Second-order stochastic leapfrog algorithm for multiplicative noise Brownian motion

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A stochastic leapfrog algorithm for the numerical integration of Brownian motion stochastic differential equations with multiplicative noise is proposed and tested. The algorithm has a second-order convergence of moments in a finite time interval and requires the sampling of only one uniformly distributed random variable per time step. The noise may be white or colored. We apply the algorithm to a study of the approach towards equilibrium of an oscillator coupled nonlinearly to a heat bath and investigate the effect of the multiplicative noise (arising from the nonlinear coupling) on the relaxation time. This allows us to test the regime of validity of the energy-envelope approximation method.

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I. INTRODUCTION

Noise terms in stochastic differential equations come in two varieties: additive and multiplicative. In the general case, noise terms can enter the equations of motion coupled directly to some function of the stochastic variable. This is the case of multiplicative noise. The special case of additive noise occurs when the noise term does not couple directly to the stochastic variable. (In the case of stochastic *partial* differential equations, the noises can be spatiotemporal, but here we restrict attention to ordinary stochastic differential equations in which the noises are only temporal.) For reasons of simplicity, additive noise tends to be employed in most modeling applications.

Nevertheless, in many situations, stochastic differential equations with multiplicative noise are physically relevant. In addition, they also have interesting mathematical properties. Consequently such equations have attracted substantial attention over the years [1–11]. The key point lies in the fundamental difference between additive and multiplicative noises: because additive noise does not couple directly to the system variables, it disappears from the noise-averaged form of the dynamical equations. However, in the case of multiplicative noise, the system variables do couple directly to the noise (alternatively, we may say that the noise amplitude depends on the system variables). This fact can lead to dramatic changes of system behavior that cannot occur in the presence of additive noise alone. Two classic illustrations are the Kubo oscillator [12] and the existence of long-time tails in transport theory [13]. In this paper we will investigate another example, that of an oscillator nonlinearly coupled to a heat bath, in which the effects of multiplicative noise can significantly alter the qualitative nature, as well as the rate [2], of the equilibration process (relative to that of an oscillator subjected only to additive noise).

The dynamical behavior of systems subjected to noise can be studied in two different ways: we may either solve stochastic differential equations and average over realizations to obtain statistical information, or we may directly solve the Fokker-Planck equation which describes the evolution of the corresponding probability distribution function. Both approaches have their share of advantages and disadvantages. Fokker-Planck equations are partial-differential equations and their mathematical properties are still not fully understood. Moreover, they are very expensive to solve numerically even for dynamical systems possessing only a very modest number of degrees of freedom. Truncation schemes or closures (such as cumulant truncations) have had some success in extracting the behavior of low-order moments, but the systematics of these approximations remains to be elucidated. Compared to the Fokker-Planck equation, stochastic differential equations are not difficult to solve, and with the advent of modern supercomputers, it is possible to run a very large number of realizations in order to compute low-order moments accurately. (We may mention that in applications to field theories it is essentially impossible to solve the corresponding Fokker-Planck equation since the probability distribution is now a functional.) However, the extraction of the probability distribution function itself is very difficult due to the sampling noise inherent in a particle representation of a smooth distribution.

Numerical algorithms to solve stochastic differential equations have been discussed extensively in the literature [14–19]. The simplest, fastest, and still widely used algorithm is Euler's method, which yields a first-order convergence of moments for a finite time interval. Depending on the control over statistical errors arising from the necessarily finite number of realizations, in the extraction of statistical information it may or may not pay to use a higher order algorithm especially if it is computationally expensive. Because of this fact, it is rare to find high-order schemes being put to practical use for the solution of stochastic differential equations, and second-order convergence is usually considered a good compromise between efficiency and accurracy. A popular algorithm with second-order convergence of moments for additive noise but with only first-order convergence of moments for multiplicative noise is Heun's algorithm [also called stochastic RK2 (Runge-Kutta, 2nd order) by some authors] [14,17,20]. A stochastic leapfrog algorithm, which has the same order convergence of moments as

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Heun's method, was suggested in Ref. [21] to study particle motion in a stochastic potential without damping. Several other algorithms for particle motion in a quasiconservative stochastic system were proposed in Ref. [16] and in the book by Allen and Tildesley [22]. At every time step, these methods all require sampling two Gaussian random variables which adds to the computational cost. A modified algorithm suggested in Ref. [19] requires only one Gaussian random variable but applies only to white Gaussian noise. In the following sections, we present a stochastic leapfrog algorithm for multiplicative Gaussian white noise and Ornstein-Uhlenbeck colored noise which not only has second-order convergence of moments but also requires the sampling of only one random uniform variable per time step.

The organization of this paper is as follows: General numerical integration of a system of stochastic differential equations with Gaussian white noise is discussed in Sec. II. The stochastic leapfrog algorithms for Brownian motion with Gaussian white noise and colored Ornstein-Uhlenbeck noise are given in Sec. III. Numerical tests of these algorithms using a one-dimensional harmonic oscillator are presented in Sec. IV. A physical application of the algorithm to the multiplicative-noise Brownian oscillator is given in Sec. V. Section VI contains the final conclusions and a short discussion.

