

GENERALIZED KRAMERS' PROBLEM FOR LÉVY PARTICLE

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We consider a generalization of the classical stochastic problem, namely, how to evaluate the mean escape time and escape probability law of a macroscopic particle, being under the influence of the surrounding medium, from a potential well (Kramers problem). The calculations are executed using the method of numerical integration of an overdamped Langevin equation, in which the random force obeys Lévy stable probability law. The detailed description of the method is given, paying much attention to the correct Langevin equation time-quantization and to creating noise generator for the simulations. The mean escape times and escape probability density functions for the case of a truncated harmonic potential and for the whole admitted region of Lévy indices α are evaluated.

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1. INTRODUCTION

Brownian motion of a macroscopic particle has become a classical problem of physics. It has found numerous applications in physics, astronomy, chemistry, biology etc., see [1-3], therefore being a worth object for theoretical challenges. One of the problems raised by Brownian motion is the Kramers problem that is evaluation of the mean escape time of a particle from the potential well due to thermal impact of the surrounding medium [2]. There are several approaches for obtaining the mean escape time. For an overdamped case the first one is solving the Langevin equation with Gaussian white noise in the right-hand side:

$$\frac{dx}{dt} = -\frac{1}{m\gamma} \frac{dU(x)}{dx} + \xi(t), \quad (1)$$

where $x(t)$ is the particle's coordinate, m its mass, γ a viscosity constant, $U(x)$ is the potential, $\xi(t)$ is the Gaussian white noise,

$$\langle \xi(t)\xi(\tau) \rangle = D\delta(t-\tau). \quad (2)$$

D is the noise intensity, $D = 2k_B T / m\gamma$, k_B is Boltzmann constant, T is the surrounding medium temperature.

Another approach, which allows not only a numerical solution, as the one above, is based on integrating the Fokker-Planck equation.

Most well-known solving procedures are based on the idea the potential barrier is high enough in comparison to the thermal fluctuations. They give the result in dimensionless variables (see, e.g. [2]):

$$T_{esc} = \frac{2\pi \exp(|U(x_{max}) - U(x_{min})|/D)}{\sqrt{U''(x_{min})|U''(x_{max})|}}, \quad (3)$$

where x_{max} and x_{min} are the points where the potential has its maximum and minimum, respectively.

An approach that does not assume the barrier to be high was proposed by A.N. Malakhov [4]. It is based on

the solution of the Fokker-Planck equation using Laplace transformation and defining the timescales for the PDF. It gives

$$T_{esc} = \frac{1}{D} \int_{x_0}^{l_2} e^{U(v)/\gamma D} dv \int_{l_1}^v e^{-U(u)/\gamma D} du + \frac{1}{D} \int_{l_2}^{\infty} e^{U(v)/\gamma D} dv \int_{l_1}^{l_2} e^{-U(u)/\gamma D} du. \quad (4)$$

Here $[l_1, l_2]$ is the escape interval, that is the particle needs T_{esc} time to escape from it.

However, a number of experimental observations discovered a violation of this law. Is it was revealed, that is due to the non-Gaussian nature of the external random force $\xi(t)$. The probability distribution function (PDF) of that noise belongs to the class of so-called α -stable, or Lévy, distributions. The peculiarity of these PDFs are the power-law asymptotics $f(x) \propto 1/|x|^{1+\alpha}$, where α is the Lévy index. This means, that the Lévy noise has strong "outliers" alongside with small Gaussian-like noise. Even though due to this fact, the mean squared displacement for Lévy motion diverges, such a motion can be found in non-physical space (e.g. energy diffusion), where no finite variance is required.

A generalization of the Kramers problem for the case of external random force with Lévy PDF was primarily studied in [5] for the particle in the quartic double-well potential. Here we suggest the problem of a particle in the truncated harmonic potential.

