Kramers escape rate in nonlinear diffusive media

Zhao JiangLin[a)]
Institute of Mechanics (IMECH), Chinese Academy of Sciences, Beijing, 100080, China

Jing-Dong Bao and Gong Wenping
Physics Department, Beijing Normal University, Beijing 100875, China

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In this paper, we study nonlinear Kramers problem by investigating overdamped systems ruled by the one-dimensional nonlinear Fokker-Planck equation. We obtain an analytic expression for the Kramers escape rate under quasistationary conditions by employing a metastable potential and its predictions are in excellent agreement with numerical simulations. The results exhibit the anomalies due to the nonlinearity in W that the escape rate grows with D and drops as μ becomes large at a fixed D. Indeed, particles in the subdiffusive media $(\mu>1)$ can escape over the barrier only when D is above a critical value, while this confinement does not exist in the superdiffusive media $(\mu<1)$. © *2006 American Institute of Physics*. [DOI: 10.1063/1.2150433]

I. INTRODUCTION

Ever since Kramers reported his seminal work[1] on Brownian motion in phase space, the problem of noise-induced escape from metastable states has played a significant role in several areas of physical, chemical, biological, and even financial sciences. In particular, much attention has been paid to research on the Kramers escape rate from one state to another, which is nearly relevant in phase transitions in many systems. Diverse physical applications of this quantity, for example, stochastic resonance, ratchets, kink motion, and even transport induced by chaos-generated fluctuations. An overview can be found in Refs. 2–4.

However, most studies are concentrated in systems in ordinary media, where a particle exhibits standard Brownian motion and has a escape rate of the Arrhenius form. More complex systems require a generalized expression for the Kramers escape rate. For example, diffusion models deviating from Brownian motion show distinct nonlinear transport features. These stochastically driven mechanisms would result in an anomalous escape behavior. In this paper, we will focus on the problem of calculating the escape rate governed by the anomalous diffusion of the correlated type (not Levy-type diffusion).

The correlated anomalous diffusion can be described through the following nonlinear Fokker-Planck (FP) equation:

$$\frac{\partial}{\partial t}W(x,t)=\frac{\partial}{\partial x}[f'(x)W(x,t)]+D\frac{\partial^2}{\partial x^2}W^{\mu}(x,t), \qquad (1)$$

where (x,t) is a dimensionless $1+1$ space time, $f(x)$ is an external potential, μ and D are real parameters, and $D>0$ is diffusion contant. This equation recovers the ordinary Fokker-Planck equation when $\mu=1$. Other values of μ correspond to different physical systems with the W-dependent diffusion.[5–7]

II. MODEL AND ANOMALOUS KRAMERS RATE

We now consider a set of identical particles which are subject to an external metastable potential $f(x)$, shown as Fig. 1, and are couple to an anomalous diffusive environment. The density distribution of the particles can be solved from Eq. (1) which has been fully studied in Refs. 6, 8, and 9. The stationary solution of Eq. (1) is

$$W_s(x)=[1-(\mu-1)\beta_{\mu}f(x)]_+^{1/(\mu-1)}/Z, \qquad (2)$$

where $[g]_+=\max\{g,0\}$, Z is a normalization constant, and $\beta_{\mu}=Z^{\mu-1}/(\mu D)$. We are led back to the Boltzmann-Gibbs distribution $W_s(x)\sim\exp[-f(x)/D]$ in the limit $\mu\to1$. For $\mu\neq1$, the stationary solution of Eq. (1) can attain a maximum Tsallis entropy. The Tsallis entropy which was proposed in Refs. 10 has initiated extensive study of the nonextensive statistics. Particularly, it has been applied to reassociation in folded proteins,[11] fluxes of cosmic rays,[12] turbulence,[13] electron-positron annihilation,[14] and finance and economics.[15] Note that the condition $\mu>-1$ must hold so

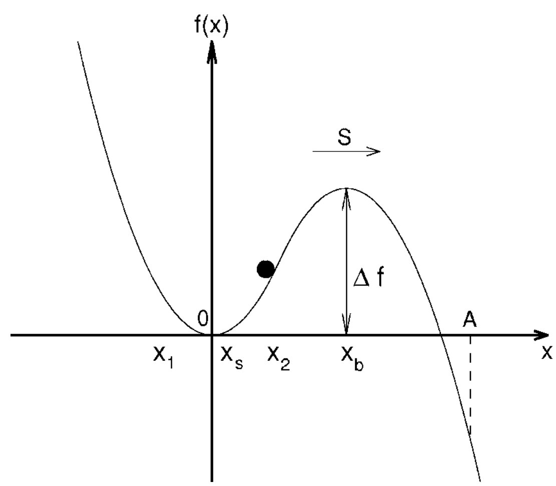

FIG. 1. A metastable potential for calculating the escape rate.

