Color-Induced Transition to a Nonconventional Diffusion Regime

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It is shown that the negative diffusion coefficients exhibited by the current approaches to the Fokker-Planck equation for non-Markovian and bistable processes result from assuming the diffusion process to be stationary. The rejection of this assumption leads to predictions on the escape over a barrier agreeing with the physical arguments pertaining to the extremely colored-noise regime.

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Many groups[1-13] have recently focused their attention on physical systems described by the stochastic differential equation,

$$\dot{x}=\phi(x)+\psi(x)\xi(t), \tag{1}$$

where $\xi(t)$ is a colored Gaussian noise, with vanishing mean value, and correlation function defined by

$$\langle\xi(0)\xi(t)\rangle=(D_0/\tau)e^{-t/\tau}, \tag{2}$$

where τ is the correlation time. It has also more recently been shown that the results of seemingly different theories can be recovered within the context of the projection operator method,[1,2] which leads to the following Fokker-Planck-type equation for $\sigma(x;t)$, the probability distribution of x:

$$\frac{\partial}{\partial t}\sigma(x;t)=\left[-\frac{\partial}{\partial x}\phi(x)+\frac{D_0}{\tau}\frac{\partial}{\partial x}\psi(x)\frac{\partial}{\partial x}\psi(x)\int_0^t ds\exp\{-[\tau^{-1}-\Pi(x)]s\}\right]\sigma(x;t)+\cdots. \tag{3}$$

For the definition of $\Pi(x)$ see Ref. 2. It must be remarked (a) that this equation is the result of a perturbation calculation at the second order in the interaction between x and ξ where the higher-order terms result in nonstandard Fokker-Planck terms,[1,2] and (b) that it is based on the initial condition $\rho(x,\xi;0)=\sigma(x;0)\rho_{eq}(\xi)$, where $\rho(x,\xi;0)$ is the initial probability distribution of the whole system and $\rho_{eq}(\xi)$ is the equilibrium distribution of the variable ξ [$\rho_{eq}(\xi)\sim\exp(-\xi^2\tau/2D_0)$]. This means that the x and ξ systems, originally statistically independent, are brought into contact with one another at time $t=0$. Equation (3) allows us to predict the subsequent behavior of the x system.

It is usually assumed[1-7] that a steady state is reached by the system for $t\to\infty$. Thus the time t appearing as the upper integration limit on the right-hand side of Eq. (3) is replaced by ∞. The resulting equation, from now on referred to as standard Fokker-Planck form (SFPF), is affected by this basic fault: There are critical regions where the diffusion coefficient turns out to be negative. This fault essentially affects the short-time expansions of Refs. 7-9 and, after a critical value of τ, τ_c, even the Fox theory.[5,6]

This difficulty has so far elicited two different kinds of reactions: Peacock-López, West, and Lindenberg[10] showed that those properties that do not specifically involve $\sigma(x;t)$, in the critical region may be well represented by the SFPF. Fox and Roy,[11] on the contrary, to bypass this difficulty had recourse to a generalized version of the so-called decoupling theory,[12] which consists of replacing $\Pi(x)$ with a suitable negative value independent of x. An approximation of this kind, however, does not reproduce interesting effects of colored noise such as, for instance, the transition from one- to two-mode distributions.[13]

The basic aim of this Letter is to show that if Eq. (3) is left as it is (i.e., the upper limit of the time integration is not replaced by ∞) the artifact of negative diffusion coefficients is bypassed. Furthermore, this allows us safely to attain the large-τ region, *where its predictions on the escape process are seen to fit the physical arguments rigorously valid for* $\tau\to\infty$.