2. MAIN EQUATION

We start from the Langevin equation

$$\frac{dx}{dt} = -\frac{1}{m\gamma} \frac{dU(x)}{dx} + \xi_{\alpha,D}(t), \quad (5)$$

where α in $\xi_{\alpha,D}(t)$ denotes the Lévy index. If we integrate Eq. (5) by time within the limits $[t; t + \delta t]$, we get:

$$x(t+\delta t) - x(t) = -\frac{1}{m\gamma} \int_t^{t+\delta t} \frac{dU(x)}{dx} dt + \int_t^{t+\delta t} \xi_{\alpha,D}(t) dt. \quad (6)$$

If we assume $U(x)$ is a slowly changing function in time:

$$x(t+\delta t) - x(t) = -\frac{1}{m\gamma} \frac{dU(x)}{dx} \delta t + \int_t^{t+\delta t} \xi_{\alpha,D}(t) dt. \quad (7)$$

The value $\int_t^{t+\delta t} \xi_{\alpha,D}(t) dt \equiv L_{\alpha,D}$ is a Lévy process with characteristic function

$$\hat{f}_{\alpha,D}(k, \delta t) = \int_{-\infty}^{\infty} \exp(ikL_{\alpha,D}) f(L_{\alpha,D}, \delta t) dL_{\alpha,D} \equiv \langle \exp(ikL_{\alpha,D}) \rangle = \exp(-D|k|^\alpha \delta t). \quad (8)$$

Let us introduce a Lévy process with unit noise intensity:

$$\hat{f}_{\alpha,1}(k, \delta t) = \langle \exp(ikL_{\alpha,1}) \rangle = \exp(-|k|^\alpha \delta t), \quad (9)$$

and find the relation between $L_{\alpha,D}$ and $L_{\alpha,1}$. Since $D > 0$ we can write $D|k|^\alpha = |D^{1/\alpha}k|^\alpha$. Then, making the change of variable $D^{1/\alpha}k \rightarrow k$ in Eq. (8) we get

$$\langle \exp(ikD^{-1/\alpha}L_{\alpha,D}) \rangle = \exp(-|k|^\alpha \delta t). \quad (10)$$

Then, comparing Eqs. (9) and (10) we find

$$L_{\alpha,D} = D^{1/\alpha}L_{\alpha,1}. \quad (11)$$

Now our Langevin equation (7) reads as

$$x(t+\delta t) - x(t) = -\frac{1}{m\gamma} \frac{dU(x)}{dx} \delta t + D^{1/\alpha} \int_t^{t+\delta t} \xi_{\alpha,1}(t') dt'. \quad (12)$$

where $\xi_{\alpha,1}(t)$ is Lévy noise with a unit intensity.

Now, let us pass to the dimensionless variables. To do this it is necessary to specify the potential $U(x)$. In the paper we will dwell on the potential

$$U(x) = \begin{cases} a \frac{x^2}{2}, & |x| < b, \quad a, b > 0; \\ 0, & \text{otherwise.} \end{cases} \quad (13)$$

Making the substitutions $x \rightarrow x\tilde{x}$, $t \rightarrow t\tilde{t}$, $D \rightarrow D\tilde{D}$ in Eq. (12) we get:

$$\frac{x^\alpha}{\tilde{D}} = \tilde{t} = \frac{m\gamma}{a};$$

$$x(t+\delta t) - x(t) = -\frac{dU(x)}{dx} \delta t$$

$$+ D^{1/\alpha} \int_t^{t+\delta t} \xi_{\alpha,1}(t') dt'.$$

Next, let us obtain the time-discrete Langevin equation. That is, the noise should depend on the number of time step. We will write such a discrete noise as