II. NUMERICAL INTEGRATION OF STOCHASTIC DIFFERENTIAL EQUATIONS

A general system of continuous-time stochastic differential equations (Langevin equations), with i labeling the stochastic variables, can be written as

$$\dot{x}_i = F_i(x_1, \ldots, x_n) + \sigma_{ij}(x_1, \ldots, x_n)\xi_j(t), \tag{1}$$

where $i = 1, \ldots, n$ and $\xi_j(t)$ is a Gaussian white noise with

$$\langle \xi_j(t) \rangle = 0, \tag{2}$$

$$\langle \xi_j(t)\xi_j(t') \rangle = \delta(t-t'), \tag{3}$$

and the symbol $\langle \cdots \rangle$ represents an average over realizations of the inscribed variable (ensemble average). The generalized force F_i contains all the systematic terms, including damping effects. The noise is said to be additive when σ_{ij} is not a function of the x_i, otherwise it is said to be multiplicative. In the case of multiplicative noises, a mathematical subtlety arises in interpreting stochastic integrals, the so-called Ito-Stratonovich ambiguity [23] [i.e., whether, given two stochastic processes $\mathbf{Y}$ and $\mathbf{X}$, to define the formal stochastic integral $\int_0^t \mathbf{Y} d\mathbf{X}$ as $\lim_{\Delta t \to 0} \Sigma_0^l \mathbf{Y}_{t_i}(\mathbf{X}_{t_{i+1}} - \mathbf{X}_{t_i})$ (Ito) or as $\lim_{\Delta t \to 0} \Sigma_0^l \mathbf{Y}_{(t_i + t_{i+1})/2}(\mathbf{X}_{t_{i+1}} - \mathbf{X}_{t_i})$ (Stratonovich)]. It should be stressed that this is a point of mathematics and not of physics. Once it is clear how a particular Langevin equation has been derived and what it is supposed to represent, it should either be free of this ambiguity (as in the case of the example we study later) or it should be clear that there must exist two different stochastic equations, one written in the Ito form, the other in Stratonovich, both representing the same physical process and hence yielding identical answers for the variables of interest. (Another way to state this is that there should be only one unique Fokker-Planck equation.) It is important to note that the vast majority of numerical update schemes for Langevin equations use the Ito form of the equation.

The integral representation of the set of equations (1) is

$$x_i(t) = x_i(0) + \int_0^t ds F_i(x_1(s), \ldots, x_n(s)) + \int_0^t ds \sigma_{ij}(x_1(s), \ldots, x_n(s))\xi_j(s), \tag{4}$$

where $x_i(0)$ is a given sharp initial condition at $t=0$. The infinitesimal update form of this equation may be derived by replacing t with an infinitesimal time step h,

$$\begin{aligned} x_i(h) = x_i(0) + \int_0^h dt' F_i\Big[x_k(0) + \int_0^{t'} ds F_k(x(s)) \\ + \int_0^{t'} ds \sigma_{kl}(x(s))\xi_l(s) \Big] + \int_0^h dt' \sigma_{ij} \\ \times \Big[x_k(0) + \int_0^{t'} ds F_k(x(s)) + \int_0^{t'} ds \sigma_{kl}(x(s))\xi_l(s) \Big] \\ \times \xi_j(t'). \end{aligned} \tag{5}$$

Since F_i and σ_{ij} are smooth functions of the x_i, they may be expanded about their values at $t=0$, in which case we can write the exact solution for $x_i(h)$ as

$$x_i(h) = D_i(h) + S_i(h), \tag{6}$$

where $D_i(h)$ and $S_i(h)$ denote the deterministic and stochastic contributions, respectively. The deterministic contribution $D_i(h)$ is

$$D_i(h) = x_i(0) + hF_i + \tfrac{1}{2}h^2 F_{i,k}F_k + O(h^3), \tag{7}$$

where $F_{i,k} = \partial F_i / \partial x_k$, the summation convention for the repeated indices having being employed. The stochastic contribution $S_i(h)$ is

$$\begin{aligned} S_i(h) = \sigma_{ij}W_j(h) + \sigma_{ij,k}\sigma_{kl}C_{lj}(h) + F_{i,k}\sigma_{kl}Z_l(h) \\ + \sigma_{ij,k}F_k(hW_j(h) - Z_j(h)) \\ + \tfrac{1}{2}\sigma_{ij,kl}\sigma_{km}\sigma_{ln}H_{mnj}(h) + \tfrac{1}{2}F_{i,kl}\sigma_{ks}\sigma_{lt}G_{st}(h) \\ + \tfrac{1}{2}F_k\sigma_{ij,kl}\sigma_{lm}K_{mj}(h) + \tfrac{1}{2}F_l\sigma_{ij,kl}\sigma_{km}K_{mj}(h) \\ + \tfrac{1}{6}\sigma_{ij,klm}\sigma_{kn}\sigma_{lo}\sigma_{mp}I_{nopj} + O(h^{5/2}). \end{aligned} \tag{8}$$

The quantities W_i, C_{ij}, H_{ijk}, Z_i, G_{ij}, K_{ij}, and I_{ijkl} are random variables which can be written as stochastic integrals over the Gaussian white noise $\xi(t)$,

$$W_i(h) = \int_0^h dt \xi_i(t) \sim O(h^{1/2}), \tag{9}$$

$$C_{ij}(h)=\int_0^h dtW_i(t)\xi_j(t),\sim O(h), \tag{10}$$

$$H_{ijk}(h)=\int_0^h dtW_i(t)W_j(t)\xi_k(t)\sim O(h^{3/2}), \tag{11}$$

$$Z_i(h)=\int_0^h dtW_i(t)\sim O(h^{3/2}), \tag{12}$$

$$G_{ij}(h)=\int_0^h dtW_i(t)W_j(t)\sim O(h^2), \tag{13}$$

$$K_{ij}(h)=\int_0^h tdtW_i(t)\xi_j(t)\sim O(h^2), \tag{14}$$

$$I_{ijkl}(h)=\int_0^h dtW_i(t)W_j(t)W_k(t)\xi_l(t)\sim O(h^2). \tag{15}$$

Ito integration has been employed in the derivation of the above equations.

