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Tests of Numerical Simulation Algorithms for the Kubo Oscillator

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Numerical simulation algorithms for multiplicative noise (white or colored) are tested for accuracy against closed-form expressions for the Kubo oscillator. Direct white noise simulations lead to spurious decay of the modulus of the oscillator amplitude. A straightforward colored noise algorithm greatly reduces this decay and also provides highly accurate results in the white noise limit.

KEY WORDS: Numerical simulation; multiplicative noise; Kubo oscillator.

The widespread availability of rapid, large-scale computing has made Monte Carlo simulations an extremely powerful technique for investigating the properties of stochastic differential equations. The stochasticity appears in these equations as either additive or multiplicative noise terms. While simulations of additive noise have been thoroughly tested for their accuracy,[(1,2)] this is not the case for multiplicative noise. In addition, colored noise simulations have gained increased importance because of their relevance in a variety of physical situations. This has been especially true in the study of dye laser intensity fluctuations.[(3)]

In this paper, we show results of tests of numerical algorithms that simulate colored and white, multiplicative noise for a stochastic differential equation that possesses closed-form, analytic solutions. This equation describes the so-called Kubo oscillator,[(4)] which is the prototype for all multiplicative stochastic processes, and has seen application in the theory of nuclear magnetic resonance and elsewhere.

The Kubo oscillator is described by the complex stochastic differential equation

$$\frac{\partial}{\partial t} a(t) = i(\omega_0 + \omega(t))\, a(t) \tag{1}$$

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in which $a(t)$ is a complex amplitude and $\omega(t)$ is a real, stochastic frequency. In the colored noise regime $\omega(t)$ satisfies an additive stochastic differential equation

$$\frac{\partial}{\partial t}\omega(t) = -\lambda\omega(t) + \lambda\xi(t) \tag{2}$$

in which $\xi(t)$ is white noise, with correlation formula

$$\langle \xi(t)\,\xi(s)\rangle = Q\delta(t-s) \tag{3}$$

and zero mean. This engenders in $\omega(t)$ the correlation formula

$$\langle \omega(t)\,\omega(s)\rangle = \tfrac{1}{2}Q\lambda e^{-\lambda|t-s|} \tag{4}$$

In the limit $\lambda \to \infty$, $\omega(t)$ becomes white noise with correlation formula identical with (3), and (1) is to be interpreted in the sense of Stratonovich.[5]

Converting $a(t)$ to polar coordinates

$$a = re^{i\phi} \tag{5}$$

results in the exact differential equation for the probability density for the phase ϕ:

$$\frac{\partial}{\partial t}P(\phi, t) = \left[-\omega_0\frac{\partial}{\partial\phi} + D(t)\frac{\partial^2}{\partial\phi^2}\right]P(\phi, t) \tag{6}$$

in which $D(t)$ is defined by

$$D(t) = \tfrac{1}{2}Q(1-e^{-\lambda t}) \tag{7}$$

and the initial condition is $P(\phi, 0) = \delta(\phi - \phi_0)$. The modulus of $a(t)$, r, is a constant of the dynamics described by (1).

Our studies focused on the mean phase $\langle\phi\rangle$, the normalized variance $\langle\Delta\phi^2\rangle/\langle\phi\rangle^2$, and the skewness $\langle\Delta\phi^3\rangle/\langle\Delta\phi^2\rangle^{3/2}$. These quantities may be determined in closed form from Eq. (6), which has the explicit solution

$$P(\phi, t) = \frac{1}{2\pi}\sum_{m=-\infty}^{\infty}\exp\left[im\phi - im\phi_0 - im\omega_0 t - m^2\int_0^t ds\, D(s)\right] \tag{8}$$