We shall focus on the bistable system

$$\phi(x)=\alpha x-\beta x^3 \tag{4}$$

in the additive case [$\psi(x)=1$]. Then we shall adopt the local linearization approximation[2,14] $\Pi(x)\approx\phi'(x)\equiv d\phi(x)/dx$. This approximation holds for $D_0\to 0$ and it has the nice effect of making the terms higher than second order in Eq. (3) vanish. This local linearization is consistent with the spirit of the Kramers theory.[15]

Thus we must solve the following equation of motion:

$$\frac{\partial}{\partial t}\sigma(x;t)=\left[-\frac{\partial\phi}{\partial x}+\frac{D_0}{\tau}\frac{\partial^2}{\partial x^2}\frac{\exp\{[\phi'(x)-\tau^{-1}]t\}-1}{\phi'(x)-\tau^{-1}}\right]\sigma(x;t). \tag{5}$$

The function $\phi'(x)$ changes sign at $x=\pm b$ where $b \equiv (\alpha/3\beta)^{1/2}$. In the side regions $-\infty < x < -b$, $b < x < \infty$, the function $\phi'(x)$ is always negative thereby leading the space- and time-dependent diffusion coefficient to a finite stationary value. In contrast, in the region around the barrier $-b \le x \le b$, $\phi'(x)$ is always positive semidefinite with values ranging from 0 (at the boundary) to α (at $x=0$). Thus, when the critical condition $\tau=\tau_c \equiv 1/\alpha$ is reached, the diffusion process at the top of the barrier is prevented from attaining the kind of stationary state that is conventionally evaluated by one's setting $\partial\sigma(x;t)/\partial t=0$.

The divergence of the diffusion coefficient for $t\rightarrow\infty$, triggered by the color of the noise ($\tau > \tau_c$), is not a theoretical artifact: In the linear case of the inverted parabola, Eq. (5) is easily proven to lead to an exact result.[14]

To prove that with Eq. (5) a correct equilibrium distribution can be reached even in the critical region $\tau > \tau_c$, we used as initial distributions the steady-state solutions of the SFPF with $\psi(x)=1$ and $\Pi(x)=\phi'(x)$, but with the population of the region where the SFPF results in negative diffusion coefficients set to vanish (note that a vanishing population in this region is rigorously exact only in the limiting case $\tau\rightarrow\infty$, as it has been proved[9] that the region around the barrier at finite values of τ is characterized by a finite population). Thus by construction, the initial population at $x=0$, $\sigma(x;0)$, vanishes throughout the whole critical region $\tau_c < \tau < \infty$. Figure 1 shows that $\sigma(0,t)$ is always semidefinite positive even beyond the threshold τ_c, where negative values of the population should be reached according to the SFPF.

A basic tenet of all the theories of chemical reaction processes is the assumption that the reaction process is characterized by a stationary current.[15,16] However, we see from Eq. (5) that when the critical value τ_c is reached, the diffusion coefficient diverges for $\tau\rightarrow\infty$ over a region the size of which increases upon increase of τ from the point $x=0$ (at $\tau=\tau_c$) till it covers the whole interval $-b<x<b$ (at $\tau=\infty$). This makes it impossible to use the standard analytical approaches.[15,16]

We thus carried out the following idealized experiment. At the initial time $t=0$ the system is placed in an initial distribution obtained from those used to obtain the results of Fig. 1 by our setting the population equal to zero at $x>0$, and the interaction with the ξ system is switched on. We then solve Eq. (5) numerically and monitored the time variation of the reactant population, $n(t)=\int_{-\infty}^{0}\sigma(x;t)dx$, which after a transient time of the order $1/\alpha$ turned out to be a perfectly exponential function of time. The results of Figs. 2 and 3 were obtained by the assumption that the inverse of the rate of this exponential decay can be compared with the mean first-passage time T.

In the long-τ region, it is possible to derive an analytical formula for the mean first-passage time with use of the following physical arguments. When the condition $\tau \gg 1/\alpha$ applies, the Brownian particle is virtually always found to be in a stable equilibrium position given by one of the three roots of the equation $\phi(x)+\xi=0$. This equilibrium position gradually changes in time as an effect of the slow time dependence of ξ. When the critical value $\xi_c=\pm(4\alpha^3/27\beta)^{1/2}$, corresponding to the disappearance of the barrier, is reached, the particle jumps from the positive to the negative side of the x axis, and vice versa. By evaluating the first-passage time for ξ to reach the critical value ξ_c (ξ is a stationary Gaussian-Markov process with damping $1/\tau$) we obtain

