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Alternative Simulating Technique for Periodic Motion in the Presence of Multiplicative White Noise

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An effective approach for simulating the periodic motion of an overdamped particle subjected to a multiplicative white-noise source is described. The accurate calculations for the velocity of the particle and its correlation function can be realized by introducing an inertial term. The results show that fluctuation around a time-averaged quantity increases with decreasing time step in the overdamped white-noise algorithm, however, a massive white-noise technique greatly reduces this spurious drift. In particular, the present algorithm converges on the correct values of the calculated quantities, while the mass of the particle approaches to zero.

KEY WORDS: Langevin equation; multiplicative white noise; periodic potential; velocity; correlation function.

1. INTRODUCTION

Numerical simulations of stochastic differential equations offer a powerful technique for obtaining information in statistical physics. Usually, one uses a small time step to integrate these equations, nevertheless, in all these multiplicative noise cases, few robust algorithms are known.[1, 2] Ten years ago, Fox used a weak exponentially colored noise to mimic a white noise in the numerical tests of the Kubo oscillator,[3–5] where the noise was a multiplicative type. By using the direct white-noise algorithm, the author of refs. 3–5 observed that the same data produced a strong decay in the amplitude oscillator. Unfortunately, the result was due to a programming error, this was pointed out by Fox and Roy in Erratum.[6] It was also mentioned in ref. 1 by Drummond and Mortimer who first suspected it and

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who commented out in their work. However, for a multiplicative white noise problem one always needs to treat carefully.

In the studies of the double-well dynamics, one considers a response of the position of the particle to a periodic modulation. However, for a spatial periodic system there could be some ambiguity in the definition of the response of the system to an external time-periodic force. This is because the particles can move and diffuse very far from the origin, thus the mean velocity of a particle and its correlation function become two important output signs.[7, 8] Very recently, the transport process of an overdamped Brownian particle moving in a periodic potential subjected to various unequilibrium fluctuations has been much attracted by many researchers, which is related to the studies of molecular motors. Those operating model can be equivalently to be a multiplicative noise driven the directed motion, i.e.,

$$\dot{x}(t) = f(x) + g(x)\,\xi(t) \tag{1}$$

with $\langle \xi(t) \rangle = 0$ and $\langle \xi(t)\,\xi(t') \rangle = 2\delta(t-t')$.

For time-independent f and g and for $g \neq 0$, a multiplicative noise always becomes an additive one by a simple transformation of variable: $dy = g(x)^{-1}\,dx$, thus one can get a Langevin equation for new variable y with an additive noise force. Nevertheless, this transformation of variable does not apply to a multidimensional case or a multi-noise problem. In general, the transient velocity of the particle averaging over the realization needs to evaluate from Eq. (1), that is, $\langle \dot{x}(t) \rangle = \langle f(x(t)) \rangle + \langle g(x(t))\,\xi(t) \rangle$. It stems from the fact that during a change of $\xi(t)$ also $x(t)$ changes and therefore $\langle g(x(t))\,\xi(t) \rangle$ is no longer zero, and this average leads to the "spurious" drift. Moreover, it is impossible to plot a realization with a δ-correlated noise. So that the velocity of the particle at any time is given by $\dot{x}(t) = [x(t+\Delta t) - x(t)]/\Delta t$. It has been known that the last order of stochastic term is $(\Delta t)^{1/2}$ in numerical solutions of both Ito and Straronvich stochastic equations with a white noise. The problem is made more severe by the fact that the velocity $\dot{x}(t) \propto (\Delta t)^{-1/2}$ becomes relatively larger as $\Delta t \to 0$. This means that the resulting velocity does not convergence.

The main purpose of this work is to overcome the above difficulty. An alternative numerical technique by introducing an inertia term into an overdamped Langevin equation is proposed, and which is compared with the colored-noise approximate algorithm of Fox.[3–5]

2. MODEL AND ALGORITHM

Let us introduce an inertial term into the left-hand side of Eq. (1), and use a weak exponentially colored noise $\varepsilon(t)$ with correlation time τ to mimic the white noise $\xi(t)$, thus the equation of motion of the particle is given by

$$\mu\ddot{x}(t) + \dot{x}(t) = f(x) + g(x)\,\varepsilon(t) \tag{2}$$

$$\dot{\varepsilon} = -\frac{1}{\tau}\,\varepsilon(t) + \frac{1}{\tau}\,\xi(t) \tag{3}$$

in which μ and τ are two control parameters.