Define C, S, and T by

$$C = \sum_{m=1}^{\infty}\frac{1}{m^2}\cos m(\phi_0 + \omega_0 t)\exp\left[-m^2\int_0^t ds\, D(s)\right] \tag{9}$$

$$S = \sum_{m=1}^{\infty} \frac{1}{m} \sin m(\phi_0 + \omega_0 t) \exp\left[-m^2 \int_0^t ds\, D(s) \right] \tag{10}$$

$$T = \sum_{m=1}^{\infty} \frac{1}{m^3} \sin m(\phi_0 + \omega_0 t) \exp\left[-m^2 \int_0^t ds\, D(s) \right] \tag{11}$$

With these, we may write

$$\langle \phi \rangle = \pi - 2S \tag{12}$$

$$\langle \Delta\phi^2 \rangle = \tfrac{1}{3}\pi^2 + 4C - 4S^2 \tag{13}$$

$$\frac{\langle \Delta\phi^3 \rangle}{\langle \Delta\phi^2 \rangle^{3/2}} = \frac{12T + 24SC - 16S^3}{(\frac{1}{3}\pi^2 + 4C - 4S^2)^{3/2}} \tag{14}$$

These expressions were used to test the accuracy of multiplicative noise numerical algorithms for strongly colored, weakly colored, and white noise regimes.

In the colored noise regimes, we numerically integrate Eqs. (1) and (2) simultaneously, generating Gaussianly distributed random numbers for Eq. (2) by the Box–Mueller algorithm,[6] and treating Eq. (1) by the algorithm developed by Sancho *et al.*[7] The results of these simulations are compared with Eqs. (12)–(14) in Figs. 1–9, which cover three different values of λ. The strongly colored noise regime corresponds with $\lambda = 0.05$, the weakly colored noise regime corresponds with $\lambda = 1.0$, and for $\lambda = 10$,

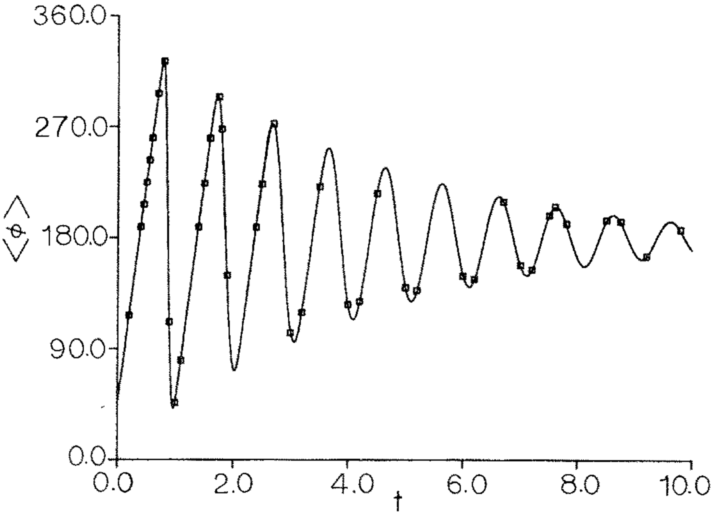

Fig. 1. Time evolution of the mean phase $\langle \phi \rangle$ for colored noise, for $Q = 0.1$ and $\lambda = 0.05$. The step size was $\Delta = 1.5915 \times 10^{-4}$ and 5000 stochastic trajectories were computed for Figs. 1–12. (□) Simulation results.

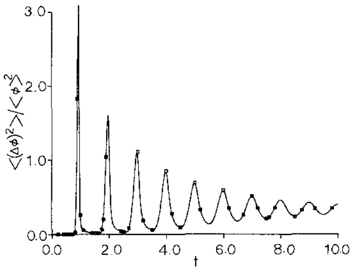

Fig. 2. Time evolution of the normalized variance $\langle(\Delta\phi)^2\rangle/\langle\phi\rangle^2$ for colored noise, for $Q=0.1$ and $\lambda=0.05$.

the results are virtually indistinguishable from the results we obtained for white noise using the algorithm described below.