$$T=(27D_0\pi\tau/8V_0\alpha)^{1/2}\exp[(8V_0/27D_0)\alpha\tau],$$

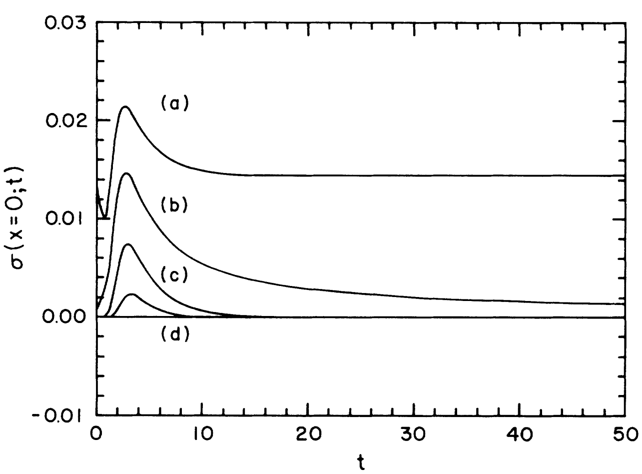

FIG. 1. The probability distribution $\sigma(x;t)$ at $x=0$ is plotted as a function of time for various correlation times τ: (curve a) 0.75, (curve b) 0.99, (curve c) 1.5, (curve d) 2.5. The value of the strength of the noise is $D_0=0.114$ and $\alpha=\beta=1$.

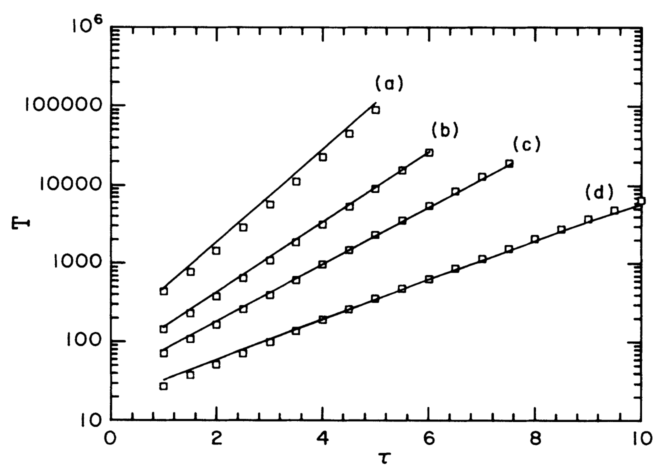

FIG. 2. T vs τ for $\alpha=\beta=1$ and D_0 equal to (curve a) 0.06, (curve b) 0.08, (curve c) 0.10, and (curve d) 0.15. Full lines denote Eq. (6), whereas squares denote the result of the numerical calculation with Eq. (5).

where the height of the barrier is given by $V_0=\alpha^2/4\beta$. This expression implies also the assumption that $\alpha\tau \gg 27D_0/8V_0$ (for the arguments of the Kramers theory to be applied). Surprisingly enough, the numerical solution of Eq. (5) shows that the slope of $\log(T/T_0)$ (T_0 is the first-passage time in the white-noise case) as a function of τ as predicted by this analytical law, i.e., $(8V_0/27D_0)\alpha$, is already exhibited at $\alpha\tau \gtrsim 1.5$. The numerical solution of Eq. (5) results indeed in $\log(T/T_0)$ being a straight line virtually parallel to that resulting from the long-τ expression above. It turns out that in the region from $\alpha\tau \approx 1.5$ up to the largest values of τ explored with our numerical solution of Eq. (5) the numerical results are satisfactorily fitted by the following analytical expression:

$$T=\exp(V_0/D_0)[\pi/\alpha\sqrt{2}+(\pi\tau)^{1/2}(27D_0/8\alpha V_0)^{1/2}\exp(8V_0\alpha\tau)/27D_0]. \tag{6}$$

This expression satisfies the obvious condition of matching the long-τ expression above with the white-noise limit. However, it serves only the purpose of emphasizing the agreement of the numerical solution of Eq. (5) with the slope of $\log(T/T_0)$ predicted by our analytical expression for $\tau\to\infty$ (the agreement on the slope is remarkable indeed, see Fig. 2).

