Numerical simulation of generalized Langevin equation with arbitrary correlated noise

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A generalized Langevin equation with arbitrary correlated noise and associated frequency-dependent friction is simulated, which can lead to anomalous diffusion. The algorithm is realized by using the Fourier transform technique to generate noise and the stochastic Runge-Kutta method to solve the whole equation. Application to an acoustic phonon model, initial preparation-dependent ballistic diffusion, is shown.

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The generalized Langevin equation (GLE) is an equation of motion for the non-Markovian stochastic process where the particle has a memory effect to its velocity. Recently, GLE has been used to govern the dynamics of a system in a non-Ohmic environment that presents anomalous diffusion [1–3]. The noise is defined by its spectral density proportional to $\omega^{\delta-1}$ at low frequencies, where δ is the power exponent. The frequency-dependent friction is deduced from the correction function of the noise by means of the Kubo second fluctuation-dissipation theorem (FDT) [4]. This model yields the mean square displacement of a force-free particle of the form $\langle x^2(t)\rangle \propto t^{\delta}$, a subdiffusion for $0<\delta<1$, a normal diffusion for $\delta=1$, a superdiffusion for $1<\delta<2$, and a ballistic diffusion for $\delta=2$. It is known that dynamical behaviors of the system depend strongly on the properties of the correlation function of noise and of the memory friction kernel. Unfortunately, systematic studies on anomalous transport in external fields so far have not been presented yet, because numerical solving the fractional Fokker-Planck equation [5] and numerical solving the fractional Langevin equation [6] leads to anomalous diffusions, which is a difficult task.

Usually, a numerical scheme for GLE simulates a set of Markovian Langevin equations by introducing variable transforms [7], or usually the thermal colored noise appearing in GLE can be simulated directly [8]. Several algorithms have been proposed in the last few years to generate correlated colored noises [9–11], most of which obey a linear Langevin equation driven by a Gaussian white noise. Nevertheless, quite often in stochastic dynamics, such as in the study of anomalous diffusion, one needs to generate a Gaussian noise with a particular time correlation function, but with unknown Langevin-like dynamics [12,13]. In this paper, we propose an effective algorithm to simulate the time-dependent transport process of an anomalously diffusing particle. The non-Ohmic and acoustic phonon models are considered.

The GLE for a classical particle of mass m in the presence of a potential reads

$$\dot{x} = v(t),$$

$$\dot{v} = -\int_0^t \gamma(t-t')v(t')dt' - \frac{U'(x(t))}{m} + \sqrt{\frac{k_B T}{m}}\xi(t), \quad (1)$$

where k_B is the Boltzmann constant, T is the temperature of the environment, $\gamma(t)$ is the friction kernel function and $\langle \xi(t)\xi(0)\rangle = \gamma(t)$ is related to the noise $\xi(t)$ through FDT.

If GLE (1) cannot be transferred into a set of Markonian LEs, we need to use the second-order stochastic Runge-Kutta method [14] to solve Eq. (1) itself. The key point of the algorithm is to simulate arbitrary correlated noise with time-translation invariance. Here we consider a general case that the noise $\xi(t)$ cannot be generated by a stochastic differential equation driven by a Gaussian white noise. García and Sancho have developed an approach to generate time-correlated noise in Ref. [12]. In the following we will adopt their scheme.

In the ω-Fourier space, the correlation function of the noise is written as

$$\langle \xi(\omega)\xi(\omega')\rangle = 2\pi\gamma(\omega)\delta(\omega+\omega'), \quad (2)$$

where $\xi(\omega)$ and $\gamma(\omega)$ are the Fourier transforms of $\xi(t)$ and $\gamma(t)$, respectively. We discretize time in $N=2^n$ intervals of the mesh size Δt. Every one of those intervals will be denoted by a Roman index in the real space and by a Greek index in the Fourier space. So the discrete Fourier version of Eq. (2) is given by

$$\langle \xi(\omega_\mu)\xi(\omega_\nu)\rangle = \gamma(\omega_\mu)N\Delta t\,\delta_{\mu+\nu,0}. \quad (3)$$

Then the noise in the Fourier space is constructed as

$$\xi(\omega_\mu) = \sqrt{N\Delta t\,\gamma(\omega_\mu)}\,\alpha_\mu, \quad \mu = 1, \ldots, N-1,$$

$$\xi(\omega_0) = \gamma(\omega_N), \quad (4)$$

where α_μ are Gaussian random numbers with the zero mean and correlation

$$\langle \alpha_\mu \alpha_\nu \rangle = \delta_{\mu,-\nu}. \quad (5)$$

α_μ can be expressed in terms of its real and imaginary parts $\alpha_\mu = a_\mu + i b_\mu$, where a_μ and b_μ are Gaussian random numbers with zero mean and variance given by [2]

$$\begin{cases} \langle a_\mu^2\rangle = \langle b_\mu^2\rangle = \frac{1}{2}, & \text{for } \mu = 1,2,\ldots,N-1; \\ \langle a_\mu^2\rangle = 1,\ \langle b_\mu^2\rangle = 0, & \text{for } \mu = N. \end{cases}$$