The nth moment of the x_i is

$$\langle x_i(h)^n\rangle=\langle[D_i(h)+S_i(h)]^n\rangle=D_i(h)^n+nD_i(h)^{n-1}\langle S_i(h)\rangle + C_n^2 D_i(h)^{n-2}\langle[S_i(h)]^2\rangle+\cdots, \tag{16}$$

where

$$C_n^i=\binom{i}{n}=\frac{n!}{i!(n-i)!} \tag{17}$$

and

$$\langle S_i(h)\rangle=\tfrac{1}{4}F^i_{,kl}\sigma^{ks}\sigma^{ls}h^2+O(h^3), \tag{18}$$

$$\langle S_i(h)S_j(h)\rangle=\sigma^{il}\sigma^{jl}h+\tfrac{1}{2}\sigma^{im}_{,k}\sigma^{kl}\sigma^{jm}_{,p}\sigma^{pl}h^2+\tfrac{1}{2}\sigma^{il}F^j_{,k}\sigma^{kl}h^2 + \tfrac{1}{2}\sigma^{jl}F^i_{,k}\sigma^{kl}h^2+\tfrac{1}{2}\sigma^{il}\sigma^{jl}_{,k}F^k h^2 + \tfrac{1}{2}\sigma^{jl}\sigma^{il}_{,k}F^k h^2+\tfrac{1}{4}\sigma^{ip}\sigma^{jp}_{,kl}\sigma^{km}\sigma^{lm}h^2 + \tfrac{1}{4}\sigma^{jp}\sigma^{ip}_{,kl}\sigma^{km}\sigma^{lm}h^2+O(h^3), \tag{19}$$

$$\langle S_i(h)S_j(h)S_k(h)\rangle=O(h^3), \tag{20}$$

$$\langle S_i(h)^4\rangle=3(\sigma^{ii})^4+O(h^3), \tag{21}$$

$$\langle(S_i(h))^5\rangle=O(h^3). \tag{22}$$

Suppose that the results from a numerical algorithm were written as

$$\overline{x_i}(h)=\overline{D}_i(h)+\overline{S}_i(h), \tag{23}$$

where the $\overline{x_i}$ are approximations to the exact solutions x_i. The nth moment of $\overline{x_i}$ is

$$\langle\overline{x_i}(h)^n\rangle=\langle[\overline{D}_i(h)+\overline{S}_i(h)]^n\rangle=\overline{D}_i(h)^n+n\overline{D}_i(h)^{n-1}\langle\overline{S}_i(h)\rangle + C_n^2\overline{D}_i(h)^{n-2}\langle[\overline{S}_i(h)]^2\rangle+\cdots. \tag{24}$$

Comparing Eqs. (16) and (24), we see that if $D_i(h)$ and $\overline{D}_i(h)$, and $S_i(h)$ and $\overline{S}_i(h)$ coincide up to h^2, we will have

$$x_i(h)-\overline{x_i}(h)=O(h^3) \tag{25}$$

and for a finite time interval

$$\langle x_i(t)^n\rangle-\langle\overline{x_i}(t)^n\rangle=O(h^2). \tag{26}$$

III. STOCHASTIC LEAPFROG ALGORITHM FOR BROWNIAN MOTION

The approach to modeling Brownian motion that we consider here is that of a particle coupled to the environment through its position variable [1]. When this is the case, noise terms enter only in the dynamical equations for the particle momenta. In Eq. (27) below, the indices are single-particle phase-space coordinate indices; the convention used here is that the odd indices correspond to momenta, and the even indices to the spatial coordinate. In the case of three dimensions, the dynamical equations then take the general form

$$\dot{x}_1=F_1(x_1,x_2,x_3,x_4,x_5,x_6)+\sigma_{11}(x_2,x_4,x_6)\xi_1(t),$$

$$\dot{x}_2=F_2(x_1),$$

$$\dot{x}_3=F_3(x_1,x_2,x_3,x_4,x_5,x_6)+\sigma_{33}(x_2,x_4,x_6)\xi_3(t),$$

$$\dot{x}_4=F_4(x_3),$$

$$\dot{x}_5=F_5(x_1,x_2,x_3,x_4,x_5,x_6)+\sigma_{55}(x_2,x_4,x_6)\xi_5(t),$$

$$\dot{x}_6=F_6(x_5). \tag{27}$$

In the dynamical equations for the momenta, the first term on the right-hand side is a systematic drift term which includes the effects due to external forces and damping. The second term is stochastic in nature and describes a noise force which, in general, is a function of position. The noise $\xi(t)$ is first assumed to be Gaussian and white as defined by Eqs. (2) and (3). The stochastic leapfrog algorithm for Eqs. (27) is written as

$$\overline{x_i}(h)=\overline{D}_i(h)+\overline{S}_i(h). \tag{28}$$

The deterministic contribution $\overline{D}_i(h)$ can be obtained using the deterministic leapfrog algorithm [defined by keeping only the first two terms in Eq. (29) below]. The stochastic contribution $\overline{S}_i(h)$ can be obtained by applying Eq. (8) on Eq. (27). The stochastic integration defined by Eqs. (9)–(15) can be approximated so that the moment relationships defined by Eqs. (18) to (22) are satisfied. After some calculation, the deterministic contribution $\overline{D}_i(h)$ and the stochastic

contribution $\overline{S_i}(h)$ of the above recursion formula for one-step integration are found to be

$$\overline{D_i}(h)=\overline{x_i}(0)+hF_i(\overline{x_1^*},\overline{x_2^*},\overline{x_3^*},\overline{x_4^*},\overline{x_5^*},\overline{x_6^*}) \quad (i=1,3,5),$$

$$\overline{D_i}(h)=\overline{x_i^*}+\tfrac{1}{2}hF_i[x_{i-1}+hF_{i-1}(\overline{x_1^*},\overline{x_2^*},\overline{x_3^*},\overline{x_4^*},\overline{x_5^*},\overline{x_6^*})] \quad (i=2,4,6),$$

$$\overline{S_i}(h)=\sigma_{ii}\sqrt{h}W_i(h)+\tfrac{1}{2}F_{i,k}\sigma_{kk}h^{3/2}\tilde{W}_i(h)+\tfrac{1}{2}\sigma_{ii,j}F_jh^{3/2}\tilde{W}_i(h)+\tfrac{1}{4}F_{i,kl}\sigma_{kk}\sigma_{ll}h^2\tilde{W}_i(h)\tilde{W}_i(h) \quad (i=1,3,5;\ j=2,4,6;\ k,l=1,3,5),$$

$$\overline{S_i}(h)=\frac{1}{\sqrt{3}}F_{i,j}\sigma_{jj}h^{3/2}\tilde{W}_j(h)+\frac{1}{4}F_{i,jj}\sigma_{jj}^2h^2\tilde{W}_j(h)\tilde{W}_j(h) \quad (i=2,4,6;\ j=1,3,5),$$

$$\overline{x_i^*}=\overline{x_i}(0)+\tfrac{1}{2}hF_i(\overline{x_1},\overline{x_2},\overline{x_3},\overline{x_4},\overline{x_5},\overline{x_6}) \quad (i=1,2,3,4,5,6), \tag{29}$$

where $\tilde{W}_i(h)$ is a series of random numbers with the moments

$$\langle\tilde{W}_i(h)\rangle=\langle[\tilde{W}_i(h)]^3\rangle=\langle(\tilde{W}_i(h))^5\rangle=0, \tag{30}$$

$$\langle(\tilde{W}_i(h))^2\rangle=1, \quad \langle(\tilde{W}_i(h))^4\rangle=3. \tag{31}$$

