Cancellation phenomenon of barrier escape driven by a non-Gaussian noise

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The Lévy noise, with a long-tail distribution induced particle escape from a metastable potential, is shown to display a feature called a cancellation phenomenon, as compared to the Brownian motion case. As a consequence, the escape rate is found to be a nonmonotonous function of the Lévy index μ and the Arrhenius law is not obeyed. We have also derived a rate expression using the reactive flux method, which supports our numerical findings, namely, with the decrease of μ, a large positive flow is allowed to establish at the barrier, however, the probability passing over the saddle point decreases. This implies that the particles outside the barrier come back to the inside and cancel with themselves.

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The process of noise-driven escape of particles over a potential barrier, i.e., the well-known Kramers problem, is ubiquitous in natural science [1,2]. The inverse of the steady escape rate, varying on a logarithmic scale, is a linear function of the inverse noise intensity at weak noise. This is called the Arrhenius law [3]. The key point in the barrier escape dynamics was assumed by Caldeira and Leggett [4] that *the phase relationship between the amplitudes for being on different sides of the barrier(s) can be neglected, since once outside the barrier the system never comes back and interferes with itself*. This procedure relies on the single-event probability of the reaction coordinate. However, this raises the question if the noise is a non-Gaussian one, whether the rate constant will still follow the Arrhenius law and increase when diffusion becomes fast. The barrier passage process driven by a structured noise needs to be studied in detail, which may play a dominant role in many processes, for instance, collision of molecular systems, atomic clusters, biomolecules, fusion of massive nuclei, stability of a metastable state, etc.

In the ordinary Brownian motion, the statistics of a random walk is given by a Gaussian distribution. There are, however, many processes in nature which are characterized by anomalous diffusion due to various statistical properties of the environments. Lévy flights of a force-free particle constitute a generalization of ordinary Brownian motion with a mean square displacement $\langle x^2(t)\rangle \propto t^{2/\mu}$ [5–7] where μ is the Lévy index taking the values $0<\mu<2$. In fact, the second moment of a Lévy flight diverges. This is an effective scaling only, which has been used to model a variety of processes [6] such as bulk-mediated surface diffusion and application in porous glasses and eye lenses, transport in micelle system, single molecule spectroscopy, and even the flight of an albatross. The dynamics driven by a Lévy noise differs from the regular Brownian motion by the occurrence of extremely long jumps. Recently, Chechkin *et al.* [8] found that Lévy noise induced a crossover from unimodal to bimodal behavior at stationarity in a nonlinear oscillator. Romero *et al.* studied the first passage time statistics for a system driven by a long-range correlation Gaussian noise [9]. Ditlevsen [10] considered a particle subjected to Lévy noise jumping between asymmetrical double-stable wells, the result shows that the waiting time scale is a power function of μ and the height of the barrier has no influence on the transition probability. To our knowledge, application of long-tailed Lévy statistics to barrier escape has not been discussed yet.

In this paper, we report a cancellation phenomenon of the barrier via Langevin simulations of a particle subjected to a Lévy noise in a metastable potential. Physical understanding of the process is provided, which differs from normal Brownian motion [2] in that the low-friction regime (i.e., the energy-diffusion limited regime), the reaction rate is very low and even more so as it approaches to zero [11]. An expression of the rate constant is obtained using the reactive flux method. Here, the metastable case is also different from the bistable case because the two reflecting boundaries will influence the barrier passage with a long jump induced by Lévy noise in the latter case. The theoretical predication supports our numerical findings.

The equation of the motion of an overdamped particle reads

$$\dot{x}(t) = -U'(x) + L(t), \tag{1}$$

where the zero-mean noise $L(t)$ obeys Lévy statistics. In the Fourier space one defines the characteristic function $p(k)$ of the noise variable $L(t)$ [5,7],

$$p(k) = \int dL \exp(-ikL)p(L) = \exp(-D|k|^{\mu}), \tag{2}$$

where D is the intensity of Lévy noise and $p(L)$ is a Gaussian distribution when $\mu=2$.