Equation (1) can be numerically simulated by itself in the white noise case (in the Stratonovich interpretation).[7,8] In Figs. 10–12 we show the comparison for these simulations. We note that the agreement is equally good. However, in Fig. 13 we show the behavior of one trajectory for real and imaginary components of $a(t)$. In Fig. 14a the same information is shown for $r(t)$, a supposed constant of the motion! The white noise algorithm generates a spurious decay in the amplitude of each stochastic trajectory, although, as noted above, the phase behaves faithfully. In Fig. 14b we show $r(t)$ for one trajectory calculated with the colored noise algorithm. No decay is visible and $r(t)$ remains almost constant.

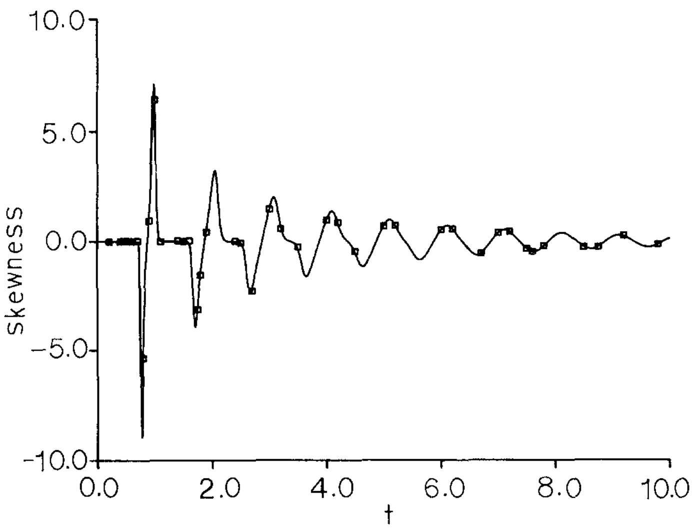

Fig. 3. Skewness versus t, for $Q=0.1$ and $\lambda=0.05$.

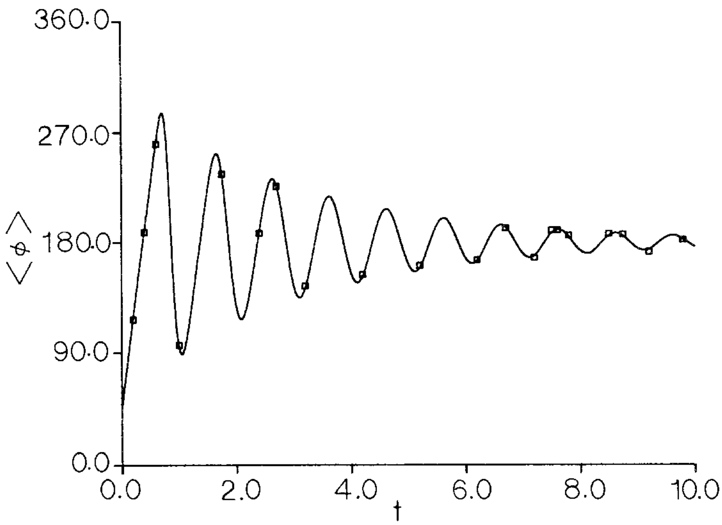

Fig. 4. Plot of $\langle \phi \rangle$ versus t, for $Q=0.1$ and $\lambda=1.0$. This represents weakly colored noise.