This can not only be achieved by choosing true Gaussian random numbers, but also by using the sequence of random numbers following:

$$\tilde{W}_i(h)=\begin{cases}-\sqrt{3}, & R<1/6\\ 0, & 1/6\leqslant R<5/6\\ \sqrt{3}, & 5/6\leqslant R\end{cases} \tag{32}$$

where R is a uniformly distributed random number on the interval (0,1). This trick significantly reduces the computational cost in generating random numbers.

Next we consider the case that the noise in Eqs. (27) is a colored Ornstein-Uhlenbeck process which obeys

$$\langle\xi_i(t)\rangle=0, \tag{33}$$

$$\langle\xi_i(t)\xi_i(t')\rangle=\frac{k_i}{2}\exp(-k_i|t-t'|), \tag{34}$$

where the correlation factor k_i is the reciprocal of the correlation time. In the limit of $k_i\to\infty$, the Ornstein-Uhlenbeck process reduces to Gaussian white noise. The above process can be generated by using a white Gaussian noise from a stochastic differential equation

$$\dot{\xi}_i(t)=-k_i\xi_i(t)+k_i\zeta_i(t), \tag{35}$$

where $\zeta_i(t)$ is a standard Gaussian white noise. The initial value $\xi_i(0)$ is chosen to be a Gaussian random number with $\langle\xi_i(0)\rangle=0$ and $\langle\xi_i(0)^2\rangle=k_i/2$.

For the stochastic process with colored noise, the leapfrog algorithm for Eqs. (27) is of the same form as that for white noise [cf. Eq. (29)], but with

$$\overline{D_i}(h)=\overline{x_i}(0)+hF_i(\overline{x_1^*},\overline{x_2^*},\overline{x_3^*},\overline{x_4^*},\overline{x_5^*},\overline{x_6^*})+h\sigma_{ii}(\overline{x_2^*},\overline{x_4^*},\overline{x_6^*})\xi_i^* \quad (i=1,3,5),$$

$$\overline{D_i}(h)=\overline{x_i^*}+\tfrac{1}{2}hF_i[\overline{x_{i-1}}+hF_{i-1}(\overline{x_1^*},\overline{x_2^*},\overline{x_3^*},\overline{x_4^*},\overline{x_5^*},\overline{x_6^*})+h\sigma_{i-1i-1}(\overline{x_2^*},\overline{x_4^*},\overline{x_6^*})\xi_{i-1}^*] \quad (i=2,4,6),$$

$$\overline{D_{\xi_i}}(h)=\xi_i(0)\exp(-k_ih) \quad (i=1,3,5),$$

$$\overline{S_i}(h)=\frac{1}{\sqrt{3}}\sigma_{ii}(\overline{x_2},\overline{x_4},\overline{x_6})k_ih^{3/2}\tilde{W}_i(h) \quad (i=1,3,5),$$

$$\overline{S_i}(h)=0 \quad (i=2,4,6),$$

$$\overline{S_{\xi_i}}=k_i\sqrt{h}\tilde{W}_i(h)-\tfrac{1}{2}k_i^2h^{3/2}\tilde{W}_i(h) \quad (i=1,3,5), \tag{36}$$

where

$$\overline{x_i^*}=\overline{x_i}(0)+\tfrac{1}{2}h[F_i(\overline{x_1},\overline{x_2},\overline{x_3},\overline{x_4},\overline{x_5},\overline{x_6})+\sigma_{ii}(\overline{x_2},\overline{x_4},\overline{x_6})\xi_i] \quad (i=1,3,5),$$

$$\overline{x_i^*}=\overline{x_i}(0)+\tfrac{1}{2}hF_i(\overline{x_1},\overline{x_2},\overline{x_3},\overline{x_4},\overline{x_5},\overline{x_6}) \quad (i=2,4,6),$$

$$\xi_i^*=\xi_i(0)\exp(-\tfrac{1}{2}k_ih) \quad (i=1,3,5). \tag{37}$$

IV. NUMERICAL TESTS

The above algorithms were tested on a one-dimensional stochastic harmonic oscillator with a simple form of the multiplicative noise. The equations of motion were

$$\dot{p}=F_1(p,x)+\sigma(x)\xi(t),$$

$$\dot{x}=p, \tag{38}$$

where $F_1(p,x)=-\gamma p-\eta^2x$ and $\sigma(x)=-\alpha x$. The stochastic leapfrog integrator for this case is given by Eqs. (29) (white noise) and Eq. (36) (colored noise) with the substitutions $x_1=p$, $x_2=x$. A comparison was also run against the Heun algorithm described in Appendix A.