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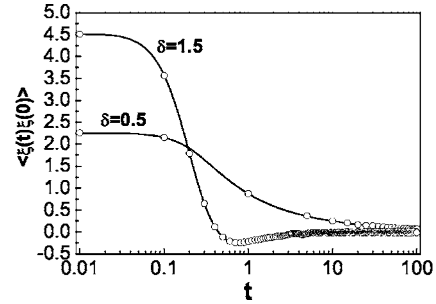

FIG. 1. The correlation function of non-Ohmic noise for two power exponents. The solid lines and open circles are theoretical and numerical results, respectively.

The discrete inverse Fourier transform of Eq. (4) gives a string of N numbers, $\xi(t)$, which are correlated with the requested time correlation by construction. Then the friction kernel function and the corresponding correlation function of the noise are numerically evaluated by

$$\gamma(t_i) = \frac{\sum_{j=0}^{N_0} \langle \xi(t_j + i\Delta t)\xi(t_j)\rangle}{N_0 + 1}, \tag{6}$$

where the numbers of the network $N=2^{25}$ and $N_0=N/4$ are used in our simulations.

It is known that the non-Ohmic model [1] can describe a rich variety of frequency-dependent friction mechanisms, which arises from a spectral density $J(\omega)=\gamma_\delta(\omega/\tilde{\omega})^{\delta-1}f_c$, where f_c is a high frequency cut-off function of typical width ω_c; $\tilde{\omega}$ denotes a reference frequency allowing for the friction constant $m\gamma_\delta$ to have the dimension of a viscosity of any δ. The friction kernel function in the spectral space reads

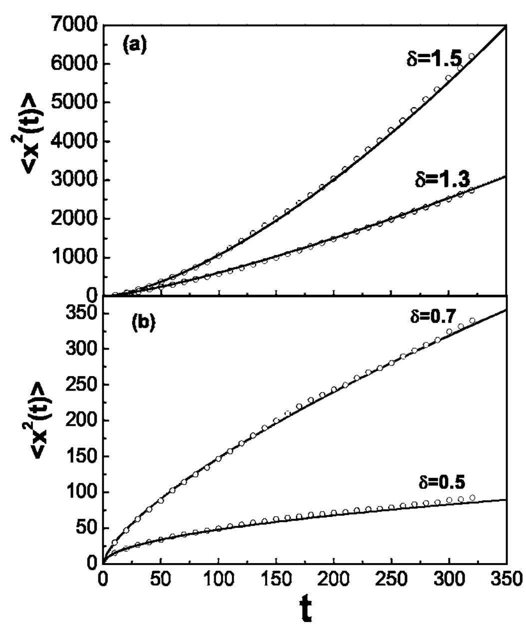

FIG. 2. The mean square displacement of the particle calculated by numerical simulation (open circles) and theoretical expression (lines) for various δ. The parameters used are the same as Fig. 1.

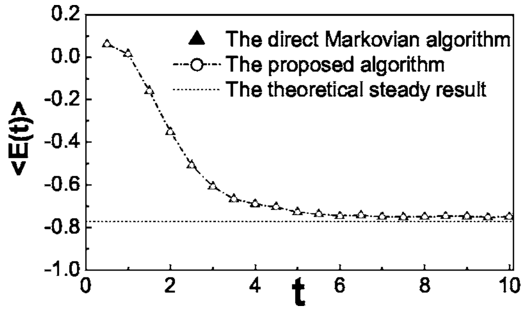

FIG. 3. The mean temporal energy of the particle in a double-well potential. The straight line is the stationary analytical result. The parameters used are $\gamma_0=1.0$, $T=0.2$, and $\tau=0.005$.

$$\gamma(\omega) = 2\gamma_\delta\left(\frac{|\omega|}{\tilde{\omega}}\right)^{\delta-1} f_c\left(\frac{|\omega|}{\omega_c}\right). \tag{7}$$

When $\delta=1$, $\gamma(\omega)$ is equal to a constant at least in the frequency range $|\omega| \ll \omega_c$, which reduces to the Ohmic friction, i.e., the usual Gaussian white noise case.