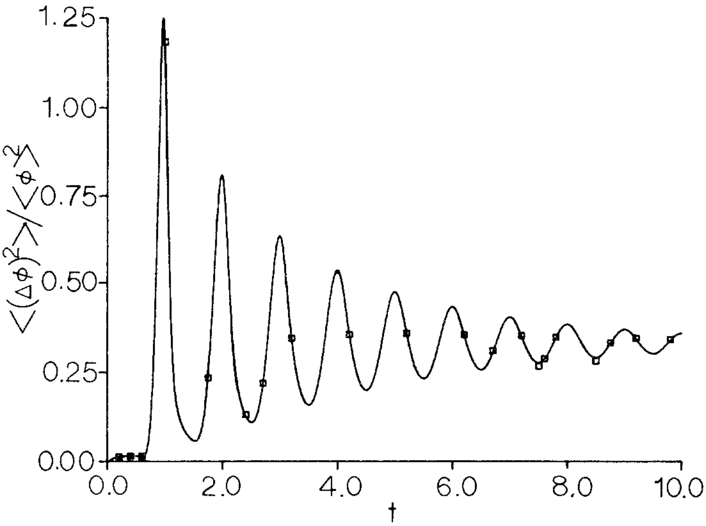

Fig. 5. Plot of $\langle (\Delta\phi)^2 \rangle / \langle \phi \rangle^2$ versus t, for $Q=0.1$ and $\lambda=1.0$.

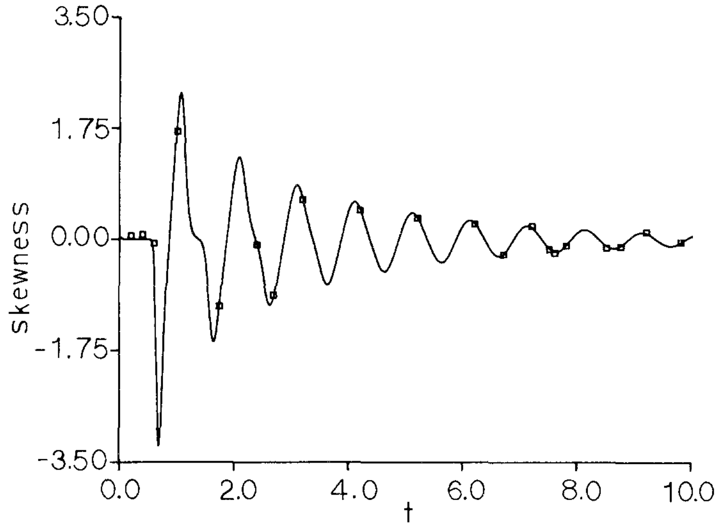

Fig. 6. Skewness versus t, for $Q = 0.1$ and $\lambda = 1.0$.

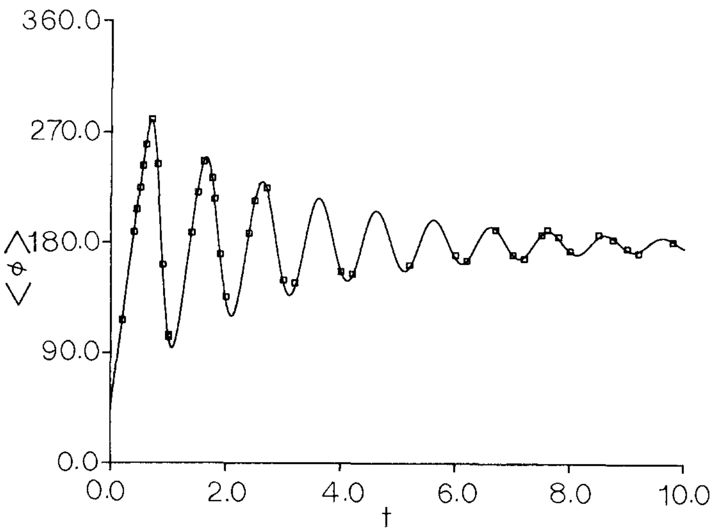

Fig. 7. Plot of $\langle \phi \rangle$ versus t, for $Q = 0.1$ and $\lambda = 10.0$. This represents very weakly colored noise. The curves in Figs. 7–9 are indistinguishable from those for white noise (Figs. 10–12).

