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Simulation of one-dimensional noisy Hamiltonian systems and their application to particle storage rings

M. Seeßelberg[1], H.P. Breuer[1], H. Mais[2], F. Petruccione[1], J. Honerkamp[1]

[1] Albert-Ludwings-Universität, Fakultät für Physik, Hermann-Herder Strasse 3, D-79104 Freiburg, Germany (FAX: 0761/203 5821)
[2] Deutsches Elektronen-Synchrotron DESY, Notkestrasse 85, D-22607 Hamburg, Germany (FAX: 040/8994 4305)

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Abstract. Stochastic differential equations are investigated which reduce in the deterministic limit to the canonical equations of motion of a Hamiltonian system with one degree of freedom. For example, stochastic differential equations of this type describe synchrotron oscillations of particles in storage rings under the influence of external fluctuating electromagnetic fields. In the first part of the article new numerical integration algorithms are proposed which take into account the symplectic structure of the deterministic Hamiltonian system. It is demonstrated that in the case of small white noise the algorithm is more efficient than conventional schemes for the integration of stochastic differential equations. In the second part the algorithms are applied to synchrotron oscillations. Analytical approximations for the expectation value of the squared longitudinal phase difference between the particle and the reference particle on the design orbit are derived. These approximations are tested by comparison with numerical results which are obtained by use of the symplectic integration algorithms.

1 Introduction

In this article we propose new algorithms for the numerical integration of a set of two stochastic differential equations which reduce in the deterministic limit to the canonical equations of motion of an autonomous Hamiltonian system with one degree of freedom. Equations of this type arise when synchrotron oscillations of a particle in a storage ring are investigated [1, 2]. Under the influence of fluctuating electromagnetic fields a particle performs stochastically perturbed oscillations with respect to a reference particle which travels with fixed energy along the design orbit of the accelerator. The oscillations in the plane transverse to the design orbit are called betatron oscillations; the energy or phase oscillations with respect to the reference particle are referred to as synchrotron oscillations. To a first approximation the coupling between these oscillatory degrees of freedom is negligible and the equations of motion governing synchrotron oscillations can be written as canonical equations of motion of an autonomous Hamiltonian function with one degree of freedom driven by random forces [3, 4, 5].

Let us consider the following set of stochastic differential equations

$$\dot{p}(t)=F(x)+\sigma(x)\xi(t), \quad F(x)\overset{\text{def}}{=}-\frac{\partial V}{\partial x}(x),$$

$$\dot{x}(t)=\frac{p(t)}{m}. \tag{1}$$

The variables p and x denote momentum and position of a particle with mass m. Random forces are described by the stochastic process $\xi(t)$ which is assumed to be either a Gaussian colored or white noise process. The function $\sigma(x)$ specifies the influence of the random forces on the motion of the particle. In the deterministic limit $\sigma=0$ the differential equations (1) reduce to a set of canonical equations of motion. Note that there is no Ito–Stratonovich interpretation problem [6, 7] since we assume that $\sigma(x)$ does not depend on momentum p and, therefore, both kinds of interpretation are equivalent.

Given these equations, expectation values $\langle M(p,x)\rangle(t)$ of a function $M(p,x)$ are of interest. For example when investigating synchrotron oscillations the second moment $\langle x^2\rangle(t)$ represents the mean of the squared longitudinal phase difference of particles with respect to the reference particle on the design orbit. Since these expectation values can be calculated analytically only in very few cases, numerical methods are required. The usual approach is as follows [8, 9]. An ensemble of approximate solutions of the set of stochastic differential equations is generated by use of an appropriate numerical integration algorithm; then the expectation value $\langle M(p,x)\rangle(t)$ is estimated as an ensemble average.

In this paper we suggest new algorithms for the numerical integration of system (1) in the case of Gaussian colored and white noise $\xi(t)$. Provided the influence of noise on the macroscopic variables p and x is small they allow a more efficient estimation of the expectation values $\langle M(p,x)\rangle(t)$ than conventional algorithms, e.g., the

stochastic Heun method [8, 9]. Our algorithms are particularly well suited to the numerical integration of system (1) because in the deterministic limit $\sigma=0$ they become identical with symplectic integration algorithms. Conventional stochastic integration algorithms lack this property. In the case of a Gaussian white noise process $\xi(t)$ we demonstrate the efficiency of our algorithm.

As an example we study synchrotron oscillations which may be described by the following equations of motion [3, 4]

$$\dot{p}(t)=-\omega^2\sin(x)+\sigma(x)\xi(t),$$

$$\dot{x}(t)=p.$$

In this context p is proportional to the energy deviation of the particle from the reference particle travelling on the design orbit; x measures the longitudinal phase difference of both particles. We consider phase noise ($\sigma(x)=\lambda\cos(x)$) and amplitude noise ($\sigma(x)=\lambda\sin(x)$) with Gaussian white and colored noise processes $\xi(t)$. In accelerator physics the growth of the moment $\langle x^2\rangle(t)$ with time and its dependence on statistical properties of the noise term $\sigma(x)\xi(t)$ is of interest. In order to obtain a general view of the behaviour of $\langle x^2\rangle(t)$ this moment is determined analytically for an ensemble of harmonic oscillators driven by random forces. This approximation is expected to yield acceptable results for smalll values of x which is the typical situation in accelerator physics since small values of x correspond to small deviations of the particle from the reference particle. In order to demonstrate the validity of our analytical approximations we estimate $\langle x^2\rangle(t)$ by use of our symplectic algorithms and compare these results with the analytical approximations.

This paper is divided into five sections. Section 2 contains a brief review of symplectic algorithms for the numerical integration of the canonical equations of motion of a deterministic Hamiltonian function with one degree of freedom. In Sect. 3 these algorithms are generalized to allow the integration of canonical equations of motion with Gaussian white or colored noise terms. We restrict ourselves to stochastic differential equations which reduce in the deterministic limit to the canonical equations of an autonomous Hamiltonian system with one degree of freedom. In the white noise case, an example demonstrates the efficiency of our algorithm. Section 4 is devoted to the study of synchrotron oscillations. For Gaussian white and colored noise we evaluate approximations of the moment $\langle x^2\rangle(t)$ and examine their validity by comparing with numerical estimations obtained with our algorithms. Section 5 contains a summary and a discussion of the results of the article.

2 Symplectic integration of deterministic canonical equations of motion

Difference schemes such as the well-known Runge–Kutta algorithms [10] are frequently used for the numerical integration of deterministic Hamiltonian equations of motion. These algorithms do not take into account the fact that the phase flow of the corresponding canonical equations of motion is a symplectic map. Therefore, some authors (e.g. [11–13]) proposed symplectic algorithms which are well suited for the integration of these equations. In this section, we briefly summarize some facts concerning the symplectic integration of deterministic one-dimensional Hamiltonian systems.

Let us consider a Hamilton function $H(p, x)$ and the corresponding canonical equations

$$\dot{p}(t)=-\frac{\partial H}{\partial x},\quad \dot{x}(t)=\frac{\partial H}{\partial p}. \tag{2}$$

Given initial values (p^0, x^0) at time $t=0$ the state of the system $(p(t), x(t))$ is uniquely determined. If we introduce the phase flow f_H^t corresponding to Hamilton's function $H(p, x)$ we may write

$$\begin{pmatrix} p(t) \\ x(t) \end{pmatrix}=f_H^t\begin{pmatrix} p^0 \\ x^0 \end{pmatrix}.$$

The phase flow f_H^t is a symplectic map which means in our case that the determinant of the corresponding Jacobi matrix $\mathbf{Df_H^t}$ is equal to one:

$$\det(\mathbf{Df_H^t})=1. \tag{3}$$

In order to solve numerically the system of differential equations (2) one proceeds as follows. We choose a small time step h and replace the exact phase flow f_H^h by an approximation $\bar{f}_H^h$. Then the recursion formula

$$\begin{pmatrix} \bar{p}_h(k+1) \\ \bar{x}_h(k+1) \end{pmatrix}=\bar{f}_H^h\begin{pmatrix} \bar{p}_h(k) \\ \bar{x}_h(k) \end{pmatrix},\quad \bar{p}_h(0)\overset{\text{def}}{=}p^0,\quad \bar{x}_h(0)\overset{\text{def}}{=}x^0$$

is iterated. Supposing $\bar{f}_H^h$ is a good approximation of f_H^h then the quantities $\bar{p}_h(k)$, $\bar{x}_h(k)$ are good approximations of the state of the system $p(t=kh)$, $x(t=kh)$.