[a)]Electronic mail: ydqc@eyou.com

that the solution can be normalized, but here we restrict our discussion to the regime of $\mu > 0$.

We are mainly interested in the case where the probability current S over the top of a potential barrier near x_b can be taken as a small value and the time change of the density $W(x,t)$ as well. For this quasistationary state the small current S must then be approximately independent of x. We want to calculate the escape rate for particles sitting in a deep well near $x_s(=0)$ but have to obtain the current S at first. To this end, we employ the continuity equation

$$\frac{\partial}{\partial t}W(x,t) + \frac{\partial}{\partial x}S(x,t) = 0. \tag{3}$$

Equation (1) together with Eq. (3) will give the expressions for the probability current S in the case of both normal diffusion [$\mu=1$ in Eq. (1)] and anomalous diffusion [$\mu \neq 1$ in Eq. (1)].

A. $\mu=1$ case

For the normal diffusion case, using Eq. (1) with Eq. (3), we can easily obtain the analytic expression for the current as well as for the escape rate according to Ref. 16. But here we would apply an alternative method to calculate them in order to research conveniently the case of $\mu \neq 1$ later.

Putting Eq. (3) into Eq. (1), we have

$$-\frac{\partial}{\partial x}S(x,t) = \frac{\partial}{\partial x}[f'(x)W(x,t)] + D\frac{\partial^2}{\partial x^2}W(x,t), \tag{4}$$

namely,

$$S(x,t) = -f'(x)W(x,t) - D\frac{\partial}{\partial x}W(x,t). \tag{5}$$

Let us assume

$$W_m(x,t) = F(x)W(x,t), \quad S_m(x,t) = F(x)S(x,t), \tag{6}$$

where $F(x)$ is a factor function. Neglecting the mathematical proof, we assume that there certainly exists the proper $W_m(x,t)$ and $S_m(x,t)$ satisfying diffusion law,

$$S_m(x,t) = -D\frac{\partial}{\partial x}W_m(x,t), \tag{7}$$

if $W(x,t)$ can be solved from Eq. (4). Thus, expanding Eq. (7) with Eq. (6), we have

$$S(x,t) = -DW(x,t)\frac{\partial}{\partial x}[\ln F(x)] - D\frac{\partial}{\partial x}W(x,t). \tag{8}$$

Comparing Eq. (8) with Eq. (5), we get

$$F(x) = \exp\left(\frac{f(x)}{D}\right), \tag{9}$$

and then Eq. (7) becomes

$$S(x,t) = -D\exp\left(-\frac{f(x)}{D}\right)\frac{\partial}{\partial x}\left[\exp\left(\frac{f(x)}{D}\right)W(x,t)\right]. \tag{10}$$

This is the exact expression for the current S. Then, according to the same treatment as Ref. 16 and the definition of Kramers' escape rate,

$$r_k = \frac{S}{\int_{x_1}^{x_2}W(x,t)dx'} \tag{11}$$

as well as the approximative conditions that D is sufficiently small and $f(x)$ presents the sharp peaks at x_s and x_b, we obtain the well-known Kramers' escape rate

$$r_k = \frac{\sqrt{f''(x_s)|f''(x_b)|}}{2\pi}\exp\left(-\frac{f(x_b)-f(x_s)}{D}\right). \tag{12}$$

B. $\mu \neq 1$ case

In this case, the problem may be a little complicated but can be still solved in the spirit of the above approach. When $\mu \neq 1$, Eq. (4) becomes

$$-\frac{\partial}{\partial x}S(x,t) = \frac{\partial}{\partial x}[f'(x)W(x,t)] + D\frac{\partial^2}{\partial x^2}W^{\mu}(x,t). \tag{13}$$

Integrating over x, we have

$$S(x,t) = -f'(x)W(x,t) - D\frac{\partial}{\partial x}W^{\mu}(x,t). \tag{14}$$

Now $W_m(x,t)$ and $S_m(x,t)$ are assumed as follows:

$$W_m(x,t) = F(x,t)W^{\mu}(x,t), \quad S_m(x,t) = F(x,t)S(x,t), \tag{15}$$

respectively. Thus Eq. (7) becomes

$$S(x,t) = -DW^{\mu}(x,t)\frac{\partial}{\partial x}[\ln F(x,t)] - D\frac{\partial}{\partial x}W^{\mu}(x,t). \tag{16}$$