$\xi_{\alpha,1}(1)$. Making variable change in Eq. (9) $((\delta t)^{1/\alpha} k \rightarrow k)$ similarly to the variable change performed above with Eq. (8), and taking into account $\int_t^{t+\delta t} \xi_{\alpha,1}(1) dt' \equiv \xi_{\alpha,1}(n)$, we get:

$$x_{n+1} - x_n = -\frac{dU(x)}{dx} \delta t + (D\delta t)^{1/\alpha} \xi_{\alpha,1}(n), \quad (14)$$

or, substituting the potential (13)

$$x_{n+1} - x_n = -x_n \delta t + (D\delta t)^{1/\alpha} \xi_{\alpha,1}(n). \quad (15)$$

The numerical generator producing the set $\{\xi_{\alpha,1}(n)\}$ can be taken from [6]. The authors suggest calculating the value

$$X = \frac{\sin(\alpha\gamma)}{(\cos(\gamma))^{1/\alpha}} \left(\frac{\cos((1-\alpha)\gamma)}{W} \right)^{(1-\alpha)/\alpha}, \quad (16)$$

where γ is a uniformly distributed on the range $(-\frac{\pi}{2}; \frac{\pi}{2})$ random value; W is an independent random value possessing exponential PDF with mean equal unity; α is the Lévy index, $0 < \alpha \leq 2$.

To prove that such a value X will possess a Lévy PDF we will firstly consider the case $0 < \alpha < 1$. When $\gamma > 0$, Eq. (16) can be written as

$$X = \left(\frac{a(\gamma)}{W} \right)^{(1-\alpha)/\alpha}, \quad (17)$$

where

$$a(\gamma) = \left(\frac{\sin \alpha \gamma}{\cos \gamma} \right)^{\alpha/(1-\alpha)} \cos((1-\alpha)\gamma). \quad (18)$$

Then

$$P(0 \leq X \leq x) = P(0 \leq X \leq x, \gamma > 0)$$

$$= P\left(0 \leq \left(\frac{a(\gamma)}{W}\right)^{(1-\alpha)/\alpha} \leq x, \gamma > 0\right)$$

$$= P\left(W \geq x^{-\alpha/(1-\alpha)} a(\gamma), \gamma > 0\right) \equiv$$

$$\equiv \frac{1}{\pi} \int_0^{\frac{\pi}{2}} d\gamma \int_{x^{-\alpha/(1-\alpha)} a(\gamma)}^{\infty} d\xi e^{-\xi}$$

$$= \frac{1}{\pi} \int_0^{\frac{\pi}{2}} d\gamma \exp\left(-x^{-\alpha/(1-\alpha)} a(\gamma)\right).$$

The received expression, according to [7] is an integral representation of the Lévy PDF.

When $1 < \alpha \leq 2$ the proof is analogous to that presented above. In the case $\alpha = 1$ the expression for X transforms into $X = \text{tg}(\gamma)$ that is a random variable

with Cauchy PDF. The case $\gamma < 0$ just gives the negative values of X .

The noise, produced with such generator, is depicted in Fig. 1. It is seen, that the less the Lévy index is, the larger and thicker the “outliers” become. Fig. 2 represents the comparison of the Lévy PDFs with $\alpha = 1, 1.3, 1.6, 1.8$ and 2 . As one can notice, Lévy PDFs possess long power-law tails.

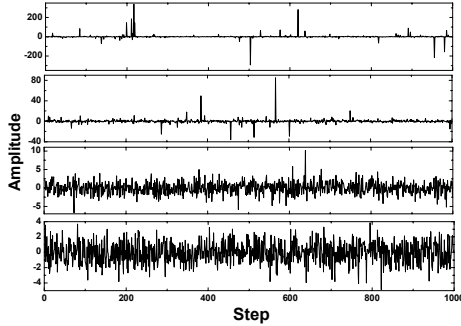


Fig. 1. Lévy noise with different α (downwards $\alpha = 1.0, 1.5, 1.8, 2.0$). The less the Lévy index is, the larger the “outliers” become