Given a system of differential equations, an algorithm for its numerical solution yields an approximate phase flow $\bar{f}_H^h$. One expects an algorithm to be best suited for the approximation of Hamiltonian systems (2) if the approximation $\bar{f}_H^h$ is a symplectic map which obeys condition (3). These algorithms are referred to as symplectic algorithms. As mentioned above common integration schemes lack this property [12].

These considerations can be generalized to yield symplectic algorithms for the numerical integration of the canonical equations of motion of a time-dependent Hamiltonian function with several degrees of freedom. Efficient symplectic algorithms for a Hamilton function $H(\mathbf{p}, \mathbf{x}, t)=T(\mathbf{p})+V(\mathbf{x}, t)$ with kinetic energy $T(\mathbf{p})$ and potential energy $V(\mathbf{x}, t)$ are investigated in reference [12]. Restricting ourselves to time-dependent Hamiltonian functions $H(p, x, t)=T(p)+V(x, t)$ with one degree of freedom we introduce the force $F(x, t)=-\partial V/\partial x$ and the derivative of the kinetic energy $P(p)=\partial T/\partial p$. Then an n-th order scheme for an integration from time $t_0=kh$ to $t=(k+1)h$ is given by the following recursion formula which must be iterated from $i=1$ to $i=n$:

$$\bar{p}_h\left(k+\frac{i}{n}\right)=\bar{p}_h\left(k+\frac{i-1}{n}\right)+b_i hF\left(\bar{x}_h\left(k+\frac{i-1}{n}\right), t_{i-1}\right),$$

$$\bar{x}_h\left(k+\frac{i}{n}\right)=\bar{x}_h\left(k+\frac{i-1}{n}\right)+a_i hP\left(\bar{p}_h\left(k+\frac{i}{n}\right)\right),$$

$$t_i=t_{i-1}+a_i h. \tag{4}$$

The leapfrog algorithm is obtained by choosing $n=2$. In this case the coefficients a_i, b_i are [12]

$$a_1=a_2=\tfrac{1}{2},\quad b_1=0,\quad b_2=1,$$

whereas in the case of the fourth order algorithm these coefficients are [12]

$$a_1=a_4=\tfrac{1}{6}(2+2^{1/3}+2^{-1/3}),\quad a_2=a_3=\tfrac{1}{6}(1-2^{1/3}-2^{-1/3}),$$

$$b_1=0,\quad b_2=b_4=(2-2^{1/3})^{-1},\quad b_3=(1-2^{2/3})^{-1}.$$

We will employ the second order leapfrog algorithm when Hamiltonian systems driven by white noise forces are investigated. The fourth order algorithm will form the basis for the integration of Hamiltonian systems under the influence of colored noise.

3 Integration of canonical equations with noise

This section deals with algorithms for the numerical integration of the system of stochastic differential equations (1). The stochastic term $\xi(t)$ is assumed to be either a standard Gaussian white noise process with the expectation values

$$\langle\xi(t)\rangle=0,\quad \text{and}\quad \langle\xi(t)\xi(t')\rangle=\delta(t-t'),$$

or a Gaussian colored noise process. In this paper, for Gaussian colored noise we always use the Ornstein–Uhlenbeck process [7] obeying

$$\langle\xi(t)\rangle=0,\quad \text{and}\quad \langle\xi(t)\xi(t')\rangle=\frac{\kappa}{2}\exp(-\kappa|t-t'|).$$

The Ornstein–Uhlenbeck process is characterized by a correlation factor κ; its reciprocal $1/\kappa$ is the correlation time. In the limit $\kappa\to\infty$ the Ornstein–Uhlenbeck process becomes identical with Gaussian white noise.

The essential difference between Gaussian white noise and the Ornstein–Uhlenbeck process is that realizations of Gaussian white noise are discontinuous at ach time t while those of the Ornstein–Uhlenbeck process are continuous functions [7]. Therefore, the deterministic integration schemes of the previous section are easily generalized to cope with colored noise; for white noise the generalization turns out to be more complicated.

3.1 Colored noise

Since realizations of colored noise are continuous functions the fourth order symplectic algorithm (4) is appropriate for the integration of the stochastic system (1) provided that trajectories $\xi(t)$ of the Ornstein–Uhlenbeck process can be generated. This can easily be done by use of the following stochastic differential equation [7]

$$\dot{\xi}(t)=-\kappa\xi(t)+\kappa\zeta(t),$$

$$\zeta(t)\ \text{standard Gaussian white noise},\qquad (5)$$

where the initial value $\xi(0)$ is chosen as Gaussian random number with $\langle\xi(0)\rangle=0$ and $\langle\xi(0)^2\rangle=\kappa/2$. With the help of the stochastic Euler-algorithm [8, 9] approximations $\bar{\xi}_h(k)$ of individual trajectories $\xi_h(t=kh)$ are generated by iteration of the recursion formula

$$\bar{\xi}_h(k+1)=\bar{\xi}_h(k)\exp(-\kappa h)+\kappa\sqrt{h}\eta(k)$$

where the symbol $\eta(k)$ denotes a sequence of equally distributed random numbers with zero mean and variance 1.

Thus, defining a time-dependent force $F(x,t)$ as the sum of the deterministic force $F(x)$ and the stochastic contribution $\sigma(x)\xi(t)$

$$F(x,t)=F(x)+\sigma(x)\xi(t),$$

we can use the fourth order algorithm of Sect. 2 to obtain a realization of the stochastic differential equation (1) in the case of colored noise $\xi(t)$.

3.2 The stochastic leapfrog algorithm for white noise

For the sake of clarity we will omit lengthy calculations at this point; in Appendix A we give a proof that the following algorithm is suited for the approximation of system (1) in the case of Gaussian white noise. The recursion formula reads

$$\begin{pmatrix}\bar{p}_h(k+1)\\ \bar{x}_h(k+1)\end{pmatrix}=\begin{pmatrix}\bar{p}_h(k)\\ \bar{x}_h(k)\end{pmatrix}+h\begin{pmatrix}F(\chi(k))\\ \bar{p}_h(k)/m+hF(\chi(k))/(2m)\end{pmatrix}+\sigma(\bar{x}_h(k))\eta(k)\begin{pmatrix}\sqrt{h}\\ h^{3/2}/(m\sqrt{3})\end{pmatrix}\qquad (6)$$

where we have introduced the abbreviation

$$\chi(k)\overset{\text{def}}{=}\bar{x}_h(k)+\frac{h}{2m}\bar{p}_h(k).$$

$\eta(k)$ denotes a sequence of random numbers with the moments

$$\langle\eta(k)\rangle=\langle\eta(k)^3\rangle=\langle\eta(k)^5\rangle=0,$$

$$\langle\eta(k)^2\rangle=1,\quad \langle\eta(k)^4\rangle=3.$$

This can be achieved by choosing Gaussian random numbers as well as using

$$\eta(k)=\begin{cases}4\sqrt{3+\sqrt{6}}(\vartheta(k)-0.25), & \text{if } \vartheta(k)<0.5,\\ 4\sqrt{3-\sqrt{6}}(\vartheta(k)-0.75), & \text{if } \vartheta(k)\geq 0.5,\end{cases}\qquad (7)$$

where $\vartheta(k)$ are equally distributed random numbers in [0, 1]. The generation of a sequence $\eta(k)$ according to this definition is much faster than the generation of Gaussian random numbers; thus the CPU-time required for the iteration of recursion formula (6) is reduced.

In Appendix A it is shown that the difference between the exact expectation value $\mathcal{M}(t)$ and its estimation $\mathcal{M}_h(t)$ obeys

$$\mathcal{M}_h(t)-\mathcal{M}(t)=\begin{cases}\mathcal{O}(h), & \text{if } \sigma(x) \text{ is a function of } x,\\ \mathcal{O}(h^2), & \text{if } \sigma \text{ is constant},\end{cases}\qquad (8)$$

where h denotes the time step and $\mathcal{O}(h^m)$ represents terms of order h^m.