Comparing Eq. (16) with Eq. (14), we have

$$F(x,t) = \exp\left[\frac{\phi_\mu(x,t)}{D}\right], \tag{17}$$

where

$$\phi_\mu(x,t) = \int f'(x)W^{1-\mu}(x,t)dx. \tag{18}$$

We see that ϕ_μ represents an effective W-dependent potential resulting from the nonlinear diffusive media, particularly, the ordinary potential $f(x)$ can be recovered when $\mu \to 1$. For a quasistationary state, we utilize the solution of Eq. (2) and get

$$\phi_\mu(x) = \frac{\mu D}{1-\mu}\ln[1-(\mu-1)\beta_\mu f(x)]. \tag{19}$$

Then Eq. (7) is rewritten as

$$S(x,t) = -D\exp\left[-\frac{\phi_\mu(x)}{D}\right]\frac{\partial}{\partial x}\left[\exp\left(\frac{\phi_\mu(x)}{D}\right)W^{\mu}(x,t)\right]. \tag{20}$$

Applying the same treatment, we obtain the expression for the current,

$$S = \frac{D/Z^{\mu}}{\int_{x_s}^{A}[1-(\mu-1)\beta_\mu f(x)]^{\mu/(1-\mu)}dx}, \tag{21}$$

and thus the escape rate $r_k = S/P$, where $P = \int_{x_1}^{x_2}W_s^{\mu}(x)dx$, can be arrived at, namely,

$$r_k = \frac{D}{\int_{x_1}^{x_2}[1-(\mu-1)\beta_\mu f(x)]^{\mu/(\mu-1)}dx \int_{x_s}^{A}[1-(\mu-1)\beta_\mu f(x)]^{\mu/(1-\mu)}dx}. \tag{22}$$

It is evident that we can find an approximate expression for the current S and the escape rate r_k when D is sufficiently small and the potential $f(x)$ has sharp peaks at x_s and x_b. Then we extend the integration boundaries in integrals in Eqs. (21) and (22) to the whole space and thus obtain

$$S \simeq \frac{D\sqrt{\mu\beta_\mu|f''(x_b)|}}{\sqrt{\pi}Z^{\mu}[1-(\mu-1)\beta_\mu f(x_b)]^{(1+\mu)/2(1-\mu)}}, \tag{23}$$

$$r_k \simeq \frac{Z^{\mu-1}\sqrt{f''(x_s)|f''(x_b)|}}{\pi[1-(\mu-1)\beta_\mu f(x_b)]^{(1+\mu)/2(1-\mu)}[1-(\mu-1)\beta_\mu f(x_s)]^{(3\mu-1)/2(\mu-1)}}. \tag{24}$$

The expression (24) is a generalized Kramers escape rate formula, which can be recovered to the normal Kramers rate expression in the limit $\mu \to 1$. It is clearly seen that Eq. (22) is the reciprocal of escape time obtained by Ref. 17 where the escape problem is treated directly by considering a linear approximation of Eq. (1) and employing the corresponding backward FP, which conforms soundly to our expectation.

In fact, for a more generalized nonlinear FPE,

$$\frac{\partial}{\partial t}W^{\nu}(x,t) = \frac{\partial}{\partial x}[f'(x)W^{\nu}(x,t)] + D\frac{\partial^2}{\partial x^2}W^{\mu}(x,t), \tag{25}$$

we can also obtain the analytic expressions for the current and the escape rate by renaming $\widetilde{W}(x,t)=W^{\nu}(x,t)$ and $\widetilde{\mu}=\mu/\nu$. They are written as follows, respectively,

$$S \simeq \frac{D\sqrt{(\mu/\nu)\beta_{\mu\nu}|f''(x_b)|}}{\sqrt{\pi}Z^{\mu/\nu}[1-[(\mu-\nu)/\nu]\beta_{\mu\nu}f(x_b)]^{(\mu+\nu)/2(\nu-\mu)}}, \tag{26}$$

$$r_k \simeq \frac{Z^{(\mu-\nu)/\nu}\sqrt{f''(x_s)|f''(x_b)|}}{\pi[1-[(\mu-\nu)/\nu]\beta_{\mu\nu}f(x_b)]^{(\mu+\nu)/2(\nu-\mu)}[1-[(\mu-\nu)/\nu]\beta_{\mu\nu}f(x_s)]^{(3\mu-\nu)/2(\mu-\nu)}}, \tag{27}$$

where $\beta_{\mu\nu}=\nu Z^{(\mu-\nu)/\nu}/(\mu D)$.