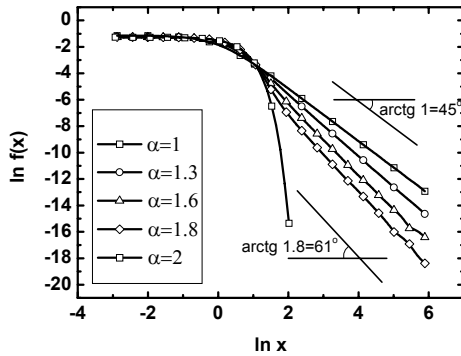


Fig. 2. Comparison of Lévy PDFs with different indices α . For $\alpha < 2$ there are power-law asymptotics

3. NUMERICAL SIMULATION

Now let us describe the numerical simulation of Kramers problem. We start from the time-discretized Langevin equation (15) obtained in the previous section. The simulation algorithm is as follows:

1. We place a “particle” into the potential’s minimum $x = 0$.
2. Fixing alpha we make the iterations of Eq. (15) for D ’s ranging from 10^{-5} to 10^5 , with the time-step $\delta t = 10^{-2}$;
3. The iterations for current D stop when the particle reaches a border of the potential ($x = \pm 1$) and the needed time is denoted;
4. For each D we do the calculations 10000 times, and then average.

The results of these iterations are shown in Fig. 3 in lg-lg scale. As one can see the curves for $\alpha \neq 2$ have power-law asymptotics at small D ’s. At large D ’s the curves in Fig. 3 tend to $\lg T_{esc} = -2$, in fact evaluating $T_{esc} = \delta t$, since the particle here needs only one step to

exit the well. The numerical simulation data for $\alpha = 2$ is fitted using formula (4) (a solid bold line in the Fig. 3). To examine the asymptotic power-law dependence we introduce the following formula:

$$T_{esc} = \frac{C(\alpha)}{D^{\mu(\alpha)}}. \quad (19)$$

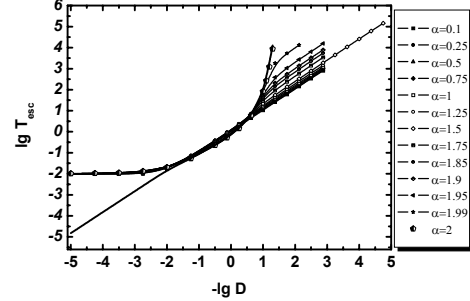


Fig. 3. Simulation results for the truncated harmonic potential (lg-lg scale). In contrast with the Gaussian case ($\alpha = 2$) the curves with $\alpha \neq 2$ possess power-law asymptotics

The values $C(\alpha)$ and $\mu(\alpha)$ can be easily found numerically from the data plotted in Fig. 3. Indeed, fitting the dependencies for small D ’s in lg-lg scale with a straight line by using the least-squared method, we obtain them instantly from the equation for this line:

$$\lg T_{esc} = -\mu(\alpha) \cdot \lg D + \lg C(\alpha).$$

Then, building the curves for the exponent $\mu(\alpha)$ and prefactor $C(\alpha)$ as functions of Lévy index (see Fig. 4), we discover they are monotonic functions. Moreover, the value $\mu(\alpha)$ exhibits a step-like behavior, being almost constant at α ’s not very close to 2 and tending to infinity while $\alpha \rightarrow 2$. The latter is a natural result, since there are no power-law asymptotics for the Gaussian case.

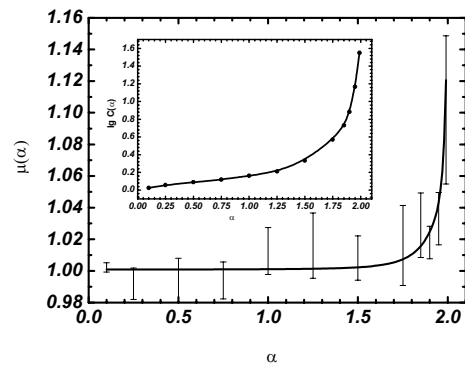


Fig. 4. Exponent $\mu(\alpha)$ and prefactor $C(\alpha)$ for small values of noise intensity D