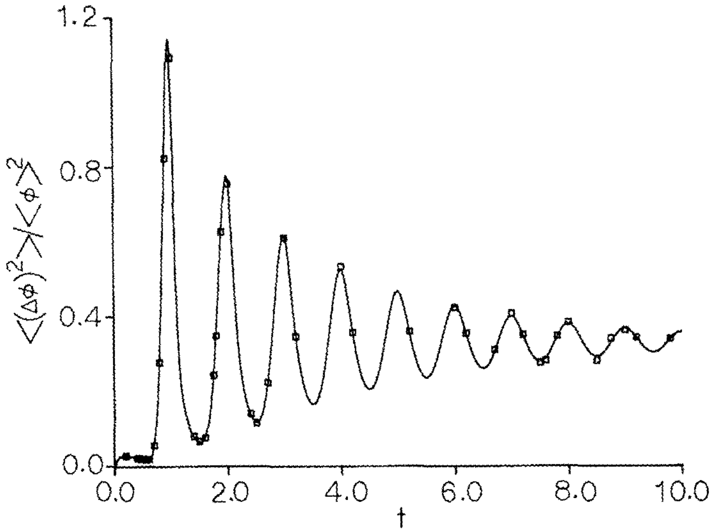

Fig. 8. Plot of $\langle(\Delta\phi)^2\rangle/\langle\phi\rangle^2$ versus t, for $Q=0.1$ and $\lambda=10.0$.

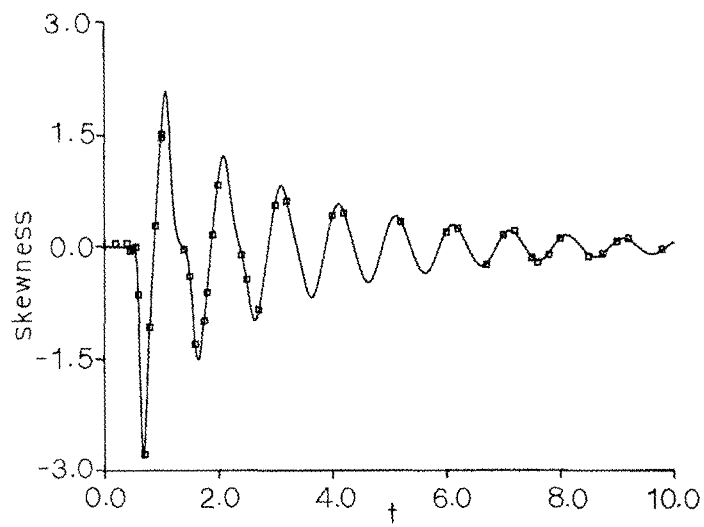

Fig. 9. Skewness versus t, for $Q=0.1$ and $\lambda=10.0$.

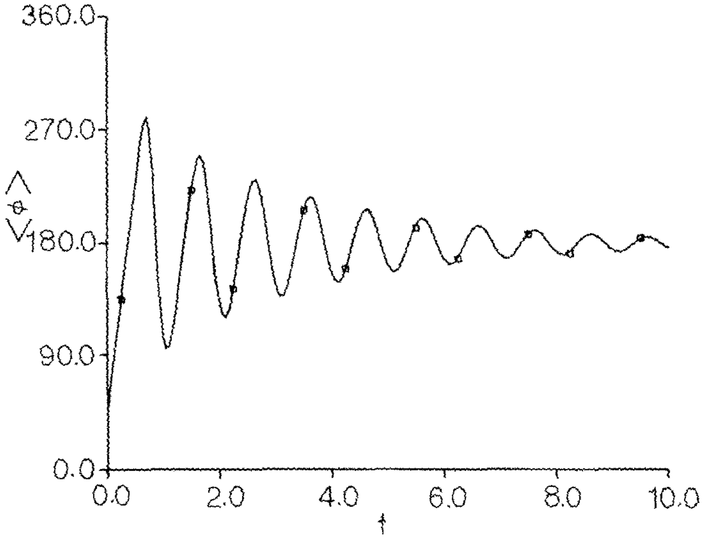

Fig. 10. Plot of $\langle \phi \rangle$ versus t, for the integration is done using the white noise algorithm, with $Q = 0.1$.