In the deterministic limit $\sigma=0$ the recursion formula (6) takes the form

$$\begin{pmatrix}\bar{p}_h(k+1)\\ \bar{x}_h(k+1)\end{pmatrix}=\begin{pmatrix}\bar{p}_h(k)\\ \bar{x}_h(k)\end{pmatrix}+h\begin{pmatrix}F(\chi(k))\\ \bar{p}_h(k)/m+hF(\chi(k))/(2m)\end{pmatrix}.$$

This recursion formula is easily seen to be equivalent to that of the deterministic leapfrog algorithm (4). Therefore we designate recursion formula (6) as stochastic leapfrog algorithm. In the deterministic limit it is symplectic as its Jacobi matrix

$$\mathbf{D}\bar{\mathbf{f}}_{\mathbf{H}}^{\mathbf{h}}=\begin{pmatrix}1+h^2F'(\chi(k))/(2m) & hF'(\chi(k))\\ h/m+h^3F'(\chi(k))/(4m^2) & 1+h^2F'(\chi(k))/(2m)\end{pmatrix}$$

fulfills the condition $\det(\mathbf{D}\bar{\mathbf{f}}_{\mathbf{H}}^{\mathbf{h}})=1$ of a symplectic flow.

3.3 Comparison of Heun's method with the stochastic leapfrog algorithm

In order to illustrate the efficiency of the stochastic leapfrog algorithm we estimate the energy expectation value of a Hamiltonian system driven by Gaussian white noise with the stochastic leapfrog algorithm and Heun's method. Heun's method is a standard algorithm for the numerical integration of stochastic differential equations which is described in detail elsewhere (see, e.g. [8, 9]). In this subsection we treat system (1) when σ is constant. By use of the corresponding Fokker–Planck equation we show in Appendix B that in this case the energy expectation value $\mathscr{E}(t)=\langle p^2/2m+V(x)\rangle$ can be evaluated analytically. We obtain (see (26))

$$\mathscr{E}(t)=\frac{(p^0)^2}{2m}+V(x^0)+\frac{\sigma^2}{2m}t. \tag{9}$$

As is to be expected in the deterministic limit $\sigma=0$ the energy is constant. However, under the influence of Gaussian white noise the energy increases linearly with time. At a first glance the growth of energy may be surprising but it simply reflects the fact that the Fokker–Planck equation does not converge to a stationary solution because there is no damping force in the underlying system of stochastic differential equations [14]. Furthermore, the energy growth is independent of the potential $V(x)$.

Now we estimate numerically the energy expectation value of an ensemble of particles with potential energy $V(x)=\gamma x^4$ under the influence of Gaussian white noise:

$$\dot{p}(t)=-4\gamma x(t)^3+\sigma\xi(t),$$

$$\dot{x}(t)=\frac{p(t)}{m_p}. \tag{10}$$

In this example m_p is the proton mass. We choose initial values $p^0=0$ and $x^0=10\,l$ where l denotes the unit of length. The constants σ and γ are $\gamma=1\,m_p l^{-2}\,\mathrm{s}^{-2}$ and $\sigma=2m_p l\,\mathrm{s}^{-3/2}$. Then a period of oscillation takes approximately the time $T=0.37$ s. From time $t=0$ to $t=20$ s we generated $N=80000$ approximate solutions for several values of the time step h with both Heun's method and the stochastic leapfrog algorithm (6). From these solutions we estimated the energy expectation value $\mathscr{E}(t=20\,\mathrm{s})$ and its standard error. The results are shown in Fig. 1: The triangles represent estimations by Heun's method, the squares show estimations obtained by the stochastic leapfrog algorithm (6). The continuous line is the analytical energy expectation value $\mathscr{E}(t=20\,\mathrm{s})=10040\,m_p l^2\,\mathrm{s}^{-2}$ given by (9). The energy expectation value can be correctly estimated with both Heun's method and the stochastic leapfrog algorithm if the time step h is small.

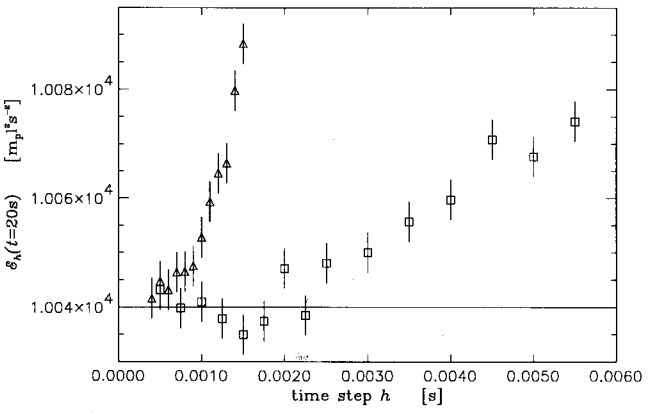

Fig. 1. The energy expectation value $\mathscr{E}(t)$ of system (10) at time $t=20$s is estimated with different values of the time step h. Parameters are $\gamma=1\,m_p l^{-2}\,\mathrm{s}^{-2}$, $\sigma=2m_p l\,\mathrm{s}^{-3/2}$, $x(0)=10l$, $p(0)=0$. The triangles and squares represent estimations obtained by Heun's method and the stochastic leapfrog algorithm respectively. The full line shows the analytical result (9) which is $\mathscr{E}(t=20\,\mathrm{s})=10040\,m_p l^2\,\mathrm{s}^{-2}$

As one can see from Fig. 1 already for a time step $h=0.00175$ s the exact value $\mathscr{E}(t=20\,\mathrm{s})$ lies within the error bars of the estimated energy expectation value when the stochastic leapfrog algorithm is employed. In order to obtain an estimation with Heun's method which is of the same accuracy one is forced to use the smaller time step $h=0.0006$ s. This is the reason for the efficiency of the stochastic leapfrog algorithm. Using the same time step h, the generation of trajectories with both algorithms requires the same CPU-time. Since the CPU-time is inversely proportional to the time step h, we expect that in our example the estimation with the stochastic leapfrog algorithm using $h=0.00175$ s takes only about a third of the CPU-time required by Heun's method using $h=0.0006$ s. Indeed, the estimation of the energy expectation value with the leapfrog algorithm using $h=0.00175$s took 121 minutes CPU-time on an IBM Risc 6000/320 workstation whereas the estimation with Heun's method and $h=0.0006$ s required 352 minutes CPU-time on the same machine.

Our example shows that the stochastic leapfrog algorithm is more efficient than the stochastic Heun method. Since (8) which describes the convergence of estimations $\mathscr{M}_h(t)$ obtained with the stochastic leapfrog algorithm is also valid for Heun's method [8, 9] both methods are of the same order. Therefore, the efficiency of the stochastic leapfrog algorithm is due to the fact that in the deterministic limit the approximate phase flow is a symplectic map.

4 Synchrotron oscillations

In this section we study synchrotron oscillations in particle storage rings which can be described by a stochastically perturbed Hamiltonian function of a pendulum [3]

$$H(p, x, t)=\frac{p^2}{2}-\omega^2\,(1+\lambda_A\xi_A(t))\cos(x)$$
$$+\omega^2\sin(x)\lambda_{\mathrm{Ph}}\xi_{\mathrm{Ph}}(t).$$

The stochastic terms $\lambda_A\xi_A(t)$ and $\lambda_{\mathrm{Ph}}\xi_{\mathrm{Ph}}(t)$ are called amplitude noise and phase noise respectively. The dimensionless variable x denotes the longitudinal phase difference between the particle and the reference particle on the design orbit. p is measured in units of s^{-1} and is proporional to the energy deviation of the particle from the reference particle.

In the case of pure phase noise ($\lambda_A=0$) the equations of motion are

$$\dot{p}(t)=-\omega^2\sin(x)-\lambda_{\mathrm{Ph}}\omega^2\cos(x)\,\xi_{\mathrm{Ph}}(t),\quad \dot{x}(t)=p, \tag{11}$$

whereas for pure amplitude noise ($\lambda_{\mathrm{Ph}}=0$) we obtain

$$\dot{p}(t)=-\omega^2\sin(x)-\lambda_A\omega^2\sin(x)\,\xi_A(t),\quad \dot{x}(t)=p. \tag{12}$$

In the remainder of this paper we are concerned with the behaviour of the expectation value $\langle x^2\rangle(t)$ in the case of colored and white phase and amplitude noise. Since the numerical estimation of the moment $\langle x^2\rangle(t)$ requires typically more than one day of CPU-time we would like to have analytical approximations which enable us to obtain quickly a general view of the dependence of $\langle x^2\rangle(t)$ on statistical properties of the stochastic terms $\lambda_A\xi_A(t)$ and $\lambda_{\mathrm{Ph}}\xi_{\mathrm{Ph}}(t)$. We evaluate analytically the moment $\langle x^2\rangle(t)$ for an ensemble of stochastically driven harmonic oscillators. This approximation is expected to yield acceptable results for small vlaues of x, i.e., small deviations of the particle from the reference particle which is the typical situation in accelerator physics. We examine the range of validity of our approximation by comparison with numerical estimations of $\langle x^2\rangle(t)$.