As a first test, we computed $\langle x^2\rangle$ as a function of time step size. To begin, we took the case of zero damping constant ($\gamma=0$), where $\langle x^2\rangle$ can be determined analytically. The top curve in Fig. 1 shows $\langle x^2\rangle$ at $t=6.0$ as a function of time step size with white Gaussian noise. Here, the parameters η and α are set to 1.0 and 0.1. The ensemble averages were taken over 10^6 independent simulations. The analytically determined value of $\langle x^2\rangle$ at $t=6.0$ is 2.095 222 (the derivation of the analytical results is given in the Appendix). The quadratic convergence of the stochastic leapfrog algorithm is clearly seen in the numerical results. We then considered the case of colored Ornstein-Uhlenbeck noise as a function of time step size using the same parameters as in the white Gaussian noise case and with the correlation parameter k

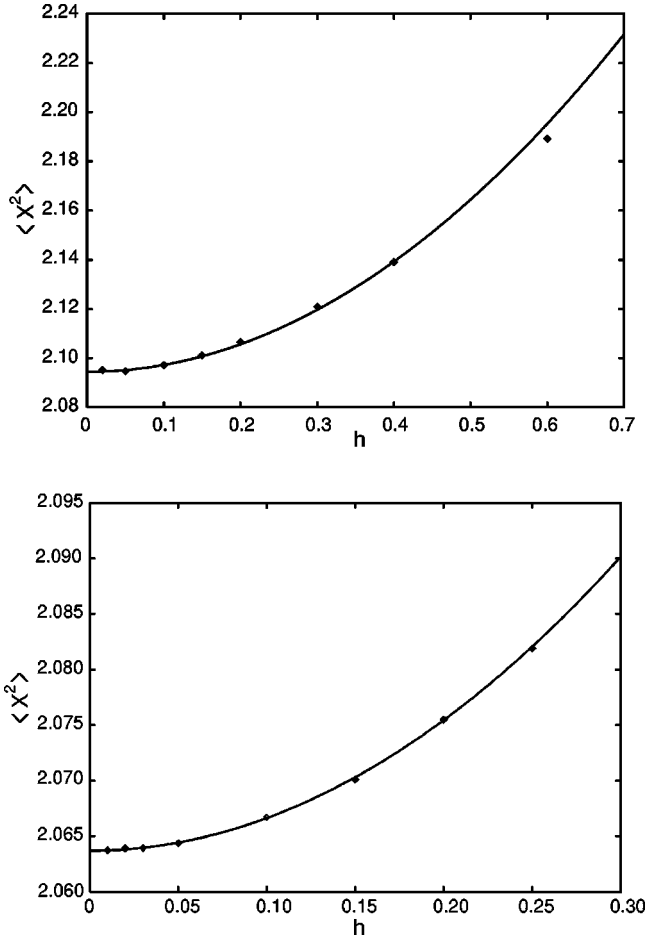

FIG. 1. Zero damping convergence test. Top: $\langle x^2(t)\rangle$ at $t=6$ as a function of step size with white Gaussian noise. Bottom: $\langle x^2(t)\rangle$ at $t=6$ as a function of step size with colored Ornstein-Uhlenbeck noise. Solid lines represent quadratic fits to the data points (diamonds).

$=0.16$. The result is shown as the bottom curve in Fig. 1 and the quadratic convergence is again apparent.

We verified that the quadratic convergence is present for nonzero damping ($\gamma=0.1$). At $t=12.0$, and with all other parameters as above, the convergence of $\langle x^2\rangle$ as a function of time step is shown by the top and bottom curves in Fig. 2 (white Gaussian noise and colored Ornstein-Uhlenbeck noise, respectively).

As a comparison against the conventional Heun's algorithm, we computed $\langle x^2\rangle$ as a function of t using 100 000 numerical realizations for a particle starting from (0.0,1.5) in the (x,p) phase space. The results along with the analytical solution and a numerical solution using Heun's algorithm are given in Fig. 3. Parameters used were $h=0.1$, $\eta=1.0$, and $\alpha=0.1$. The advantage in accuracy of the stochastic leapfrog algorithm over Heun's algorithm is clearly displayed, both in terms of error amplitude and lack of a systematic drift.

We note that while in general Heun's algorithm is only linear for multiplicative noise applications, for the particular problem at hand it turns out to be quadratic. This is due to a coincidence: the stochastic term of x does not contain $W(h)$ but does possess a higher-order term $hW(h)$. However, this higher-order term has a larger coefficient compared with our stochastic leapfrog algorithm, and this accounts for the larger errors observed in Fig. 3.

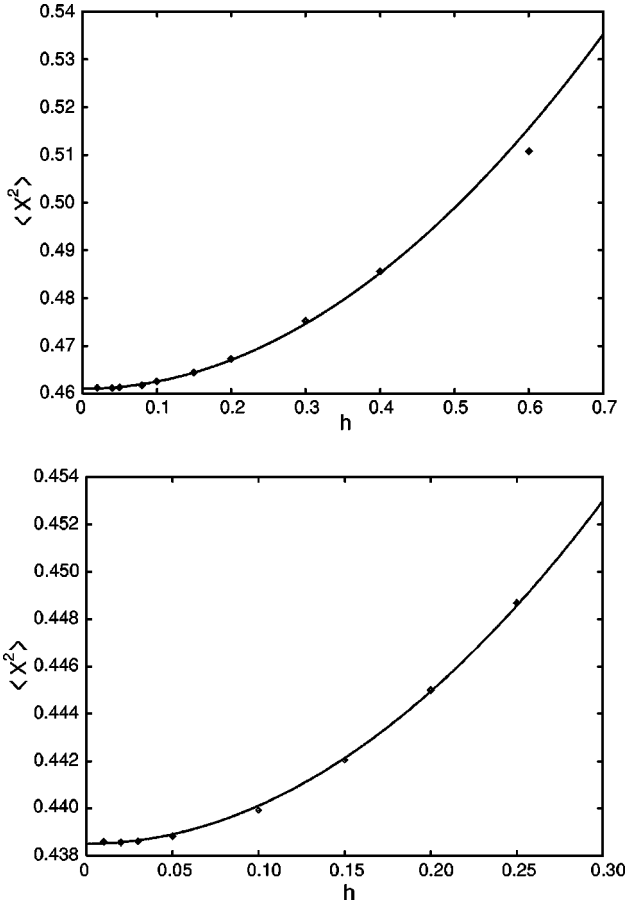

FIG. 2. Finite damping ($\gamma=0.1$) convergence test. Top: $\langle x^2(t)\rangle$ at $t=12$ as a function of step size with white Gaussian noise. Bottom: $\langle x^2(t)\rangle$ at $t=12$ as a function of step size with colored Ornstein-Uhlenbeck noise. Solid lines represent quadratic fits to the data points (diamonds).