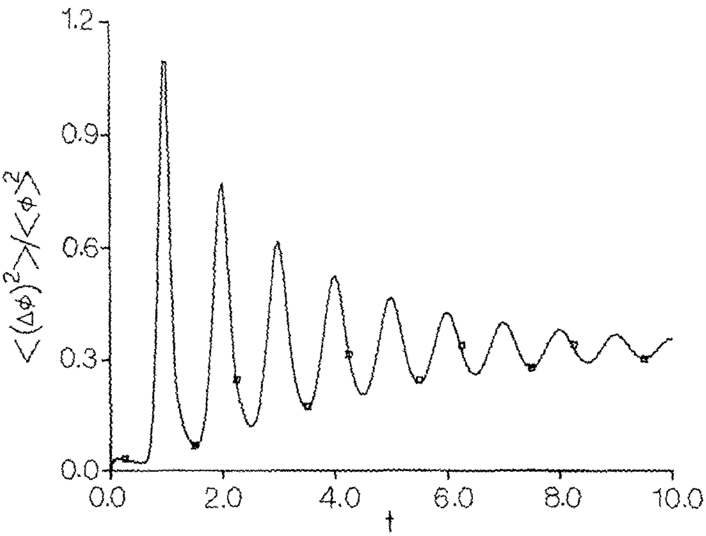

Fig. 11. Plot of $\langle (\Delta\phi)^2 \rangle / \langle \phi \rangle^2$ versus t, for the integration is done using the white noise algorithm.

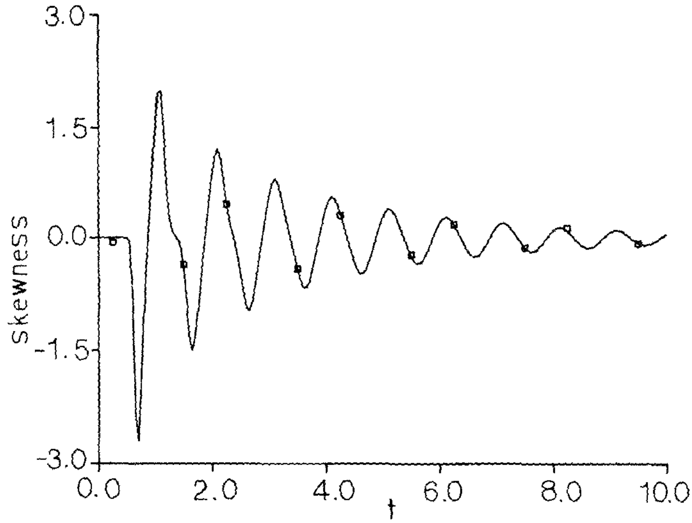

Fig. 12. Skewness versus t, for the integration is done using the white noise algorithm.

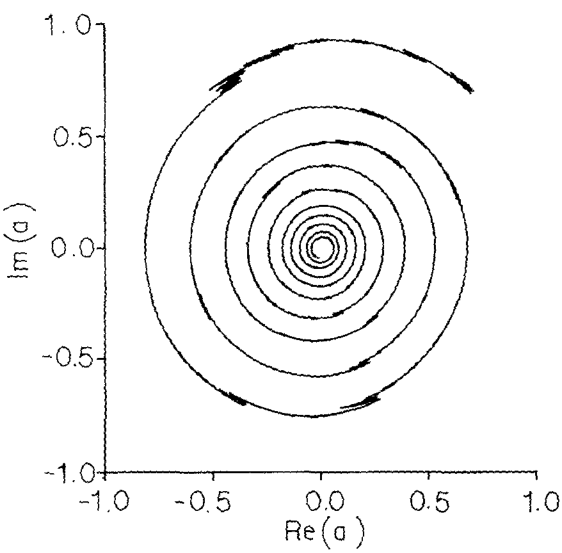

Fig. 13. The behavior of one stochastic trajectory generated by the white noise algorithm, for $Q = 0.1$. A spurious decay is evident.