4.1 Synchrotron oscillations driven by white noise

4.1.1 White phase noise. We develop an analytical approximation of $\langle x^2\rangle(t)$ in the case of small white phase noise. For this purpose the equations of motion (11) are linearized around $(p, x)=(0, 0)$. Then the system under consideration is a harmonic oscillator driven by Gaussian white noise; in full analogy to the calculation of the energy expectation value in Appendix B we obtain

$$\tilde{\mathscr{E}}(t)\overset{\mathrm{def}}{=}\left\langle\frac{p^2}{2}+\frac{\omega^2}{2}x^2\right\rangle(t)=\frac{(p^0)^2}{2}+\frac{\omega^2}{2}(x^0)^2+\frac{\lambda_{\mathrm{Ph}}^2\omega^4}{2}t.$$

Choosing initial values $p^0=x^0=0$ the virial theorem [15] ensures that the expectation value $\langle\omega^2x^2/2\rangle(t)$ is equal to $\tilde{\mathscr{E}}(t)/2$. Thus we can write

$$\langle x^2\rangle(t)=\frac{\lambda_{\mathrm{Ph}}^2\omega^2}{2}t. \tag{13}$$

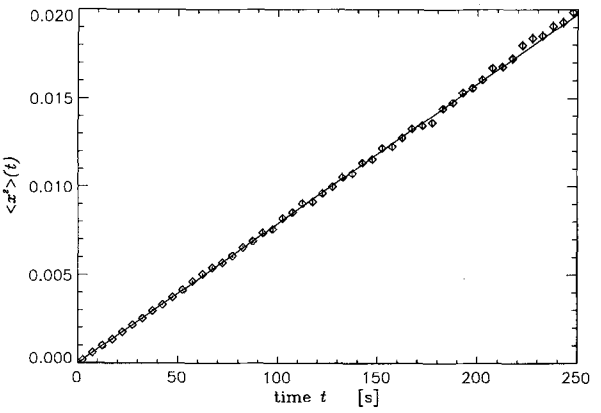

Fig. 2. The moment $\langle x^2\rangle(t)$ in the case of white phase noise. The error bars are estimations from $N=10000$ approximate solutions obtained with the stochastic leapfrog algorithm. Parameters are $\omega=40\pi\,\mathrm{s}^{-1}$, $\lambda_{\mathrm{Ph}}=10^{-4}\,\mathrm{s}^{1/2}$, time step $h=1/6000$ s, initial values $x(0)=p(0)=0$. The continuous line represents the analytical approximation (13)

The approximation of the moment $\langle x^2\rangle(t)$ grows linearly with time. In Fig. 2, the full line represents the approximation for the set of parameters $\omega=40\pi\,\mathrm{s}^{-1}$ and $\lambda_{\mathrm{Ph}}=10^{-4}\,\mathrm{s}^{1/2}$.

To examine the validity of the above approximation we estimate numerically the moment $\langle x^2\rangle(t)$ with the stochastic leapfrog algorithm from time $t=0$ to time $t=250$ s which corresponds to about 5000 periods of oscillation and to the root-mean-square of the phase difference $\langle x^2\rangle^{1/2}\approx 0.14$. To that end we generated $N=10000$ solutions of the stochastic differential equation (11) with the time step $h=1/6000$ s. This took about 46 hours CPU-time on an IBM Risc 6000/320 workstation. The error bars of Fig. 2 show our numerical results which confirm the validity of the aproximation (13).

4.1.2 White amplitude noise. In order to obtain an analytical approximation of $\langle x^2\rangle(t)$ in the case of white amplitude noise, we evaluate this moment for an ensemble of harmonic oscillators driven by white noise forces by substituting x for $\sin(x)$ in (12). Analogous to the procedure outlined in Appendix B, a set of linear ordinary differential equations for the quantities $\langle x^2\rangle(t)$, $\langle px\rangle(t)$ and $\langle p^2\rangle(t)$ can be derived from the corresponding Fokker–Planck equation. Setting $\langle px\rangle(0)\approx 0$, solving this system of ordinary differential equations in a straightforward way and performing a Taylor expansion around $\lambda_A=0$ we find up to terms of λ_A^2

$$\langle x^2\rangle(t)=\frac{1}{2}\left(\langle x^2\rangle(0)+\frac{\langle p^2\rangle(0)}{\omega^2}\right)\exp(\tau t)$$
$$+\frac{1}{2}\left(\langle x^2\rangle(0)-\frac{\langle p^2\rangle(0)}{\omega^2}\right)\exp\left(-\frac{\tau}{2}t\right)\cos(\nu t)$$
$$+\mathcal{O}(\lambda_A^2)\exp\left(-\frac{\tau}{2}t\right)\sin(\nu t), \tag{14}$$

$$\tau = \left\{ \frac{\sqrt{3}}{9} \sqrt{64\omega^6 + 27\lambda_A^4\omega^8} + \lambda_A^2\omega^4 \right\}^{1/3}$$
$$- \left\{ \frac{\sqrt{3}}{9} \sqrt{64\omega^6 + 27\lambda_A^4\omega^8} - \lambda_A^2\omega^4 \right\}^{1/3}$$
$$= \tfrac{1}{2}\omega^2\lambda_A^2 + \mathcal{O}(\lambda_A^6),$$
$$\nu = \frac{\sqrt{3}}{2} \left\{ \frac{\sqrt{3}}{9} \sqrt{64\omega^6 + 27\lambda_A^4\omega^8} + \lambda_A^2\omega^4 \right\}^{1/3}$$
$$+ \frac{\sqrt{3}}{2} \left\{ \frac{\sqrt{3}}{9} \sqrt{64\omega^6 + 27\lambda_A^4\omega^8} - \lambda_A^2\omega^4 \right\}^{1/3}$$
$$= 2\omega + \mathcal{O}(\lambda_A^4).$$

The approximation $\langle x^2\rangle(t)$ undergoes a damped fast oscillation around an exponentially growing term. Since the term proportional to sin (νt) is small we neglect it in the following.

In order to check the above approximation numerically we choose the parameters $\omega = 40\pi\,\mathrm{s}^{-1}$ and $\lambda_A = 10^{-3}\,\mathrm{s}^{1/2}$. The equations of motion (12) have the solution $p \equiv x \equiv 0$ which is stationary even in the presence of noise. Therefore, we choose the initial values $p^0 = 0$ and x^0 as a Gaussian random variable with zero mean and variance 10^{-4}. The dashed lines of Fig. 3 show the envelope of the approximation of $\langle x^2\rangle(t)$ and the intermediate line represents the exponentially growing term. In Fig. 4 the full line represents the approximation $\langle x^2\rangle(t)$ where the initial values (x^0, p^0) are chosen in such a way that the fast oscillating term vanishes: x^0 and p^0 are Gaussian random numbers with zero mean and variances $\langle x^2\rangle(0) = 10^{-4}$ and $\langle p^2\rangle(0) = 10^{-4}\omega^2$.

For a comparison with numerical results we integrated system (12) using the stochastic leapfrog algorithm; the error bars of Figs. 3 and 4 represent numerical estimations of $\langle x^2\rangle(t)$. The generation of $N = 10000$ solutions with time step $h = 1/6000$ s took 45 hours of CPU-time for each figure. In Fig. 3, the moment $\langle x^2\rangle(t)$ seems to be oscillating with low frequency. In fact, when $\langle x^2\rangle(t)$ is plotted at time $t = \Delta t, 2\Delta t, \ldots$ with Δt much smaller than the period $2\pi/\omega$, one notes that $\langle x^2\rangle(t)$ oscillates rapidly with an approximate frequency ω/π which is expected even in the deterministic limit. The apparent slow oscillation in Fig. 3 is caused by interference of the fast frequency of $\langle x^2\rangle(t)$ and the resolution time $\Delta t = 2.5025$ s between neighbouring error bars.