The temporal correlation function of the noise has been obtained by applying the inverse Fourier transform to Eq. (7). In fact, this colored noise cannot be produced by a stochastic differential equation driven by a Gaussian white noise. Here we use the parameters $\tilde{\omega}=1.0$, $\gamma_\delta=1.0$, $\Delta t=0.01$, and choose a smooth cutoff function $f_c=\exp(-\omega/\omega_c)$ [3] with $\omega_c=4.0$. Thus $\gamma(\omega)$ is written as a discrete form

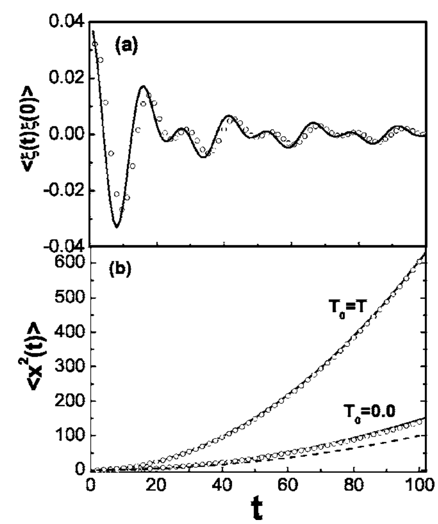

FIG. 4. (a) The simulating (open circles) and theoretical (solid lines) results for the correlation function of noise. (b) Comparison of the mean square displacement calculated by the present algorithm (open circles), the theoretical data (solid lines), and Ref. [18] (dashed line with $T_0=0$).

$$\gamma(\omega_\mu)=\begin{cases}\sqrt{2N\Delta t\gamma_\delta\left(\dfrac{2\pi\mu}{N\Delta t\tilde{\omega}}\right)^{\delta-1}}\exp(\theta), & 0\leqslant\mu\leqslant\dfrac{N}{2};\\ \gamma(\omega_{N-\mu}), & \dfrac{N}{2}\leqslant\mu\leqslant N,\end{cases} \tag{8}$$

where $\theta=2\pi\mu/(N\Delta t\omega_c)$. It is noticed that the cut-off of the noise frequency has no large influence on the result, since the long-time dynamical behavior of the system is determined by small ω spectrum of the noise.

In Fig. 1, we plot the correlation function of the noise for various power exponents δ by using the present Fourier transform technique. It is seen that the numerical results are in good agreement with the theoretical formula. This will assure the reliability of GLE driven by such thermal colored noise simulated. Figure 2 shows the mean square displacement of a force-free particle for various δ; those are calculated numerically from GLE (1) and compared with the analytical formula [3]. The particle starts from the origin of the coordinate and its initial velocity obeys a Gaussian distribution with the variance $\{v^2(0)\}=k_BT/m$ [3]. Herein we indicate by $\{\cdots\}$ the average with respect to the initial value of the state variable.

The present algorithm is not only applicable to a complex correlated noise with a frequency-dependent spectrum, but also used to simulate a non-Markovian dynamics which can be transformed into a Markovian process through introducing new variables. For comparison, we consider the energy relaxation for a particle subjected to a thermal Ornstein-Uhlenbeck noise (OUN) moving in a double-well potential [7]. The OUN $\xi(t)$ obeys the following linear Langevin equation [9,10]:

$$\dot{\xi}(t)=-\frac{\xi(t)}{\tau}+\frac{\eta(t)}{\tau}, \tag{9}$$

where $\eta(t)$ is a zero-mean Gaussian white noise with $\langle\eta(t)\eta(t')\rangle=\gamma_0\delta(t-t')$ and τ is the correlated time of noise. The stationary correlation function of the OUN is given by $\{\langle\xi(t)\xi(t')\rangle\}=(\gamma_0/\tau)\exp(-|t-t'|/\tau)$ [15]. The potential is taken to be $U(x)=x^4-2x^2$ [16,17]. The mean temporal energy of the particle is determined by $\langle E(t)\rangle=\frac{1}{2}m\langle v^2(t)\rangle+\langle U(x(t))\rangle$.

We use the present algorithm and the transforming Markovian method [7] with 10^5 trajectories to simulate the relaxation of the particle starting from $x(0)=0$ and $v(0)=0$ evolving to the stationary state, the results are shown in Fig. 3. The parameters are $\gamma_0=1.0$, $T=0.2$, $\tau=0.005$, and $\Delta t=0.0005$. The theoretical result is $\langle E(t=6)\rangle=-0.773$ [17], the system has arrived at the stationary state at this time. It is seen that the result calculated by the present algorithm is in good agreement with that of the direct simulating algorithm [7] at any time and approaches the stationary analytical data in a long-time limit.