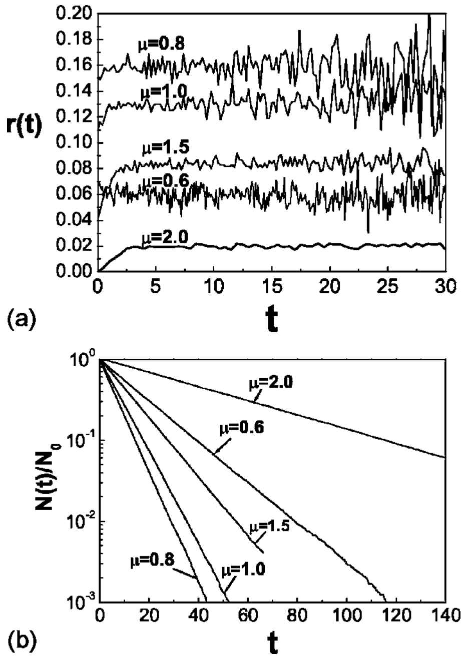

FIG. 1. Time-dependent escape rate (a) and decay probability (b) for various μ at a fixed noise intensity $D=0.5$.

We use the stochastic Runge-Kutta algorithm [12] to simulate Eq. (1) discretized in time [13]. Time-dependent escape rate is determined numerically by [14,15]

$$r(t) = -\frac{1}{N(t)}\frac{\Delta N(t)}{\Delta t}, \tag{3}$$

where $N(t)$ denotes the number of test particles that have not undergone escape at time t, and $\Delta N(t)$ is the number of test particles that have undergone escape from the barrier within a time interval $t \rightarrow t+\Delta t$ where Δt is chosen to be much larger than the interval between two successive escapes [16]. When the escape rate is introduced, the test particles are accounted in the term $N(t)$ the whole time due to the recrossing conclusions are presented.

The metastable potential is chosen in such a typical form

$$U(x) = \frac{1}{2}m\omega_0^2 x^2\left(1 - \frac{x}{x_b}\right), \tag{4}$$

we chose $x_b=1.5\sqrt{6}$ and $m\omega_0^2=1.0$ in order to make the height of potential barrier $V_b=1.0$. In the calculations, we rescale the coordinate and energy, their units are $\sqrt{D/(m\omega_0^2)}$ and D, respectively, the integration time step is $h=0.001$ for Eq. (1), $\Delta t=0.1$ in Eq. (3), and initial distribution of the system is a δ function at the well bottom with $N_0=10^5$ test particles.

Figures 1(a) and 1(b) show time-dependent escape rate and decay probability of the particle for various μ, respectively. It is seen that the transient time decreases with the decrease of μ. This is due to a fact that diffusion of the particle becomes faster when the Lévy index decreases. The larger the slope of the decay probability, the larger the escape rate is. After a transient time, the ratio of the recrossing flux at the barrier to the amount of particles remaining in the well approaches a constant. Since a statistical number of test particles within the well decreases with time, fluctuation of the rate around the average value increases. The formation of a steady escape rate is accompanied by an operation of time-dependent normalization in Eq. (3).

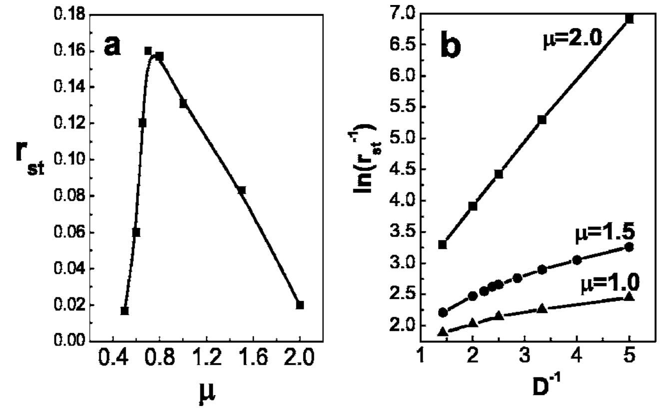

FIG. 2. (a) The stationary escape rate as a function of the Lévy index μ at a fixed noise intensity $D=0.5$. (b) The Arrhenius plotting of the rate for various μ.