In both Figs. 3 and 4, numerical estimations and the analytical approximation of $\langle x^2\rangle(t)$ agree well from time $t = 0$ to time $t \approx 150$s which corresponds to about 3000 periods of oscillation of the particle and a root-mean-square of the phase difference $\langle x^2\rangle^{1/2} \approx 0.013$ in Fig. 3 and $\langle x^2\rangle^{1/2} \approx 0.018$ in Fig. 4. For $150\,\mathrm{s} < t < 250\,\mathrm{s}$ the approximation (14) differs slightly from the numerical estimation.

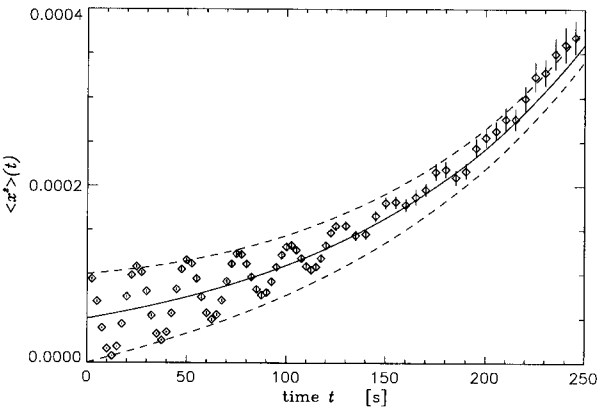

Fig. 3. The moment $\langle x^2\rangle(t)$ in the case of white amplitude noise. The error bars are estimations from $N = 10000$ approximate solutions obtained with the stochastic leapfrog algorithm. Parameters are $\omega = 40\pi\,\mathrm{s}^{-1}$, $\lambda_A = 10^{-3}\,\mathrm{s}^{1/2}$, time step $h = 1/6000$ s and $p(0) = 0$. $x(0)$ is a Gaussian random number with zero mean and variance 10^{-4}. The upper and lower curves represent the envelope of the analytical expression (14). The middle line shows the exponentially growing term of the analytic aproximation

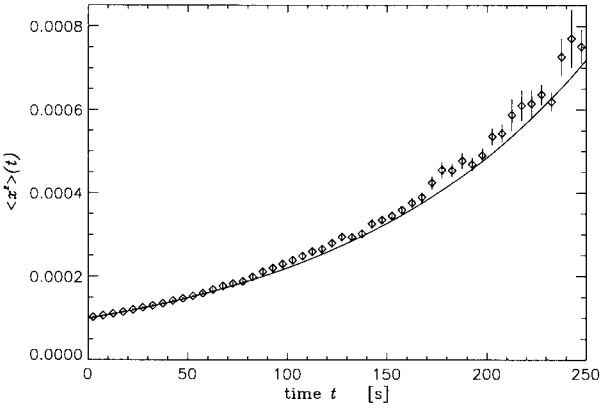

Fig. 4. The same as Fig. 3, except for the momentum initial value $p(0)$ which is now a Gaussian random number with zero mean and variance $10^{-4}\omega^2$. The continuous line represents the analytical approximation (14)

4.2 *Synchrotron oscillations driven by colored noise*

4.2.1 Colored phase noise. In the case of colored noise one obtains an analytical approximation of $\langle x^2\rangle(t)$ provided that system (11) is linearized in x, i.e., $\langle x^2\rangle(t)$ is evaluated for an ensemble of harmonic oscillators driven by colored noise. Together with (5) for colored noise $\xi_{\mathrm{Ph}}(t)$, these stochastic differential equations are equivalent to a Fokker–Planck equation governing the probability density $w(p, x, \xi_{\mathrm{Ph}}, t)$ of the random variables $p(t)$, $x(t)$ and $\xi_{\mathrm{Ph}}(t)$. Provided that $p(0) = x(0) = 0$ and $\xi_{\mathrm{Ph}}(0)$ is a Gaussian random variable with zero mean variance $\kappa/2$, a calculation analogous to the one presented in Appendix B yields

$$\langle x^2\rangle(t) = \frac{\kappa\lambda_{\mathrm{Ph}}^2\omega^2}{2(\kappa^2+\omega^2)^2} \left[\mathrm{e}^{-\kappa t}(\kappa^2 - \omega^2)\cos(\omega t) \right.$$
$$\left. - 2\mathrm{e}^{-\kappa t}\omega k \sin(\omega t) + \omega^2 - \kappa^2 \right] + \frac{1}{2}\frac{\lambda_{\mathrm{Ph}}^2\omega^2\kappa^2}{\kappa^2+\omega^2}\, t$$
$$\xrightarrow{\kappa\to\infty} \frac{\lambda_{\mathrm{Ph}}^2\omega^2}{2}\, t. \qquad (15)$$

The oscillating terms are strongly damped and vanish after a short time t. Since for $\kappa \to \infty$ colored noise becomes

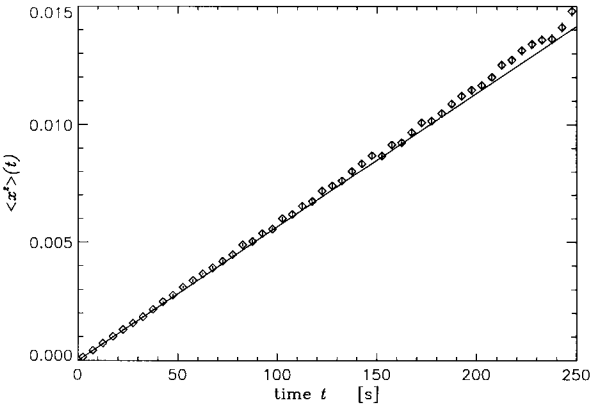

Fig. 5. The moment $\langle x^2\rangle(t)$ in the case of colored phase noise. The error bars are estimations from $N=10000$ approximate solutions obtained with the algorithm given in Sect. 3.1. Parameters are $\omega=40\pi\,s^{-1}$, $\kappa=200\,s^{-1}$, $\lambda_{Ph}=10^{-4}\,s^{1/2}$, time step $h=1/1600$ s, initial values $x(0)=p(0)=0$. The continuous line represents the analytical approximation (15)

Gaussian white noise, in this limit $\langle x^2\rangle(t)$ converges to the result (13) as expected.

To check the validity of this approximation we integrated system (11) numerically with the algorithm for colored noise of Sect. 3.1. We choose the parameters $\omega=40\pi s^{-1}$, $\kappa=200 s^{-1}$, $\lambda_{Ph}=10^{-4}s^{1/2}$, $x(0)=0$, $p(0)=0$, time step $h=1/1600$s and generated $N=10000$ solutions which required 45 hours CPU-time. The error bars of Fig. 5 represent the numerical estimations of the moment $\langle x^2\rangle(t)$ and the full line shows the approximation (15). The numerical results and the approximation agree from time $t=0$ to $t\approx 180$s which corresponds to about 3600 periods of oscillation and a root-mean-square of the phase difference $\langle x^2\rangle^{1/2}\approx 0.1$.

4.2.2 Colored amplitude noise. Finally we want to derive an analytical approximation of the moment $\langle x^2\rangle(t)$ in the case of colored amplitude noise. For this purpose we again linearize the x-dependence in (12). By use of the stochastic differential equation (5) for colored noise $\xi_A(t)$ we set up the equivalent Fokker–Planck equation. Unfortunately, the calculation of $\langle x^2\rangle(t)$ analogous to Appendix B leads to an infinite set of ordinary differential equations. However, truncating this system of moment equations by setting $\langle px\xi_A^2\rangle=0$, one derives a closed set of seven ordinary differential equations for the quantities $\langle x^2\rangle(t)$, $\langle px\rangle(t)$, $\langle x^2\xi_A\rangle(t)$, $\langle p^2\rangle(t)$, $\langle px\xi_A\rangle(t)$, $\langle x^2\xi_A^2\rangle(t)$ and $\langle p^2\xi_A\rangle(t)$. The analytical solution of this system requires the investigation of the eigensystem of a 7×7 matrix. When approximations of the eigenvalues for small values of λ_A are analysed it can be shown that the moment $\langle x^2\rangle(t)$ oscillates with approximate frequency ω/π around an exponentially growing term. Restricting ourselves to the nonoscillating part of $\langle x^2\rangle(t)$ which we denote by $\langle\langle x^2\rangle\rangle(t)$, we obtain

$$\langle\langle x^2\rangle\rangle(t)=c\exp(\tau t),$$

where c is constant and τ is given by

$$\tau=\kappa\frac{\kappa\omega^2\lambda_A^2-\kappa^2-4\omega^2+\sqrt{\kappa^2\omega^4\lambda_A^4+3\kappa^3\omega^2\lambda_A^2-4\kappa\omega^4\lambda_A^2+\kappa^4+8\kappa^2\omega^2+16\omega^4}}{4\omega^2+5\kappa^2}.$$

In the deterministic limit $\lambda_A=0$ we know that $\langle\langle x^2\rangle\rangle(t)$ depends only on the initial values:

$$\langle\langle x^2\rangle\rangle(t)=\frac{\langle x^2\rangle(0)}{2}+\frac{\langle p^2\rangle(0)}{2\omega^2}.$$

Under the assumption that during the first period the influence of the noise is negligible we may write

$$\langle\langle x^2\rangle\rangle(t)=\left(\frac{\langle x^2\rangle(0)}{2}+\frac{\langle p^2\rangle(0)}{2\omega^2}\right)\exp(\tau t). \tag{16}$$

In the limit $\kappa\to\infty$ we obtain

$$\tau\xrightarrow{\kappa\to\infty}\tfrac{1}{2}\omega^2\lambda_A^2,$$

and our result (16) becomes identical with the exponentially growing term of $\langle x^2\rangle(t)$ for white amplitude noise (14).