Next, we are interested in obtaining the escape PDF of the particle as the function of walking time. We fix D at the value $D = 10^{-2}$. The simulation algorithm is almost the same, except the fact that the values of time escape are not averaged, but treated with a routine that builds their PDF. The results of these calculations are shown in Fig. 5. In spite of the different nature of the

noise, the PDFs for the Lévy case, like these for the Gaussian case, show an exponential behavior

$$p(t) = \frac{1}{T_{esc}} \exp(-t/T_{esc}), \quad (20)$$

where $p(t)$ is the escape probability density function.

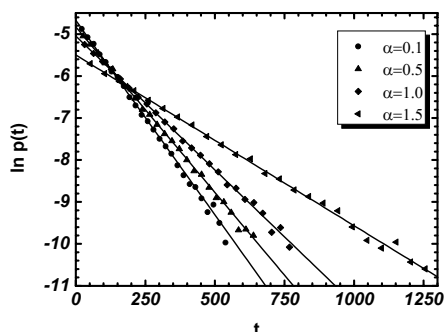


Fig. 5. Escape PDF for Lévy case. As for the Gaussian case ($\alpha = 2$), they exhibit exponential behavior

Thus, using Eq. (20) we can obtain the mean escape times:

$$T_{esc} = \frac{1}{p(0)} \equiv T_1, \quad (21)$$

or

$$T_{esc} = -\left(\frac{d \ln(p(t))}{dt}\right)^{-1} \equiv T_2. \quad (22)$$

Comparison of the escape times obtained using the escape PDFs and via the direct simulation

α	T_{esc}	T_1	T_2
0.1	108.2	107.1	107.9
0.5	127.4	125.4	126.8
1.0	159.1	155.7	156.7
1.5	250.2	244.6	245.9

A table showing the comparison of the escape times obtained using Eqs. (21), (22) and the direct simulation is available below. As one can see, the difference between the corresponding values does not exceed 2.5%.

4. CONCLUSION

The results of this paper show that in contrast with the classical Kramers' problem for Gaussian noise, the mean escape time has power-law asymptotics at small values of D , remaining a monotonic function of the Lévy index. However, the escape PDFs for different α 's still are exponential.

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ОБОБЩЕННАЯ ЗАДАЧА КРАМЕРСА ДЛЯ ЛЕВИ-ЧАСТИЦЫ

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Рассмотрено обобщение одной из типовых стохастических задач – задача о получении среднего времени вылета и функции распределения вылетов макроскопической частицы из потенциальной ямы под действием окружающей ее среды (задача Крамерса). Здесь мы останавливаемся на случае обрезанного гармонического потенциала. Вычисления производятся методом численного интегрирования передемпфированного уравнения Ланжевена, в котором случайная сила обладает законом распределения Леви. Дано детальное описание самого метода, причем особое внимание обращено на правильную дискретизацию уравнения Ланжевена во времени и построение генератора шума для численного моделирования. Получены средние времена вылета и их функции распределения для всей области значений параметра Леви.

УЗАГАЛЬНЕНА ЗАДАЧА КРАМЕРСА ДЛЯ ЧАСТИНКИ ЛЕВІ

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Розглянуто узагальнення однієї із типових стохастичних задач – задача про отримання середнього часу вильоту та функції розподілу вильотів макроскопічної частинки із потенціальної ями під дією її оточуючого середовища (задача Крамерса). Ми зупиняємося на випадку обрізаного гармонічного потенціала. Обчислення виконуються методом чисельного інтегрування передемпфованого рівняння Ланжевена, в якому випадкова сила має закон розподілу Леві. Надано детальний опис самого методу, причому особа увага приділена вірній дискретизації рівняння Ланжевена у часі та побудові генератора шуму для чисельного моделювання. Отримано середні часи вильоту та їх функції розподілу для всієї області значень параметра Леві.