods for Ornstein-Uhlenbeck processes*, Stoch. Anal. Appl., 17 (1999), pp. 463–486.

[20] E. Hairer, S.P. Norsett, and G. Wanner, *Solving Ordinary Differential Equations* I: *Non-stiff Problems*, Springer, New York, 1993.

[21] K. Burrage and J.C. Butcher, *Stability criteria for implicit Runge-Kutta methods*, SIAM J. Numer. Anal., 16 (1979), pp. 46–57.

[22] A.M. Stuart and A.R. Humphries, *Dynamical Systems and Numerical Analysis*, Cambridge University Press, London, 1996.

[23] P.E. Kloeden and E. Platen, *Numerical Solution of Stochastic Differential Equations*, Springer, New York, 1992.