In Figs. 2(a) and 2(b), we plot the stationary escape rate as functions of μ and D. As expected, the stationary escape rate increases when the noise intensity increases. The escape rate is an increasing monotonous function of D because the particle becomes active with increasing D. Indeed, we find a prominent result. The stationary escape rate is a nonmonotonous function of μ when the centered distribution of the system has moved outside the barrier and the increase of distribution width with time is faster than the movement of its peak position. Thus, a tail of the distribution behind the barrier enters in the well again, leading to a negative flux over the barrier. At the same time, the particles inside the barrier will cross over the saddle point and produce a positive flux. Therefore, the total probability flux decreases and we may call this phenomenon a cancellation one. Due to this cancellation phenomenon in the barrier region, the dependence of the stationary escape rate on the noise intensity deviates from the Arrhenius law.

We use the method of reactive flux [17,18] to derive an expression of the rate constant in a generic damped case, where trajectories of the particles are started at the top of the barrier. The rate constant is defined by

$$k(t) = \frac{\langle v_0 \delta(x_0)\, \theta_P[x(x_0,v_0,t)]\rangle}{\langle \theta_R(x_0)\rangle}, \tag{5}$$

where $\theta_R[x(x_0,v_0,t)]$ is equal to 1 for $x<0$ and 0 otherwise, and θ_P is just $1-\theta_R$. Considering the normalized phase-space distribution that corresponds to an ensemble of particles starting at (x_0,v_0) at $t=0$, and undergoing a Lévy walk, we have the steady rate constant,

$$k = \frac{1}{\langle \theta_R(x_0) \rangle} \int_{-\infty}^{\infty} dx_0 \int_{-\infty}^{\infty} dv_0 W(x_0, v_0) v_0 \delta(x_0) \cdot \chi(v_0, t \to \infty)$$
$$= \frac{1}{Q} \int_{-\infty}^{\infty} v_0 W(0, v_0) \chi(v_0, t \to \infty) dv_0, \qquad (6)$$

where Q is the partition function for reactions and the distribution $W(0,v_0)$ for the initial velocity of particles at the barrier is an even function of v_0. Here, $\chi(v_0,t)$ is called the characteristic function or the passing probability over the saddle point, given mathematically by $\chi(v_0,t)=\int_0^{\infty} W(x';t)dx'$ [18,19]. It is a number that is equal to one for reactive trajectories and zero for nonreactive trajectories. Equation (6) agrees with the well-known Kramers rate formula if $\mu=2$.

For a parabolic barrier, we adopt the analytical solution of Jespersen *et al.* for the well distribution function [7], simply by substituting ω, the frequency of the oscillator, by $i\omega$. The adopted solution reads

$$W(x;t) = W_0(x - \langle x(t) \rangle; t_{eff}), \qquad (7)$$

where W_0 is the probability density function of free Lévy flights [7] in terms of Fox's H functions,

$$W_0(x,t) = \frac{\pi}{\mu |x|} H_{2,2}^{1,1}\left[\frac{|x|}{(Dt)^{1/\mu}} \middle| \begin{matrix} (1,1/\mu),(1,1/2) \\ (1,1),(1,1/2) \end{matrix} \right]. \qquad (8)$$

Because the statistical average of Lévy noise is equal to zero, the expression of mean position of the particle is the same as that of the normal Brownian case and is written as $\langle x(t) \rangle = x_0[1+\omega_b^2 \int_0^t \Phi(t')dt'] + v_0 \Phi(t)$ [19]. Here an effective time in the inverse harmonic potential is introduced as $t_{eff}=\int_0^t [\Phi(t-t')]^{\mu} dt'$, where $\Phi(t)$ is the response function of a normal particle in the inverse harmonic potential and is given by $\Phi(t)=(a_1-a_2)^{-1}[e^{a_1 t}-e^{a_2 t}]$, where a_1 and a_2 are the two roots of the equation $a^2+\gamma a-\omega_b^2=0$ (γ is the damping coefficient) [19]. It is noticed that the inertia effect has been included in the effective time. Thus, the distribution function in an inverse harmonic potential can be obtained from that in the case of free Lévy flight at an earlier, "effective" time t_{eff} [7].

In Fig. 3, we plot time-dependent characteristic function $\chi(v_0,t)$,

$$\chi(v_0,t) = \frac{1}{2} + \int_0^{\langle x(t) \rangle} W_0(x'; t_{eff}) dx', \qquad (9)$$

for various μ. When v_0 is positive, the passing probability can arrive at 1. It is seen that the stationary value of the passing probability decreases with the decrease of μ, because the width of distribution increases with decreasing μ, namely, strong diffusion is harmful for directional motion. When v_0 is negative, the peak of distribution moves along the left direction, the passing probability is always less than $\frac{1}{2}$. However, the width of distribution increases with the decrease of μ, thus strong diffusion helps the particle crossing over the barrier along the right direction.