We start from the fact that Eq. (2) can be regarded as a first-order ordinary differential equation for the velocity variable $v(t) = \dot{x}(t)$, as the right-hand side of Eq. (2) is treated and merged as a source term. The algorithm proposed reads

$$\begin{aligned} x(t+\Delta t) = {} & x(t) + \mu[1-\exp(-\Delta t/\mu)]\,v(t) \\ & + \int_t^{t+\Delta t} \{1-\exp[-(t+\Delta t - s)/\mu]\}\,[f(x(s)) + g(x(s))\,\varepsilon(s)]\,ds \end{aligned} \tag{4}$$

$$\begin{aligned} v(t+\Delta t) = {} & \exp[-\Delta t/\mu]\,v(t) + \frac{1}{\mu}\int_t^{t+\Delta t} \exp[-(t+\Delta t - s)/\mu] \\ & \cdot \{f(x(s)) + g(x(s))\,\varepsilon(s)\}\,ds \end{aligned} \tag{5}$$

$$\varepsilon(t+\Delta t) = \exp(-\Delta t/\tau)\,\varepsilon(t) + \frac{1}{\tau}\int_t^{t+\Delta t} \exp[-(t+\Delta t - s)/\tau]\,\xi(s)\,ds \tag{6}$$

Here, the Rung–Kutta approach[9] is applied to perform the integration for the deterministic parts $f(x(s))$ and $g(x(s))$, and the stochastic parts are simulated by using Gaussian random numbers in each step.[10–12] Note that Eqs. (4)–(6) are valid to a broad range of the parameters. Clearly, when $\mu \to 0$, the above expressions can be reduced to the overdamped colored-noise algorithm.[3–5]

This study focus on the mean velocity of a particle $\langle v(t)\rangle$ and its steady correlation function $C(t_d) = \langle \delta v(t-t_d)\,\delta v(t)\rangle$, where $\delta v(t) = v(t) - \langle v(t)\rangle$. Thus the diffusion rate of the particles is determined by: $D^* = \lim_{t\to\infty} \int_0^t \langle \delta v(t-t_d)\,\delta v(t)\rangle\, dt_d$. In which the mean velocity is evaluated from an implicit form of Eq. (5) in the present massive white-noise technique (ALGO 1); this quantity can be calculated by Eq. (2) for $\mu \to 0$ and for a weakly colored noise $\varepsilon(t)$ in Fox's algorithm (ALGO 2); however, for an overdamped white-noise algorithm (ALGO 3), the time-dependent velocity needs to evaluate from $\dot{x}(t) = [x(t+\Delta t) - x(t)]/\Delta t$.

3. RESULTS AND DISCUSSION

To test the accuracy of different algorithms, we consider a state-dependent diffusion proposed by Müttiker in ref. 13, where the potential and diffusion coefficient are simply given by

$$U(x) = U_0[1 - \cos(x)], \qquad D^{-1}(x) = D_0^{-1}[1 - \alpha \cos(x - \phi)] \tag{7}$$

Here α $(0 \leqslant \alpha < 1)$ is the amplitude of the modulation, the phase ϕ plays an important role, and (U_0, D_0, α, ϕ) are a set of model parameters. It is