V. A PHYSICAL APPLICATION: THE MECHANICAL OSCILLATOR

In this section we apply our algorithm to studying the approach to thermal equilibrium of an oscillator coupled nonlinearly to a heat bath modeled by a set of noninteracting harmonic oscillators [1]. The nonlinear coupling leads to the

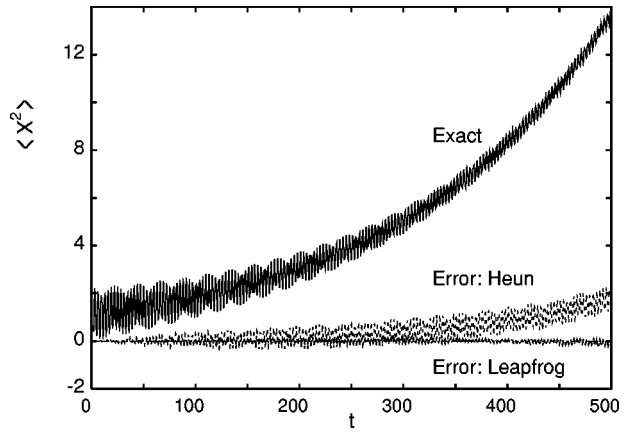

FIG. 3. Comparing the stochastic leapfrog and the Heun algorithm: $\langle x^2(t)\rangle$ as a function of t. Errors are given relative to the exact solution.

introduction of multiplicative noise into the system dynamics. Lindenberg and Seshadri have pointed out that, at weak coupling, multiplicative noise may significantly enhance the equilibration rate relative to the rate for weak linear coupling (additive noise) [2]. We will choose the same form of the coordinate couplings as in Ref. [2], in which case the additive noise equations are

$$\dot{p} = -\omega_0^2 x - \lambda_0 p + \sqrt{2D_0}\xi_0(t),$$

$$\dot{x} = p, \tag{39}$$

and for the system with multiplicative noise only

$$\dot{p} = -\omega_0^2 x - \lambda_2 x^2 p - \sqrt{2D_0}x\xi_2(t),$$

$$\dot{x} = p, \tag{40}$$

where the diffusion coefficients $D_i = \lambda_i kT$, $i = 0,2$, λ_i is the coupling constant, k is Boltzmann's constant, T is the heat bath temperature, and ω_0 is the oscillator angular frequency without damping. The approach to thermal equilibrium is guaranteed for both sorts of noises by the fluctuation-dissipation relation

$$\langle \xi_i(t)\xi_j(s)\rangle = \delta_{ij}\delta(t-s) \tag{41}$$

written here for the general case when both noises are simultaneously present. While in all cases it is clear that the final distribution is identical and has to be the thermal distribution, the precise nature of the approach to equilibrium can certainly be different. We wish to explore this issue in more detail. An important point to keep in mind is that in this particular system of equations there is no noise-induced drift in the Fokker-Planck equation obtained from the Stratonovich form of the Langevin equation, i.e., there is no Ito-Stratonovich ambiguity.

It is a simple matter to solve the Langevin equations given above applying the algorithm from Eqs. (29). As our primary diagnostic, we computed the noise-averaged energy $\langle E(t)\rangle$ of the oscillator as a function of time t, where

$$E(t) = \tfrac{1}{2}p^2 + \tfrac{1}{2}\omega_0^2 x^2. \tag{42}$$

In the weak-coupling limit and employing orbit-averaging (valid presumably when the dynamical time scale is much smaller than the relaxation time scale), one finds [2]

$$\langle E(t)\rangle = kT - (kT - E_0)e^{-\lambda_0 t} \tag{43}$$

in the case of additive noise (a result which can also be directly obtained as a limiting case from the known form of the exact solution given, e.g., in Ref. [24]). The corresponding form of the approximate solution in the case of multiplicative noise is

$$\langle E(t)\rangle = \frac{E_0 kT}{E_0 + (kT - E_0)\exp(-\lambda_2 kTt/\omega_0^2)}. \tag{44}$$

While in the case of additive noise, the exponential nature of the relaxation is already clear from the form of the exact solution (cf. Ref. [24]), the situation in the case of multiplicative noise is not obviously apparent as no exact solution is known to exist. The prediction of a relaxation process controlled by a single exponential as found in Eq. (44) is a consequence of the assumption $\langle x^2(t)\rangle \simeq kT/\omega_0^2$ at ''late'' times, this implying a constant damping coefficient in the Langevin equation (40).

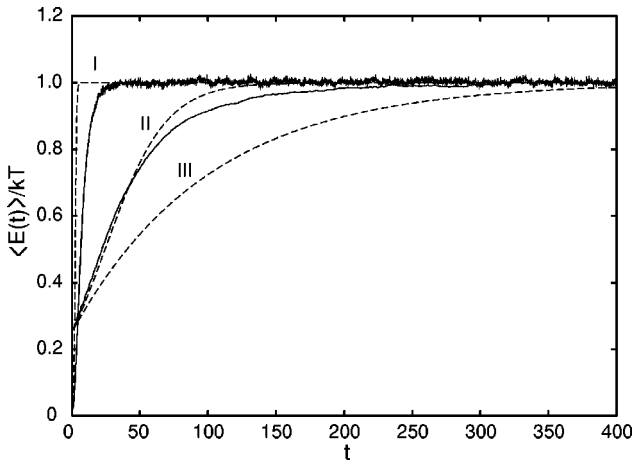

FIG. 4. Temporal evolution of the scaled average energy $\langle E(t)\rangle/kT$ with additive noise and multiplicative noise. The dashed lines I and II are the predictions from Eq. (44) for $kT = 200$ and $kT = 4.5$, respectively. The dashed line III is the theoretical prediction for additive noise with $kT = 4.5$. As predicted, the relaxation proceeds much faster with multiplicative noise: The solid lines are numerical results for multiplicative noise at $kT = 200$ and $kT = 4.5$. It is clear that at higher temperatures, the theory grossly underestimates the relaxation time.