We test the validity of approximation (16) by comparison with numerical estimations of $\langle x^2\rangle(t)$ which belong to system (12) with colored amplitude noise $\xi_A(t)$. The estimation was carried out with the methods of Sect. 2 for the parameters $\omega=40\pi\,s^{-1}$, $\kappa=200\,s^{-1}$, $\lambda_A=10^{-3}\,s^{1/2}$, time step $h=1/1600$ s and $N=10000$. We assumed $x(0)$ to be a Gaussian random variable with zero mean and variance 10^{-4}. The error bars of Fig. 6 show the results when $p(0)=0$; the error bars of Fig. 7 are obtained when $p(0)$ is Gaussian with zero mean and variance $10^{-4}\omega^2$. The estimation of $\langle x^2\rangle(t)$ took 40 and 72 hours of CPU-time respectively. In each figure the full line represents the approximation (16).

As in the case of white amplitude noise Fig. 6 exhibits a damped oscillation of $\langle x^2\rangle(t)$ which turns out to be of approximate frequency ω/π when plotted with higher resolution. In Fig. 6, numerical values agree with the approximation (16) until $t\approx 350$ s which is equivalent to

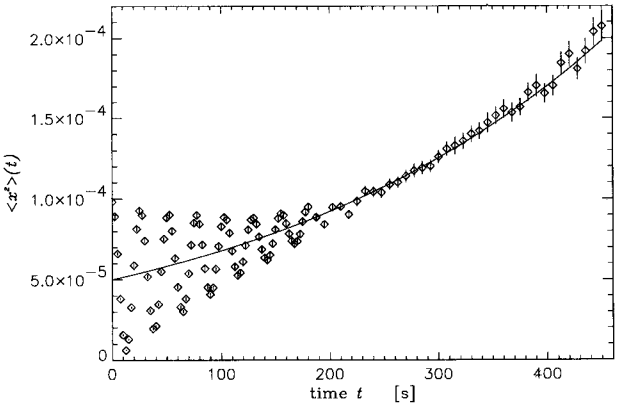

Fig. 6. The moment $\langle x^2\rangle(t)$ in the case of colored amplitude noise. The error bars are estimations from $N=10000$ approximate solutions obtained with the algorithm given in section 3.1. Parameters are $\omega=40\pi\,s^{-1}$, $\kappa=200\,s^{-1}$, $\lambda_A=10^{-3}\,s^{1/2}$, time step $h=1/1600$ s and $p(0)=0$. $x(0)$ is a Gaussian random number with zero mean and variance 10^{-4}. The continuous line represents the analytical approximation (16)

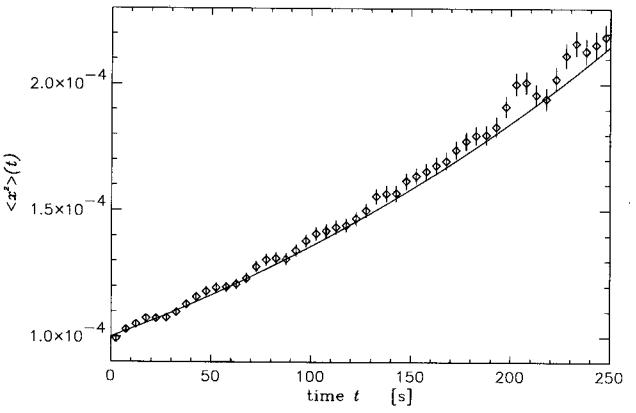

Fig. 7. The same as Fig. 6 except for the momentum initial value $p(0)$ which is now a Gaussian random number with zero mean and variance $10^{-4}\omega^2$

7000 periods of oscillation and a root-mean-square of the phase difference $\langle x^2\rangle^{1/2}\approx 0.012$. In Fig. 7, deviations of numerical values from the approximation appear for $t>150$s which corresponds to 3000 periods and a root-mean-square of the phase difference $\langle x^2\rangle^{1/2}\approx 0.013$.

5 Summary

In this article stochastic differential equations are investigated which reduce in the deterministic limit to an autonomous Hamiltonian system with one degree of freedom. Although these systems are simply described by a set of two stochastic differential equations, they are of relevance to the study of synchrotron oscillations of particles in storage rings. Given such a set of stochastic equations for the momentum p and the position x, expectation values $\langle M(p, x)\rangle(t)$ of a function M of p and x are important quantities. For example in the case of synchrotron oscillations the expectation value $\langle x^2\rangle(t)$ represents the magnitude of the squared longitudinal phase difference of an ensemble of particles with respect to the reference particle travelling along the design orbit. Expectation values can be calculated analytically only in a few cases; therefore their estimation relies on numerical tools, e.g., the stochastic Euler algorithm or Heun's method.

In Sect. 3, we suggested new algorithms suited for the numerical integration of the canonical equations of motion of a Hamiltonian function of one degree of freedom with a small stochastic force term. The stochastic term is assumed to be Gaussian white or colored noise. Our basic idea is to set up an algorithm which reduces in the deterministic limit to a symplectic algorithm which is well suited for the integration of deterministic Hamiltonian systems. Conventional stochastic integration algorithms lack this property. In the white noise case we demonstrated the efficiency of our algorithm by estimating the energy expectation value of an ensemble of stochastically driven anharmonic oscillators with our algorithm and the stochastic Heun method. It turned out that the estimation with our method took only a third of the CPU-time which was required for an estimation of equal accuracy with Heun's method.

Section 4 deals with the investigation of the equations of motion which describe synchrotron oscillations. They can be interpreted as the equations of motion of a stochastically driven pendulum. The stochastic term arises when fluctuations of external fields generated by rf cavities and various types of magnets of the storage ring are taken into consideration. Depending on the coupling of the stochastic term to the variables p and x one speaks of phase noise or amplitude noise respectively. In the four cases of Gaussian white or colored phase or amplitude noise, the behaviour of the expectation value $\langle x^2\rangle(t)$ is analysed which describes deviations of the motion of particles from the reference particle on the design orbit. Since the numerical evaluation of $\langle x^2\rangle(t)$ takes typically more than one day of CPU-time, analytical approximations of this moment are of interest which yield a general view of the dependence of $\langle x^2\rangle(t)$ on the statistical properties of the stochastic force for both phase and amplitude noise. Approximations of the moment $\langle x^2\rangle(t)$ are derived which are expected to be reasonable for small values of x. This is the situation one normally encounters in accelerator physics. The validity of the approximations is examined by comparison with numerical results which are obtained by use of our algorithms; the approximations agree with numerical estimations of $\langle x^2\rangle(t)$ for times which correspond to several thousand periods of oscillation. In the case of phase noise and for initial conditions $x(0)=p(0)=0$ the expectation value $\langle x^2\rangle(t)$ grows linearly with time whereas in the case of amplitude noise $\langle x^2\rangle(t)$ performs damped fast oscillations around an exponentially growing term.

Appendix A

In the following we give a proof that the stochastic leapfrog algorithm (6) is well suited for the approximation of the Hamiltonian system (1) driven by Gaussian white noise forces. For this purpose, we first summarize some facts concerning the numerical integration of arbitrary systems of ordinary stochastic differential equations. Subsequently the validity of the stochastic leapfrog algorithm is demonstrated.