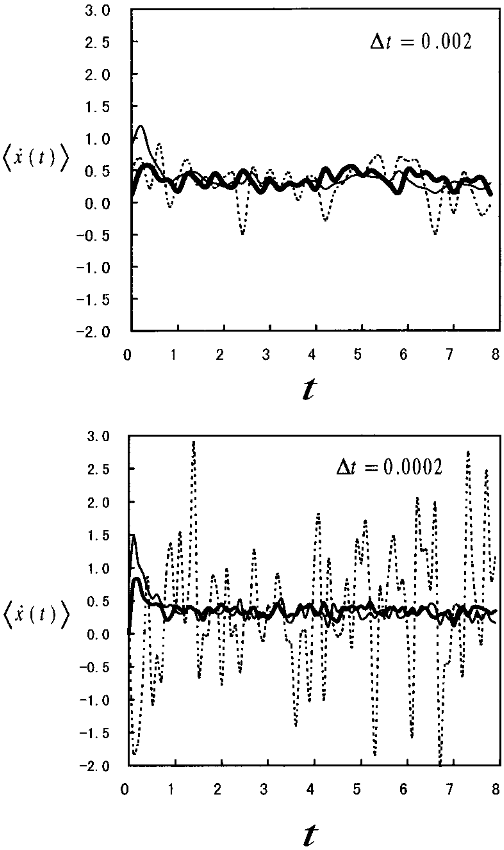

Fig. 1. Time evolution of the mean velocity simulated by three kinds of different algorithms for $D_0 = 2.0$, $\alpha = 0.7$, $\mu = 0.02$, and $\tau = 0.02$. The step sizes are (a) $\Delta t = 0.002$ and (b) $\Delta t = 0.0002$. The thick solid line, ALGO 1 ($\tau \to 0$); the thin solid line, ALGO 2 ($\mu \to 0$); and the dashed line, ALGO 3 (both μ and $\tau \to 0$).

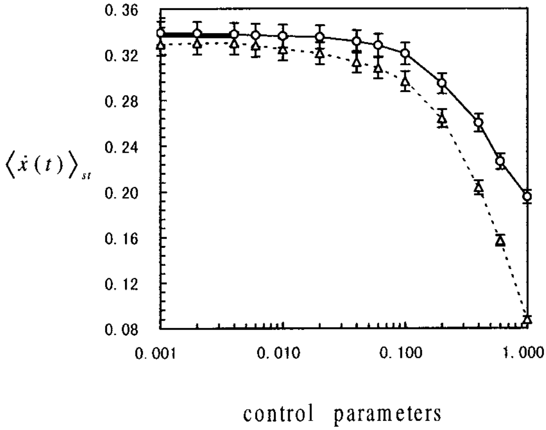

Fig. 2. The mean velocity as a function of the control parameters μ and τ, here the model parameters are the same as Fig. 1. The solid line with circles, ALGO 1 ($\tau \to 0$); the dashed line with triangles, ALGO 2 ($\mu \to 0$); and the thick short line is the realistic result.

appreciated a long time ago that the Boltzmann distribution which governs systems subjected to a state-dependent diffusion, thus one must have[8, 13]

$$f(x) = -U'(x) + \frac{1}{2}\frac{dD(x)}{dx}, \qquad g(x) = \sqrt{D(x)} \tag{8}$$

The simulation of the transport process is done starting from $x(0) = 0$, $v(0) = 0$ and a Gaussian distribution of $\varepsilon(0)$[10, 11] with averaging over $N = 2 \times 10^4$ stochastic realization for the fixed $U_0 = 1.0$ and $\phi = \pi/2$. In Figs. 1(a) and (b), we simulate the time evolution of the mean velocity by using two kinds of time steps: $\Delta t = 0.002$ in (a) and $\Delta t = 0.0002$ in (b). The weakly inertia mass of the particle corresponds with fixed $\mu = 0.02$ and the correlation time of colored noise is taken to be $\tau = 0.02$. This numerical work demonstrates that the overdamped white-noise method [Eq. (1)] is fail on calculating the derivation of the trajectories. In other wards, it does not allow to provide very small time steps.

The steady velocity of the particle as a function of the control parameters μ and τ is shown in Fig. 2 by means of massive white-noise (ALGO 1) and weakly colored-noise (ALGO 2) approaches with the same model parameters as Fig. 1. In order to eliminate the fluctuation drift of the results, the time-averaged velocity of the particle is numerically determined by

$$\langle \dot{x}(t) \rangle_{st} = \frac{1}{t - t_a} \int_{t_a}^{t} \langle \dot{x}(s) \rangle \, ds = \frac{1}{N} \sum_{n=1}^{N} \frac{x_n(t) - x_n(t_a)}{t - t_a} \tag{9}$$