This is a central result. The slope of $\log(T/T_0)$ as a function of τ as predicted by the mean-field formula[12]

$$T=\frac{\pi}{\alpha\sqrt{2}}\exp\left[\frac{V_0}{D_0}(1+2\alpha\tau)\right] \tag{7}$$

is 1 order of magnitude larger than $(8V_0/27D_0)\alpha$, thereby implying that the mean-field theory misses the basic physical aspects of that linear dependence. This linear dependence reflects the transition from a standard diffusional regime to a new one, where the particle undergoes a deterministic motion in a slowly fluctuating potential, driven by the stochastic motion of ξ. It is remarkable that this new behavior, which would seem to be incompatible with the use of a Fokker-Planck description, is actually reproduced by the numerical solution of Eq. (5). This is a central result, because it sheds light on the real physical reasons behind the linear dependence of $\log(T/T_0)$ on τ, attributed by Leiber, Marchesoni, and Risken[17] to the mean-field theory of Ref. 12 (see also Tsironis[18]).

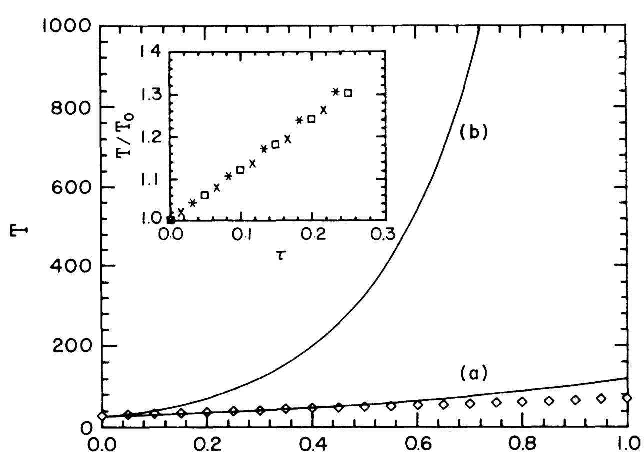

FIG. 3. First-passage time T vs the correlation time τ for $\alpha=\beta=1$ and $D_0=0.1$. Curve a represents Eq. (8), b Eq. (7), and the lozenges the values obtained from the numerical solution of Eq. (5). Inset: T/T_0 (where T_0 is the first-passage time for white noise) is plotted for D_0 equal to 0.15 (crosses), 0.10 (squares), and 0.06 (asterisks). The independence of T/T_0 from D_0 for small correlation times is evident.

In the region of $\alpha\tau \ll 1$ our Eq. (5) leads to a Fokker-Planck equation indistinguishable from that used by Masoliver, West, and Lindenberg[4] to obtain

$$T=(\pi/\alpha\sqrt{2})\exp[V_0/D_0+\tfrac{3}{2}\alpha\tau], \tag{8}$$

The linearization assumption intrinsic to the first-passage–time procedure makes the disagreement among the different groups at the order of τ^2 and larger disappear (Ref. 2) and gets the same result. A careful discussion of the whole matter can be found in a recent paper by Fox,[19] who shows that a formula originally presented by Hänggi, Marchesoni, and Grigolini[20] is correct. Further support to the analytical argument of Fox is given by the numerical solution of Eq. (5) within the same idealized experiment described above (see Fig. 3).

The mean-field theory, although it predicts a linear dependence of $\log(T/T_0)$ on τ/D_0, does not provide the correct slope[17] and does not interrupt this as an effect of the transition to a new regime at $\tau=1/\alpha$, thereby providing the suggestion[19] that this behavior also holds in the short-τ region.

The $\tau^{1/2}$ dependence of our long-τ formula must not be confused with that recently found by Doering, Hagan, and Levermore[21], in the short-τ regime. On the other hand, it seems that the short-τ behavior discovered by Doering, Hagan, and Levermore[21] does not conflict with our remarks regarding this regime, since it depends[22] on the boundary conditions different from those implicitly involved in our idealized experiment.

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