Integration of general stochastic differential equations

We summarize results of the references [8, 9]. Starting point is the general system of stochastic differential equations

$$\dot{x}_i = f_i(x_1, \ldots, x_n) + \sigma_{ij}(x_1, \ldots, x_n)\,\xi_j(t), \quad i=1, \ldots, n,$$

where $\xi_i(t)$ is standard Gaussian white noise. In the following h denotes a small time step. The exact solution $x_i(h)$ may be written as

$$x_i(h) = D_i(h) + S_i(h),$$

where $D_i(h)$ and $S_i(h)$ denote the deterministic and stochastic contribution respectively. To simplify the notation we drop arguments and write σ_{ij} and f_i instead of

$f_i(\mathbf{x}(0))$ and $\sigma_{ij}(\mathbf{x}(0))$. Then $D_i(h)$ is

$$D_i(h)=x_i(0)+hf_i+\frac{h^2}{2}\frac{\partial f_i}{\partial x_k}f_k+\mathcal{O}(h^3), \tag{17}$$

where the summation convention for the repeated indices j, k, l is employed and $\mathcal{O}(h^m)$ denotes terms of order h^m. In the case of additive noise, i.e., when σ_{ij} does not depend on $\mathbf{x}$ one obtains

$$S_i(h)=\sigma_{ij}W_j(h)+\frac{\partial f_i}{\partial x_k}\sigma_{kl}K_l(h)$$
$$+\frac{1}{2}\frac{\partial^2 f_i}{\partial x_k\partial x_l}\sigma_{km}\sigma_{ln}G_{mn}(h)+\mathcal{O}(h^{5/2}), \tag{18}$$

whereas in the case of multiplicative noise, i.e. when $\sigma_{ij}(\mathbf{x})$ is a function of $\mathbf{x}$, $S_i(h)$ is

$$S_i(h)=\sigma_{ij}W_j(h)+\frac{\partial\sigma_{ij}}{\partial x_k}\sigma_{kl}C_{lj}(h)+\mathcal{O}(h^{3/2}). \tag{19}$$

The quantities $W_j(h)$, $K_l(h)$, $G_{mn}(h)$ and $C_{lj}(h)$ are random variables which can be written as stochastic integrals of the Gaussian white noise $\xi_i(t)$. The following expectation values of $W_j(h)$ and $K_l(h)$ are important in our context:

$$\langle W_j(h)\rangle=\langle(W_j(h))^3\rangle=\langle(W_j(h))^5\rangle=0,$$
$$\langle(W_j(h))^2\rangle=h,\quad \langle(W_j(h))^4\rangle=3h^2,$$
$$\langle K_l(h)\rangle=0,\quad \langle K_l(h)K_m(h)\rangle=\frac{h^3}{3}\delta_{lm}. \tag{20}$$

An algorithm for the numerical integration of stochastic differential equations replaces the exact functionals $D_i(h)$, $S_i(h)$ by approximations $\bar{D}_i(h)$, $\bar{S}_i(h)$. Then approximations $\bar{x}_{i,h}(1)$ of exact solutions $x_i(h)$ are obtained by

$$\bar{x}_{i,h}(1)=\bar{D}_i(h)+\bar{S}_i(h).$$

If the equations

$$D_i(h)-\bar{D}_i(h)=\mathcal{O}(h^q),$$
$$\langle(S_i(h))^p\rangle-\langle(\bar{S}_i(h))^p\rangle=\mathcal{O}(h^q),$$

are valid with a fixed integer q for all integers p then the difference of the numerically estimated expectation value $\mathcal{M}_h(mh)$ of a function $M(x_1,\ldots,x_n)$ at time $t=mh$ and the corresponding exact value $\mathcal{M}(t)$ is a term of order h^{q-1}:

$$\mathcal{M}_h(t)-\mathcal{M}(t)=\langle M(\bar{x}_{1,h}(m),\ldots,\bar{x}_{n,h}(m))\rangle$$
$$-\langle M(x_1(mh),\ldots,x_n(mh))\rangle$$
$$=\mathcal{O}(h^{q-1}).$$

Thus, the quality of an algorithm is characterized by the value of q. A proper numerical method demands $q\geq 2$. Then the algorithm is said to have *convergence of moments*.

Next we give expressions for $D_i(h)$ and expectation values of $S_i(h)$ for the stochastically driven Hamiltonian system (1) which may be written as

$$\begin{pmatrix}\dot{x}_1(t)\\ \dot{x}_2(t)\end{pmatrix}=\begin{pmatrix}F(x_2)\\ x_1/m\end{pmatrix}+\begin{pmatrix}\sigma(x_2) & 0\\ 0 & 0\end{pmatrix}\begin{pmatrix}\xi_1(t)\\ \xi_2(t)\end{pmatrix}. \tag{21}$$

The deterministic contributions $D_i(h)$ can be evaluated by use of (17)

$$D_1(h)=x_1(0)+hF(x_2(0))+\frac{h^2}{2}\frac{\partial F}{\partial x_2}(x_2(0))\frac{x_1(0)}{m}+\mathcal{O}(h^3),$$

$$D_2(h)=x_2(0)+h\frac{x_1(0)}{m}+\frac{h^2}{2m}F(x_2(0))+\mathcal{O}(h^3).$$

Using (18, 19) we obtain for the stochastic contributions $S_i(h)$

$$S_1(h)=\sigma(x_2)W_1(h)+\mathcal{O}(h^{5/2},h^{3/2}),$$

$$S_2(h)=\begin{cases}\sigma K_1(h)/m+\mathcal{O}(h^{5/2}), & \text{if } \sigma \text{ is constant},\\ \mathcal{O}(h^{3/2}), & \text{if } \sigma(x) \text{ is a function of } x.\end{cases}$$

The symbol $\mathcal{O}(h^m,h^n)$ denotes terms of the order h^m for additive noise and terms of the order h^n in the case of multiplicative noise. The expectation values $\langle S_i(h)\rangle$ are

$$\langle S_1(h)\rangle=\mathcal{O}(h^3,h^2),\quad \text{and}\quad \langle S_2(h)\rangle=\mathcal{O}(h^3,h^2),$$

because the term proportional to $h^{5/2}$ or $h^{3/2}$ of $S_1(h)$ is an odd moment of Gaussian white noise with vanishing expectation value. Furthermore, using (20) we get

$$\langle(S_1(h))^2\rangle=h\sigma(x_2)^2+\mathcal{O}(h^3,h^2),$$
$$\langle(S_1(h))^3\rangle=\mathcal{O}(h^3,h^2),$$
$$\langle(S_1(h))^4\rangle=3h^2\sigma(x_2)^4+\mathcal{O}(h^3),$$
$$\langle(S_1(h))^p\rangle=\mathcal{O}(h^3),\quad p=5,6,\ldots$$
$$\langle(S_2(h))^p\rangle=\mathcal{O}(h^3),\quad p=2,3,\ldots.$$

These expressions become important when the stochastic leapfrog algorithm is investigated.

Proof of the validity of the stochastic leapfrog algorithm

The stochastic leapfrog algorithm for the numerical integration of the stochastic Hamiltonian system (21) consists of the following recursion formula for approximations $\bar{x}_{1,h}(k)$, $\bar{x}_{2,h}(k)$ of the exact solution $x_1(kh)$, $x_2(kh)$

$$\begin{pmatrix}\bar{x}_{1,h}(k+1)\\ \bar{x}_{2,h}(k+1)\end{pmatrix}$$
$$=h\begin{pmatrix}F(\bar{x}_{2,h}(k)+h\bar{x}_{1,h}(k)/(2m))\\ \bar{x}_{1,h}(k)/m+hF(\bar{x}_{2,h}(k)+h\bar{x}_{1,h}(k)/(2m))/(2m)\end{pmatrix}$$
$$+\begin{pmatrix}\bar{x}_{1,h}(k)\\ \bar{x}_{2,h}(k)\end{pmatrix}+\sigma(\bar{x}_{2,h}(k))\eta(k)\begin{pmatrix}\sqrt{h}\\ h^{3/2}/(m\sqrt{3})\end{pmatrix},$$

where $\bar{x}_{1,h}(0)$ and $\bar{x}_{2,h}(0)$ are identical with the initial values $x_1(0)$, $x_2(0)$ respectively. $\eta(k)$ denotes a series of random numbers with the moments

$$\langle\eta(k)\rangle=\langle\eta(k)^3\rangle=\langle\eta(k)^5\rangle=0,\quad \langle\eta(k)^2\rangle=1,\ \langle\eta(k)^4\rangle=3.$$

This can be achieved by choosing Gaussian random numbers as well as using the sequence of random numbers (7). Through the substitution of Gaussian random numbers a substantial amount of CPU-time is saved.