The escape rate r_k given by Eq. (24) is plotted in Fig. 2. For any μ and small D, the escape rate increases in a form of power law as the diffusion coefficient D grows, while it drops with μ at a fixed D. In the range $\mu>1$, we see that there lies a finite D_c only above which particles can escape over the barrier, otherwise the particles will be confined in the well. The value of D_c can be obtained from $\beta_{\mu c}=[(\mu-1)f(x_b)]^{-1}$. This is because a cut off of the stationary solution Eq. (2) restricts the attainable space. But the escape particles do not have such a confinement for the case of $\mu<1$.

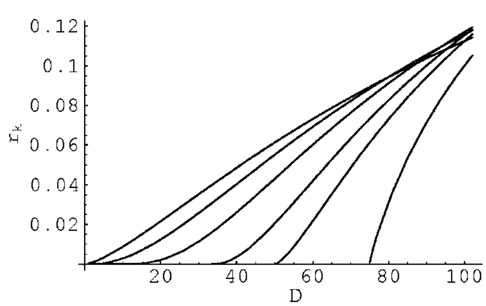

FIG. 2. The escape rate r_k obtained from Eq. (24) as a function of D for various values of $\mu>0$. Here $Z=1$, $f''(x_s)=|f''(x_b)|=1$, $f(x_s)=0$, and $f(x_b)=100$. From left to right $\mu=0.5$, 0.7, 1, 1.5, 2, and 4. All quantities are dimensionless.

III. RESULTS AND NUMERICAL SIMULATIONS

In order to verify our analytic predictions, we numerically calculate the escape rate of the system specified in the present paper. The parameters used in the metastable potential shown in Fig. 1 are $f(x_s)=0.0$, $f''(x_s)=|f''(x_b)|=1.0$, and $\Delta f=f(x_b)-f(x_s)=100.0$. The multiplicative Ito-Langevin equation corresponding to Eq. (1) reads[8,18]

$$\dot{x} = -f'(x) + \sqrt{2D}[W(x,t)]^{(\mu-1)/2}\eta(t), \tag{28}$$

where $\eta(t)$ is a δ-correlated Gaussian noise with zero mean and variance 1. For the case of $\mu=1$, the normal Langevin equation is recovered. We apply the stochastic Runge-Kutta algorithm[19] to numerically solve Eq. (28) for the multiplicative factor function $W(x,t)=W_s(x)$ with 10^5 test particles. If a Langevin trajectory starting from $x(t=0)=x_s$ finally crosses the saddle point x_b, an escape event occurs and subsequently the time-dependent escape rate is determined as[20]

$$r_k(t) = -\frac{\Delta N(t)}{N(t)\Delta t}, \tag{29}$$

where $N(t)$ denotes the number of test particles that have not undergone escape at time t; $\Delta N(t)$ is the number of test particles that have escaped within the time interval $t \to t+\Delta t$ and it is recorded through the number of test particles across the

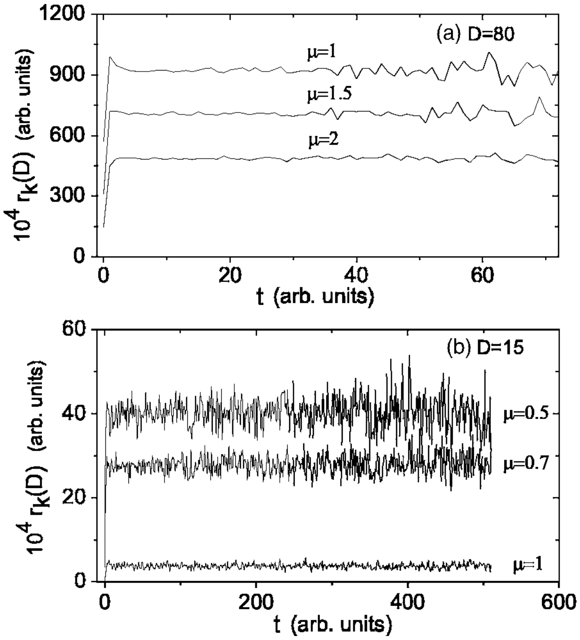

FIG. 3. The escape rate $r_k(t)$ vs time t for different values of μ at fixed D $=80.0$ (a) and 15.0 (b). Here $f''(x_s)=|f''(x_b)|=1.0$, $f(x_s)=0$, and $f(x_b)$ $=100.0$.

saddle point x_b for the last time. The results of simulation for different values of μ are shown in Figs. 3 and 4, where the escape rate is described as a function of time t and diffusion coefficient D, respectively.