The time-scale separations necessary for the energy-envelope method to be applicable are encoded in the following inequalities [2]:

$$\frac{\lambda_0}{\omega_0} \ll 1 \quad \text{additive noise}, \tag{45}$$

$$\frac{kT\lambda_2}{\omega_0^3} \ll 1 \quad \text{multiplicative noise}. \tag{46}$$

As a first check, we performed simulations with $\omega_0 = 1.0$, $\lambda_0 = \lambda_2 = 0.01$, and $kT = 4.5$, in which case both the above conditions are satisfied. Moreover, with these choices of parameter values, and within the energy-envelope approximation, the relaxation time predicted for multiplicative noise is substantially smaller than for the case of additive noise. At the same time we also ran a simulation at $kT = 200$ to see how the energy-envelope approximation for multiplicative noise breaks down at high temperatures.

In Fig. 4 we display the time evolution of the average energy (scaled by kT for convenience) with additive and multiplicative noise both from the simulations and the approximate analytical calculations. In the case of weak coupling to the environment (small λ_0, λ_2), the rate at which the average energy approaches equilibrium is significantly greater for the case of multiplicative noise relative to the case of additive noise more or less as expected. In addition, the analytic approximation resulting from the application of the energy-envelope method (44) is seen to be in reasonable

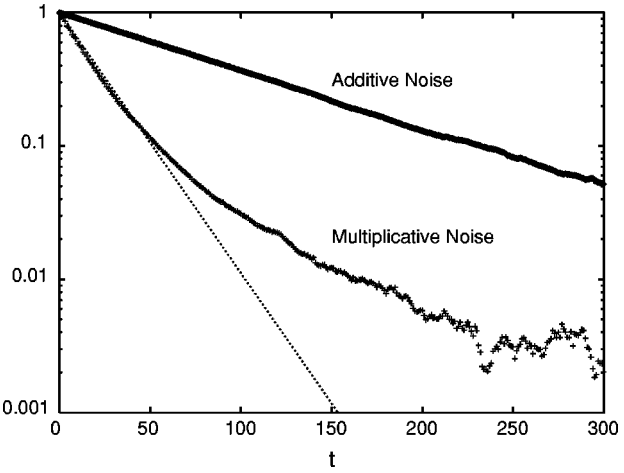

FIG. 5. The left-hand side of Eq. (47) as a function of time (straight line) compared with numerical results for $kT=4.5$. Also shown is a numerical result for the case of additive noise which is in excellent agreement with the predicted exponential relaxation with the relaxation time scale $=1/\lambda_0$.

agreement with the numerical simulations for $kT=4.5$. The slightly higher equilibration rate from the analytical calculation is due to the truncation in the energy-envelope equation using the $\langle E^2(t)\rangle \approx 2\langle E(t)\rangle^2$ relation which yields an upper bound on the rate of equilibration of the average energy [2]. Note that in the case of high temperature ($kT=200$) the relaxation time computed from the energy-envelope method is much smaller than the numerical result, consistent with the violation of the condition (46).

While the results shown in Fig. 4 do show that the energy-envelope approximation is qualitatively correct within its putative domain of validity, it is clear that the actual relaxation process is not of the precise form (44). In Fig. 5 we illustrate this point by plotting

$$\frac{E_0[kT-\langle E(t)\rangle]}{\langle E(t)\rangle(kT-E_0)}=\exp(-\lambda_2 kTt/\omega_0^2) \tag{47}$$

[equivalent to Eq. (44)] against time on a logarithmic scale: the relaxation is clearly nonexponential. The reason for the failure of the approximation is that despite the fact that equipartition of energy does take place on a relatively short time-scale, it is not true that $\langle x^2(t)\rangle$ can be treated as a constant even at relatively late times.

VI. CONCLUSIONS

We have presented a stochastic leapfrog algorithm for single-particle Brownian motion with multiplicative noise. This method has the advantages of retaining the symplectic property in the deterministic limit, ease of implementation, and second-order convergence of moments for multiplicative noise. Sampling a uniform distribution instead of a Gaussian distribution helps to significantly reduce the computational cost. A comparison with the conventional Heun's algorithm highlights the gain in acuracy due to the new method. Finally, we have applied the stochastic leapfrog algorithm to a nonlinearly coupled oscillator-heat-bath system in order to investigate the effect of multiplicative noise on the nature of the relaxation process.

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APPENDIX A

In this section we give short descriptions of the Euler and Heun algorithms referenced in the text. The Euler algorithm is defined by

$$\overline{x_i}(h)=\overline{x_i}(0)+F_i(\overline{x_1}(0),\ldots,\overline{x_n}(0))h + \sigma_{ij}((\overline{x_1}(0),\ldots,\overline{x_n}(0))\tilde{W}_j(h). \tag{A1}$$

The convergence of the moments of the Euler algorithm for a finite time interval is of order h for both additive and multiplicative noise.

The Heun algorithm is defined by

$$\overline{x_i}(h)=\overline{x_i}(0)+\tfrac{1}{2}[F_i(\overline{x_1}(0),\ldots,\overline{x_n}(0)) + F_i(\psi_1(h),\cdots,\psi_n(h))]h + \sigma_{ij}(\overline{x_1}(0),\cdots,\overline{x_n}(0))\tilde{W}_j(h), \tag{A2}$$

where

$$\psi_i(h)=\overline{x_i}(0)+F_i(\overline{x_1}(0),\ldots,\overline{x_n}(0))h + \sigma_{ij}(\overline{x_1}(0),\cdots,\overline{x_n}(0))\tilde{W}_j(h). \tag{A3}$$

This algorithm has an order h^2 convergence of the moments for a finite time interval with additive noise and, in general, the same order of convergence of the moments as the Euler algorithm in the presence of multiplicative noise. (More detailed discussions of these algorithms can be found in Ref. [14].)