Deterministic and stochastic contributions of the above recursion formula are

$$\begin{aligned}\bar{D}_1(h)&=\bar{x}_{1,h}(0)+hF\left(\bar{x}_{2,h}(0)+\frac{h}{2m}\bar{x}_{1,h}(0)\right)\\&=\bar{x}_{1,h}(0)+hF\left(\bar{x}_{2,h}(0)\right)\\&\quad+\frac{h^2}{2m}\frac{\partial F}{\partial\bar{x}_{2,h}}(\bar{x}_{2,h}(0))\bar{x}_{1,h}(0)+\mathcal{O}(h^3),\end{aligned}$$

$$\begin{aligned}\bar{D}_2(h)&=\bar{x}_{2,h}(0)+\frac{h}{m}\bar{x}_{1,h}(0)+\frac{h^2}{2m}F\left(\bar{x}_{2,h}(0)+\frac{h}{2m}\bar{x}_{1,h}(0)\right)\\&=\bar{x}_{2,h}(0)+\frac{h}{m}\bar{x}_{1,h}(0)+\frac{h^2}{2m}F(\bar{x}_{2,h}(0))+\mathcal{O}(h^3),\end{aligned}$$

$$\bar{S}_1(h)=\sigma(\bar{x}_{2,h}(0))\sqrt{h}\eta(k),$$

$$\bar{S}_2(h)=\sigma(\bar{x}_{2,h}(0))\frac{h^{3/2}}{m\sqrt{3}}\eta(k). \tag{22}$$

With the results above we obtain for the differences of approximate and exact functionals

$$\bar{D}_1(h)-D_1(h)=\mathcal{O}(h^3),\quad \bar{D}_2(h)-D_2(h)=\mathcal{O}(h^3),$$

$$\langle(\bar{S}_1(h))^p\rangle-\langle(S_1(h))^p\rangle=\mathcal{O}(h^3,h^2),\quad p\in\mathbb{N},$$

$$\langle(\bar{S}_2(h))^p\rangle-\langle(S_2(h))^p\rangle=\mathcal{O}(h^3,h^2),\quad p\in\mathbb{N}.$$

Thus, the value of q is 3 or 2 in the case of additive or multiplicative noise respectively; therefore the stochastic leapfrog algorithm is suited for the numerical integration of system (21). The order of convergence of expectation values obtained with this algorithm is

$$\mathcal{M}_h(t)-\mathcal{M}(t)=\begin{cases}\mathcal{O}(h^2), & \text{if } \sigma \text{ is constant},\\ \mathcal{O}(h), & \text{if } \sigma(x) \text{ is a function of } x.\end{cases}$$

The substitution $\bar{S}_2(h)=0$ for (22) also yields a proper algorithm. It can be shown that in the case of additive noise this algorithm has a worse *convergence in the mean square sense* [8, 9] than the stochastic leapfrog algorithm. This kind of convergence becomes important for the estimation of mean first passage times. A further investigation of this topic lies beyond the scope of our article.

Appendix B

This Appendix deals with the analytical calculation of expectation values $\langle M(p,x)\rangle(t)$ for the system of stochastic differential equations (1) in the cases of gaussian white noise when σ is constant:

$$\dot{p}(t)=F(x)+\sigma\xi(t),\quad F(x)\overset{\text{def}}{=}-\frac{\partial V}{\partial x}(x),$$

$$\dot{x}(t)=\frac{p(t)}{m}. \tag{23}$$

Initial values are assumed to be $x(t=0)=x^0$ and $p(t=0)=p^0$. As solutions of a stochastic differential equation, momentum $p(t)$ and position $x(t)$ are random variables. We replace the set of stochastic differential equations (23) by an equivalent Fokker–Planck equation [7] for the corresponding probability denity $w(p,x,t)$ which reads

$$\frac{\partial\omega}{\partial t}(p,x,t)=\left[-\frac{p}{m}\frac{\partial}{\partial x}-F(x)\frac{\partial}{\partial p}+\frac{1}{2}\sigma^2\frac{\partial^2}{\partial p^2}\right]\omega(p,x,t). \tag{24}$$

The expectation value $\mathcal{M}(t)$ of a function $M(p,x)$ at time t can be written as

$$\mathcal{M}(t)=\langle M(p,x)\rangle(t)=\int_{-\infty}^{+\infty}\mathrm{d}p\int_{-\infty}^{\infty}\mathrm{d}x\,M(p,x)w(p,x,t).$$

At least in principle $\mathcal{M}(t)$ can be obtained directly if the solution $w(p,x,t)$ of the Fokker–Planck equation is calculated which is usually a difficult task [14]. However, sometimes the calculation of $\mathcal{M}(t)$ can be reduced to the solution of a system of ordinary differential equations in the following way. The time derivative of $\mathcal{M}(t)$ is

$$\frac{\mathrm{d}\mathcal{M}}{\mathrm{d}t}(t)=\int_{-\infty}^{+\infty}\mathrm{d}p\int_{-\infty}^{\infty}\mathrm{d}x\,M(p,x)\frac{\partial w}{\partial t}(p,x,t).$$

In this expression we replace the time derivative of $w(p,x,t)$ by the right hand side of (24). Assuming that the probability density $w(p,x,t)$ as well as its derivatives vanish for $p,x\to\infty$, partial integration yields

$$\begin{aligned}\frac{\mathrm{d}\mathcal{M}}{\mathrm{d}t}(t)&=\int_{-\infty}^{+\infty}\mathrm{d}p\int_{-\infty}^{\infty}\mathrm{d}x\,w(p,x,t)\left\{\frac{p}{m}\frac{\partial M}{\partial x}(p,x)\right.\\&\quad\left.+F(x)\frac{\partial M}{\partial p}(p,x)+\frac{1}{2}\sigma^2\frac{\partial^2 M}{\partial p^2}\right\}\\&=\left\langle\frac{p}{m}\frac{\partial M}{\partial x}(p,x)\right\rangle(t)+\left\langle F(x)\frac{\partial M}{\partial p}(p,x)\right\rangle(t)\\&\quad+\frac{1}{2}\sigma^2\left\langle\frac{\partial^2 M}{\partial p^2}(p,x)\right\rangle(t).\end{aligned} \tag{25}$$

We are interested in the expectation value $\mathcal{E}(t)$ of the energy $E(p,x)=p^2/2m+V(x)$ which obeys

$$\frac{\mathrm{d}\mathcal{E}}{\mathrm{d}t}(t)=\left\langle\frac{p}{m}\frac{\partial V}{\partial x}(x)\right\rangle(t)+\left\langle F(x)\frac{p}{m}\right\rangle(t)+\frac{\sigma^2}{2m}$$

If we replace the deterministic force $F(x)$ according to its definition by the derivative of the potential $V(x)$ then the

expectation values on the right hand side cancel. We obtain

$$\frac{d\mathscr{E}}{dt}(t)=\frac{\sigma^2}{2m}.$$

Obviously the energy expectation value as a function of time t is

$$\mathscr{E}(t)=\frac{(p^0)^2}{2m}+V(x^0)+\frac{\sigma^2}{2m}t. \tag{26}$$

We want to stress that in general the evaluation of $\mathscr{M}(t)$ by use of (25) is more complicated than the calculation of the energy expectation value in our example since the expectation values

$$\mathscr{M}_1(t)\overset{\text{def}}{=}\left\langle \frac{p}{m}\frac{\partial M}{\partial x}(p,x)\right\rangle(t),$$

$$\mathscr{M}_2(t)\overset{\text{def}}{=}\left\langle F(x)\frac{\partial M}{\partial p}(p,x)\right\rangle(t),$$

$$\mathscr{M}_3(t)\overset{\text{def}}{=}\left\langle \frac{\partial^2 M}{\partial p^2}(p,x)\right\rangle(t)$$

are also unknown. If (25) is applied to calculate the time derivatives of $\mathscr{M}_1(t)$, $\mathscr{M}_2(t)$, $\mathscr{M}_3(t)$ and thus to obtain a closed set of differential equations, even more expectation values may crop up. Nevertheless, at least for a linear force $F(x)$ and $M(p,x)=p^i x^j$ with integers i, j a closed set of ordinary differential equations can be obtained which can be solved yielding $\mathscr{M}(t)$.

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