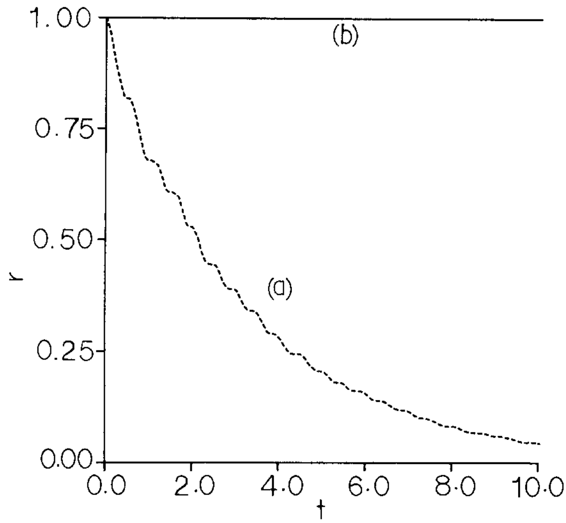

Fig. 14. (a) The same information as in Fig. 13, for the modulus $r(t)$ of a. The spurious exponential decay arises from the white noise algorithm. (b) $r(t)$ remains constant when the colored noise algorithm is used in the weakly colored noise regime ($Q = 0.1$, $\lambda = 10.0$).

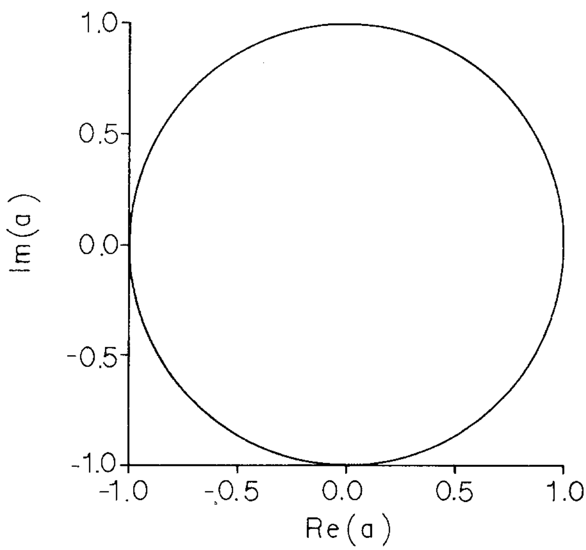

Fig. 15. The behavior of one stochastic trajectory generated by the colored noise algorithm for $Q = 0.1$ and $\lambda = 10.0$.

In Fig. 15, we show one trajectory in the complex plane for $a(t)$ when the colored noise algorithm is used instead. For this plot, $\lambda = 10$, and the time course is the same as in Figs. 13–14. Virtually no decay in amplitude can be seen.

Thus, the colored noise algorithm not only allows us to simulate strongly colored noise in the Kubo oscillator, but it also provides us with a highly accurate alternative to the white noise algorithm. Both phase and modulus are accurately portrayed.

Denote the step size by Δ. In Eq. (A10) of Sancho *et al.*[7] [or equivalently in Eq. (3.138) of Risken[8]], the multiplicative noise gives rise to terms of order $\sqrt{\Delta}$ and Δ. The latter term is responsible for the spurious decay in the modulus. The rate of decay is determined by Q. In the colored noise algorithm, Eq. (A25) of Ref. 7, the multiplicative noise terms are of order Δ and Δ^2. The Δ^2 term will still create an artifactual decay, but at a much slower rate (because Δ^2 is smaller than Δ for typically used step sizes), thus allowing us to simulate accurately the Kubo oscillation for longer times. On the other hand, reduction of step size for the algorithms of Sancho *et al.* and of Risken does not improve the situation, strongly suggesting that these algorithms are flawed for white noise.

The direct simulation of multiplicative white noise stochastic differential equations is fraught with difficulties and has recently been carefully examined by Klauder and Petersen.[9] The present study clearly indicates that the colored noise algorithm is straightforward, accurate, and even permits effective white noise simulation in its weakly colored noise regime.

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