Recently, Morgado *et al.* [18] presented a criterion for the lower part of frequency in the spectral density of noise being removed in order to produce ballistic diffusion and also performed numerical simulations, where the initial velocity of the particle was taken to be zero. The spectral density of noise in the acoustic phonon model reads

$$\rho_n(\omega)=\begin{cases}C, & \text{for } \omega_1<\omega<\omega_s;\\ 0, & \text{otherwise},\end{cases} \tag{10}$$

where C is a constant. The noise is originated from a coupled harmonic chain, ω_s is the Debye phone frequency, and ω_1 is a finite frequency. The friction kernel function of the system is given by

$$\gamma(t)=\frac{2\gamma^*}{\pi}\left(\frac{\sin(\omega_s t)}{t}-\frac{\sin(\omega_1 t)}{t}\right), \tag{11}$$

where γ^* is the friction coefficient.

However, we think that their result does not include the initial velocity of the particle and the directly simulating algorithm used by them is not accurate for such a problem. Here we report the asymptotical expression for the mean square displacement of a force-free particle as

$$\langle x^2(t)\rangle=\left[\frac{k_BT}{m}b+\left(\frac{k_BT_0}{m}-\frac{k_BT}{m}\right)b^2\right]t^2, \tag{12}$$

where the factor $b=[1+2\gamma^*/\pi(1/\omega_1-1/\omega_s)]^{-1}$ and T_0 is the initial temperature of the particle determined by its initial velocity $T_0=m\{v^2(0)\}/k_B$. In fact, the above expression is exactly according to the residue theorem [7], because there are no other nonzero roots for the equation $z+\hat{\gamma}(z)=0$ [where $\hat{\gamma}(z)$ is the Laplace transform of $\gamma(t)$], which appears in the inverse Laplace transform of the response function [19].

It is unknown for the noise with the correction (11) obeying a linear Langevin equation driven by a Gaussian white noise, but the only requirement for the algorithm to work is that the Fourier transform of the temporal correlation function can be known [12,13]. We discrete $\gamma(\omega)$ as follows

$$\gamma(\omega_\mu)=\begin{cases}\sqrt{N\Delta tC}, & \dfrac{N\Delta t\omega_1}{2\pi}+1<\mu<\dfrac{N\Delta t\omega_s}{2\pi};\\ 0, & 0\leqslant\mu\leqslant\dfrac{N\Delta t\omega_1}{2\pi}+1 \text{ or } \dfrac{N\Delta t\omega_s}{2\pi}+1\leqslant\mu<\dfrac{N}{2};\\ \gamma(\omega_{N-\mu}), & \dfrac{N}{2}\leqslant\mu\leqslant N.\end{cases} \tag{13}$$

According to the prescription (6) we generate the discrete field $\xi(\omega)$. The requested noise $\xi(t)$ can be generated by applying the Fourier transform to $\xi(\omega)$. First, we check the suitability of the procedure. The correlation function of noise is evaluated numerically based on the prescription (13) and plotted in Fig. 4(a). In comparison, the result calculated theoretically by Eq. (11) is also plotted.

Figure 4(b) shows the mean square displacement of a force-free particle calculated numerically by our algorithm and the direct method of Ref. [18]. The parameters used are $\omega_s=0.5$, $\omega_1=\frac{1}{2}\omega_s=0.25$, $\gamma^*=0.25$, $\Delta\omega=2\pi/N\Delta t$, and $\Delta t=0.01$. The particles starts from the origin of the coordinate, whose initial velocity obeys a Gaussian distribution as $W(v_0)=(2\pi m^{-1}k_BT_0)^{-1/2}\exp(-mv_0^2/2k_BT_0)$. We also plot the theoretical result [Eq. (12)] in Fig. 4(b) by choosing the initial temperatures of two kinds. The agreements between our simulation and the theoretical result are excellent, however, the error in Ref. [18] is about 40% at $t=100$. The asymptotical velocity variance of the particle is deduced as $\langle v^2(t\to\infty)\rangle=k_BT/m+b^2(k_BT_0/m-k_BT/m)$. Although the FDT does not generally hold when $b\neq 0$ it assumes validity for a special initial preparation, namely the equilibrium preparation with a Gaussian of weight k_BT/m. The breakdown of the FDT is thus connected with the breakdown of the ergodicity. Alternatively, this implies that no unique stationary probability exists for the Gaussian non-Markovian process if the initial particle velocity is not chosen to be equilibrium.

In summary, we have proposed a numerical scheme to solve the generalized Langevin equation with arbitrary correlated noise. This algorithm works in the discrete Fourier space and is not restricted to the dynamics of the noise. Because of application to the non-Ohmic model with frequency-dependent friction, we have obtained a better result for anomalous diffusion. Upon inspection from numerical and analytical calculations of the acoustic phonon model showing ballistic diffusion, we have found a prominent result: the mean square displacement and velocity of the particle are initial preparation dependent. Further, anomalous transport processes of a particle moving in a potential can be investigated by means of the present algorithm.

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