APPENDIX B

The analytic solution of Eqs. (38) for $\langle x^2(t)\rangle$ (with white Gaussian noise) as a function of time in the special case of zero damping, i.e., $\gamma=0$, can be obtained by solving the equivalent Fokker-Planck equation [24] for the probability density $f(x,p,t)$,

$$\frac{\partial}{\partial t}f(x,p,t)=\left[-p\frac{\partial}{\partial x}-\frac{\partial F_1(p,x)}{\partial p}+\frac{1}{2}\sigma^2(x)\frac{\partial^2}{\partial p^2}\right]f(x,p,t). \tag{B1}$$

The expectation value of any function $M(x,p;t)$ can be written as

$$\langle M(x,p)\rangle=\int_{-\infty}^{+\infty}dx\,dp M(x,p)f(x,p,t). \tag{B2}$$

Equations (B1) and (B2) can be used to yield a BBGKY-like heirarchy for the evolution of phase-space moments. Since the system we are considering is linear, this heirarchy truncates exactly and yields a group of coupled linear ordinary differential equations for the moments $\langle x^2\rangle$, $\langle xp\rangle$, and $\langle p^2\rangle$. These equations can be written as a single third-order time evolution equation for $\langle x^2\rangle$,

$$\frac{d^3\langle x^2\rangle}{dt^3} = -4\eta^2\frac{d\langle x^2\rangle}{dt} + 2\alpha^2\langle x^2\rangle, \tag{B3}$$

subject to the initial conditions

$$\begin{aligned}\langle x^2(0)\rangle &= x^2(0),\\ \langle \dot{x}^2(0)\rangle &= 2x(0)p(0),\\ \langle \ddot{x}^2(0)\rangle &= 2p^2(0) - 2\eta^2 x^2(0).\end{aligned} \tag{B4}$$

This equation has an analytical solution written as

$$\langle x^2(t)\rangle = c_1\exp(r_1 t) + c_2\exp(r_2 t) + c_3\exp(r_3 t), \tag{B5}$$

where c_1, c_2, and c_3 are constants depending on initial conditions, and r_1, r_2 and r_3 are the roots of a third-order alegbraic equation

$$2\alpha^2 - 4\eta^2 x - x^3 = 0, \tag{B6}$$

which gives

$$\begin{aligned} r_1 &= (\sqrt{64/27\,\eta^6 + \alpha^4} + \alpha^2)^{1/3} - (\sqrt{64/27\,\eta^6 + \alpha^4} - \alpha^2)^{1/3},\\ r_2 &= \tfrac{1}{2}(1 + \sqrt{3}i)(\sqrt{64/27\,\eta^6 + \alpha^4} - \alpha^2)^{1/3}\\ &\quad - \tfrac{1}{2}(1 - \sqrt{3}i)(\sqrt{64/27\,\eta^6 + \alpha^4} + \alpha^2)^{1/3},\\ r_3 &= r_2^*, \end{aligned} \tag{B7}$$

where the superscript * represents complex conjugation. The existence of the positive real root r_1 implies that $\langle x^2(t)\rangle$ will have an exponential growth in time.

[1] R. Zwanzig, J. Stat. Phys. **9**, 215 (1973).
[2] K. Lindenberg and V. Seshadri, Physica A **109**, 483 (1981).
[3] A. Careta and F. Sagues, Phys. Rev. A **44**, 2284 (1991).
[4] S. Habib and H. Kandrup, Phys. Rev. D **46**, 5303 (1992).
[5] S. Habib, Ann. N.Y. Acad. Sci. **706**, 111 (1993).
[6] G. Efremov, L. Mourokh, and A. Smirnov, Phys. Lett. A **175**, 89 (1993).
[7] A. Becker and L. Kramer, Phys. Rev. Lett. **73**, 955 (1994).
[8] H. Leung, Physica A **221**, 340 (1995).
[9] J. Bao, Y. Zhuo, and X. Wu, Phys. Lett. A **217**, 241 (1996).
[10] S. Mangioni, R. Deza, H. Wio, and R. Toral, Phys. Rev. Lett. **79**, 2389 (1997).
[11] W. Genovese, M. Munoz, and J. Sancho, Phys. Rev. E **57**, R2495 (1998).
[12] R. Kubo, J. Math. Phys. **4**, 174 (1963).
[13] R.W. Zwanzig, in *Statistical Mechanics; New Concepts, New Problems, New Applications*, edited by S.A. Rice, K.F. Freed, and J.C. Light (University of Chicago Press, Chicago, 1972).
[14] A. Greiner, W. Strittmatter, and J. Honerkamp, J. Stat. Phys. **51**, 94 (1988).
[15] R. Mannella and V. Palleschi, Phys. Rev. A **40**, 3381 (1989).
[16] R. Mannella, in *Noise in Nonlinear Dynamical Systems*, edited by F. Moss and P.V.E. McClintock (Cambridge University Press, Cambridge, 1989), Vol. 3.
[17] R.L. Honeycutt, Phys. Rev. A **45**, 600 (1992).
[18] P.E. Kloeden and E. Platen, *Numerical Solution of Stochastic Differential Equations* (Springer, New York, 1992).
[19] R. Mannella, in *Supercomputation in Nonlinear and Disordered Systems*, edited by L. Vazuez, F. Tirado, and I. Marun (World Scientific, 1996), p. 101.
[20] S. Habib, H.E. Kandrup, and M.E. Mahon, Phys. Rev. E **53**, 5473 (1996).
[21] M. Seesselberg, H.P. Breuer, H. Mais, F. Petruccione, and J. Honerkamp, Z. Phys. C **62**, 63 (1994).
[22] M.P. Allen and D.J. Tildesley, *Computer Simulation of Liquids* (Clarendon Press, Oxford, 1987).
[23] C.W. Gardiner, *Handbook of Stochastic Methods for Physics, Chemistry, and the Natural Sciences* (Springer, New York, 1983).
[24] H. Risken, *The Fokker-Planck Equation: Methods of Solution and Applications* (Springer, New York, 1989).