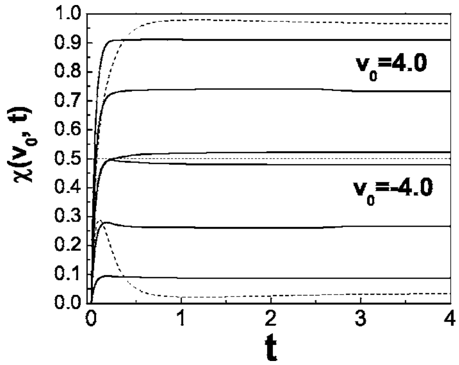

FIG. 3. Plot of time-dependent fractional reactivity index, $\chi(u_0,t)$ for two initial velocities. The solid and dashed lines are the results of Lévy noise and normal Brownian motion, respectively. $\mu=2.0$, 1.5, 1.0, 0.5 from top to bottom for $v_0=4.0$ and opposite for $v_0=-4.0$. The parameters used are $m\omega_b^2=1.0$, $D=1.0$, and $\gamma=2.0$.

Figure 4 shows the rate constant calculated by Eq. (6) as a function of μ. Here the metastable potential is chosen to be a harmonic potential with the frequency ω_0 linking with an inverse harmonic potential with the frequency ω_b. In the spurt of reactive flux rate calculation, the initial conditions are assumed at the top of the barrier [20], which correspond to the ensemble of trajectories which start with identical initial conditions but experience different stochastic histories [18]. We can analyze nonmonotonous behavior of the rate constant as a function of μ. For a large μ, the characteristic function is also large, however, the distribution of initial velocity of the particle is narrow, and thus the contribution of a large positive velocity to the saddle flux is small. On the other hand, for a small μ, the characteristic function is also small, however, $W(v_0)$ is wide and the contribution of a large positive velocity to the saddle flux cannot be neglected. Therefore there exists an optimal value of μ and the peaked position of rate curve drifts to small μ when the damping increases.

In summary, we have addressed a subject of Kramers rate theory for process driven by scale-free Lévy noise. We find a cancellation phenomenon of the barrier escape from both analytical and numerical calculations. Namely, the rate constant is shown to be a nonmonotonous function of the Lévy index, and the Arrhenius law for the rate behavior is not

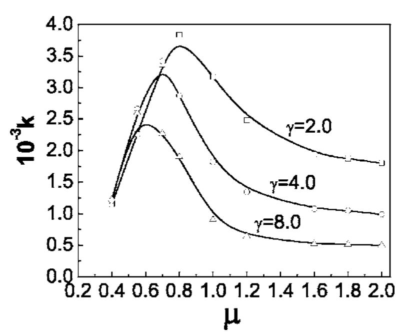

FIG. 4. The rate constant as a function of μ for various friction strengths. The parameters used are $\omega_0^2=\omega_b^2=1.0$, $D=1.0$, and the barrier height $V_b=4.0$.

obeyed at weak noise. This is due to the fact that the particles outside the barrier come back and interfere with themselves inside the barrier, so that faster diffusion does not conduce to larger barrier escape. The present phenomenon differs with the recrossing mechanism of the barrier for the regular Brownian case, the latter assures a quasi-stationary flow established at the saddle point. Of interest to us is the possibility of whether there exist other non-Gaussian cases such as an external noise source.

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[20] The exact stationary solution is

$$W_{st}(x) = \frac{\pi}{|x|} H_{2,2}^{1,1}\left[\frac{|x|^{\mu}\mu\gamma m\omega_0^2}{D} \Bigg|_{(1,\mu),(1,\mu/2)}^{(1,1),(1,\mu/2)} \right],$$

leading to the asymptotic power-law behavior $W_{st} \sim D/(\gamma\mu m\omega_0^2 |x|^{1+\mu})$. The velocity distribution at the saddle point is also taken to be this form and by substituting x by v_0 and ω_0 by 1.