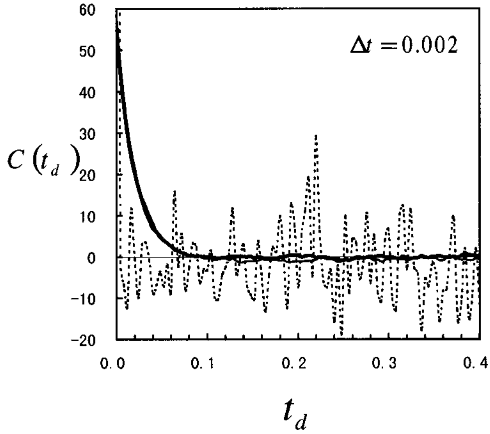

Fig. 3. The correlation function of velocity $C(t_d)$ vs. time difference t_d at $t = 6.0$. The model parameters are $D_0 = 1.0$ and $\alpha = 0.5$. The symbols are the same as Fig. 1.

where $t > t_a$ and $t_a \gg \mu$ or τ. The time step used is $\Delta t = 5 \times 10^{-4}$, $t_a = 3.0$, and $t = 8.0$. The realistic value is $\langle \dot{x} \rangle = 0.3365$ in the limit of both $\mu \to 0$ and $\tau \to 0$. It is observed that ALGO1 is more stable than ALGO2, and the former can approach to the realistic value of the steady velocity.

A further demonstration of the inefficiency of the overdamped white-noise algorithm (ALGO 3) is observed on calculating the correlation function of velocity. In Fig. 3, the correlation function of velocity is plotted as a function of time by using three kinds of algorithms. It is seen that, the fluctuations in the correlation function of velocity are large extraordinarily, while one uses the direct white-noise algorithm (ALGO 3). This is because the square term of $(\Delta t)^{-1/2}$ appearing in the correlation function. However, both ALGO 1 and ALGO 2 can give the accepted results, respectively.

Dependence of the diffusion rate D^* of the particle on the control parameters μ and τ is shown in Fig. 4. The diffusion rate can be obtained from averaging over a long time, i.e., $D^* = \frac{1}{2} \lim_{t \to \infty} (1/t) \langle [x(t) - \langle x(t) \rangle]^2 \rangle$,[8] here, the realistic value of the diffusion rate can be determined by this expression in terms of Eq. (1). It is also seen that the present technique (ALGO 1) gives accurate and convergence result comparing with the weakly colored-noise algorithm (ALGO 2).

4. SUMMARY

We are now in a position to engage in numerical simulations for the velocity-dependent quantities of an overdamped particle in a periodic potential subjected to a multiplicative white noise. The results show that,

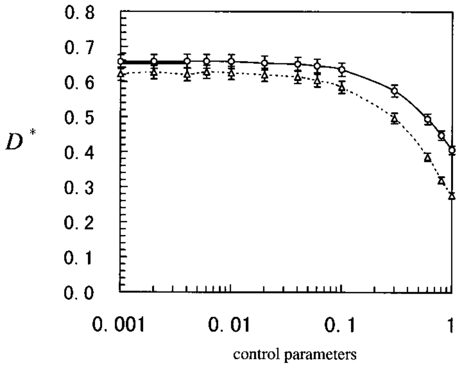

Fig. 4. The diffusion rate as a function of the control parameters μ and τ. The diffusive time $t = 80.0$, and the other model parameters are the same as Fig. 3, as well as the symbols are the same as Fig. 2.

the overdamped white-noise algorithm is generally accurate only with long-time characteristics, but which can show worse short-time behaviors of the calculated output signs, this is due to the last order of the stochastic parts of this algorithm to $(\Delta t)^{1/2}$. Namely, the errors in a transient process showed large fluctuations, although the mean values may be correct. The massive white-noise technique presented here not only avoid this difficulty, but it also provides us with highly accurate time-averaged quantities. For various improved algorithms, such as the weak colored-noise algorithm and the massive white-noise technique, the keypoint is to determine the velocity of the particle by using an extensional equation instead of a differential-quotient approximation. On the other hand, performing time averaged for the results within the stationary states, it should increase the stability and accuracy of the calculations.

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