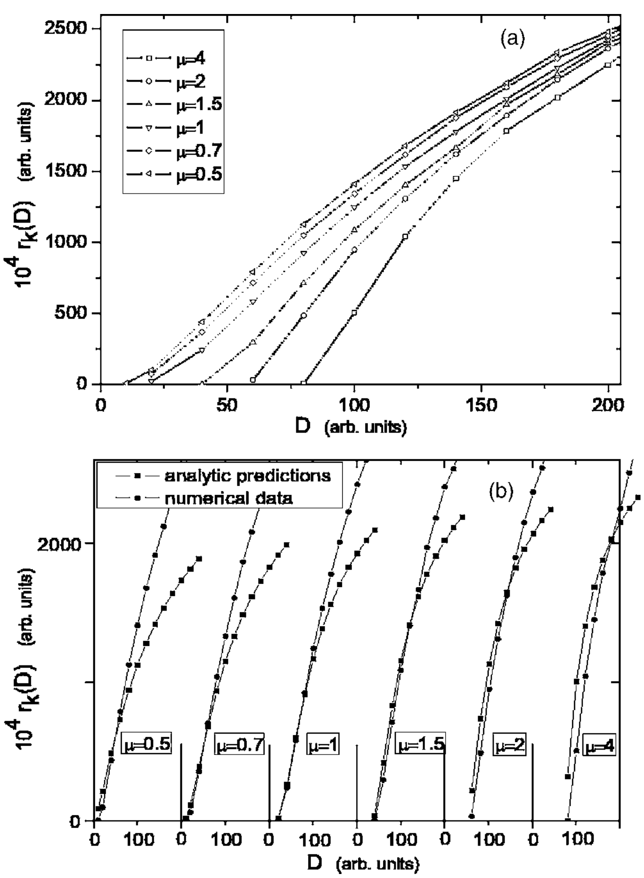

FIG. 4. The escape rate r_k numerically calculated by Eq. (29) as a function of D (a) and its comparison with the analytic prediction given by Eq. (24) (b) for different values of μ. All parameters are the same as those in Fig. 3.

We encounter long-time endless loops for the case of $\mu>1$ when D is below the critical diffusion constant D_c, as expected, and D_c is an increasing function of μ. Basically, the escape is permitted for any value of $D>0$ when $0<\mu<1$. It is clearly seen from Fig. 3 that the escape rate decreases with μ. Physically, the index μ reflects the influence of the fractal environment on the evolving particle. A fractal environment can provide the particle in that with a memory for its original state, which leads to the subdiffusive ($\mu>1$) or superdiffusive ($\mu<1$) effect. For the subdiffusive case the particle is located with a big probability in the ground state; conversely, for the superdiffusive case the particle experiences very large fluctuations so that it can escape more easily.

In Fig. 4(a), we can see that the escape rate grows with D following the power law. In fact, if $0<\mu<1$, $r_k \sim \beta_\mu^{(\mu+1)/2(\mu-1)} \sim D^{1/(1-\mu)}$ for vanishing D [whether $f(x_s)=0$ or not] and the deterministic limit is achieved. For any μ, the distinction of the escape rates due to different values of μ becomes unapparent as D increases. Theoretically, Eq. (24) indicates saturation of r_k for large D, but, in fact, when D is large enough, the stable escape state of particles collapses and curves with large fluctuations cannot be avoided. In addition, it is noteworthy that for the subdiffusive case the rate curve has a plateau before the stable escape fully disappears while the curve for the superdiffusion does not. In the limit $\mu \to 1$, the exponential growth of r_k with D is always recovered. For comparison, the approximation given by Eq. (24) is also exhibited in Fig. 4(b). The approximation is good for small D, particularly, it works better for values of μ around 1.

IV. SUMMARY

Under quasistationary conditions, we have given an analytic expression for the escape rate of particles that exhibit anomalous diffusion due to a stochastic nonlinear dependency on the density, and the theoretical predictions are in excellent agreement with numerical simulations. The escape behavior of particles in nonlinear diffusive media differs from that of the normal Brownian case. The result describes a generalized Kramers' escape process involved in the nonlinear index μ. For any μ and small D, the escape rate grows with D and drops as μ becomes large at a fixed D, but the escape starts only above a critical value of D in the subdiffusive media ($\mu>1$) while particles in the superdiffusive media ($\mu<1$) do not have this confinement. In other words, the subdiffusive media lead to a slower escape while the superdiffusive media reverse.

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