ON LÉVY FLIGHTS IN POTENTIAL WELL

O.YU. SLIUSARENKO

Karazin Kharkiv National University
(31, Kurchatov Ave., Kharkiv 61108, Ukraine; e-mail: alex_slusarenko@mail.ru)

UDC 531.19, 536.7

The motion of an overdamped Lévy particle (a particle being under the influence of an external random force with the Lévy distribution law) in a potential well (a generalized Kramers' problem) is considered. The mean crossing/escape time of the particle and the crossing/escape time probability density as a function of time are obtained. The method of numerical integration of the overdamped Langevin equation is used for two types of potential profiles and for the whole admitted region of Lévy indices of the external force.

1. Introduction

The classical Kramers' problem consists in evaluating the mean particle's escape time from a potential well under the influence of an external random force with the Gaussian distribution law. Primarily, this problem was investigated in [1]; later on, it became a part of nearly each textbook on stochastic processes and came to a regular university course due to various applications:
— the modeling of chemical reactions;
— the electroconductivity theory in crystals;
— the modeling of nucleations, etc.

Even nowadays, this classical Kramers' problem with some new peculiarities finds its place in many research works. Here, we suggest its generalization. We consider an external random force with the α-stable, or Lévy, distribution law, rather than the Gaussian one. The generic Lévy motion, which is a natural generalization of the Brownian motion, can be found, indeed, in a lot of natural phenomena, e.g. in random walks along a polymer chain, in Hamiltonian chaotic systems, and foraging movement; see also examples in [2], [3]. It is characterized by the probability distribution function (PDF) that is dependent on the special parameter, the so-called Lévy index α, $0 < \alpha \leq 2$, of the random force. This parameter may be treated as the difference degree from the Gaussian PDF: when $\alpha < 2$, the PDF exhibits a power-law decay,

$$p(x) \propto \frac{1}{|x|^{1+\alpha}}.$$

The limit case of $\alpha = 2$ corresponds to the Gaussian PDF, which decays exponentially.

Preliminarily, such a generalization was studied in [4] for an overdamped particle embedded in a symmetric double-well potential and for α ranging between 1 and 2. However, in the present work, the simulations are performed with better precision and for the two-well and metastable potential profiles in the whole domain of the Lévy indices.

The Lévy motion is closely connected with a Generalized Central Limit Theorem [5] which proves that Lévy distributions, like the Gaussian distribution, arise when the result of an experiment is determined by the influence of a large number of random factors. Due to this fact, such a generalization of the Kramers' problem appears to be quite actual. Moreover, the reason for this lies in different applications, e.g. in stochastic climate dynamics [6], single-molecule physics [7], engineering [8], etc.

2. Problem Statement

A consistent analytical approach is connected with the solution of the fractional Fokker-Planck equation with a Riesz fractional derivative (a complicated integro-differential equation in partial derivatives), thus raising substantial difficulties. Therefore, our studies are based on the numerical solution of the overdamped Langevin equation

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

where $x(t)$ is a particle's coordinate, m its mass, γ a viscosity constant, $U(x)$ an external potential, $\xi_\alpha(t)$ an α-stable noise possessing the symmetric Lévy stable probability distribution with a scale parameter equal to unity, and D the Lévy noise intensity. We consider two generic types of the potentials,

$$\text{I} \quad U_1(x) = -a\frac{x^2}{2} + b\frac{x^4}{4}, \quad a, b > 0; \tag{2}$$

$$\text{II} \quad U_2(x) = -a\frac{x^3}{3} + bx, \quad a, b > 0. \tag{3}$$

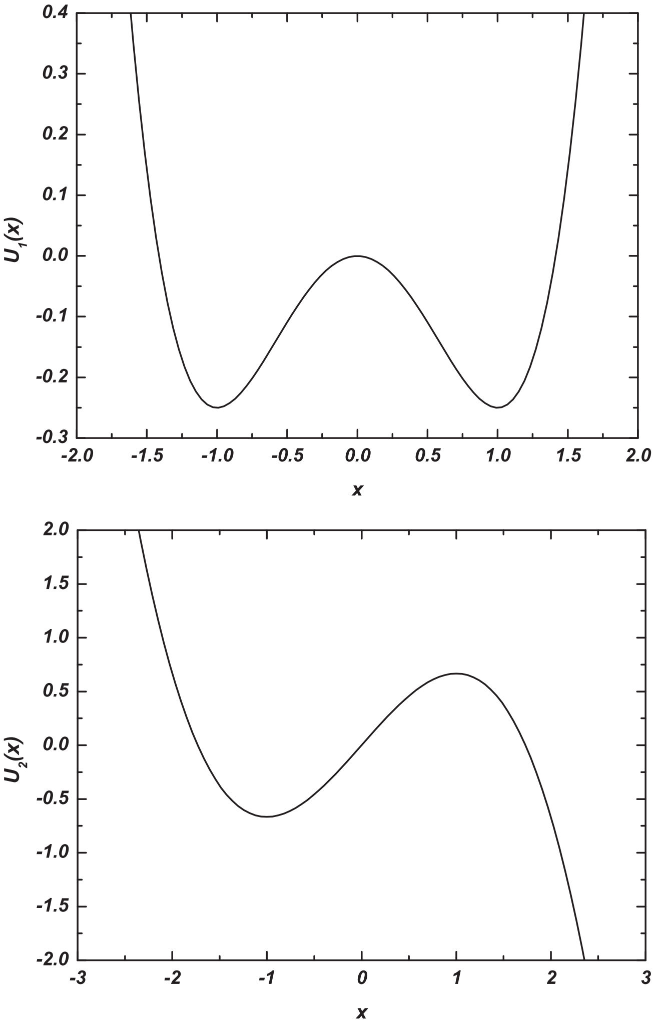


Fig. 1. Shapes of the considered potentials of type I (above) and type II (below)

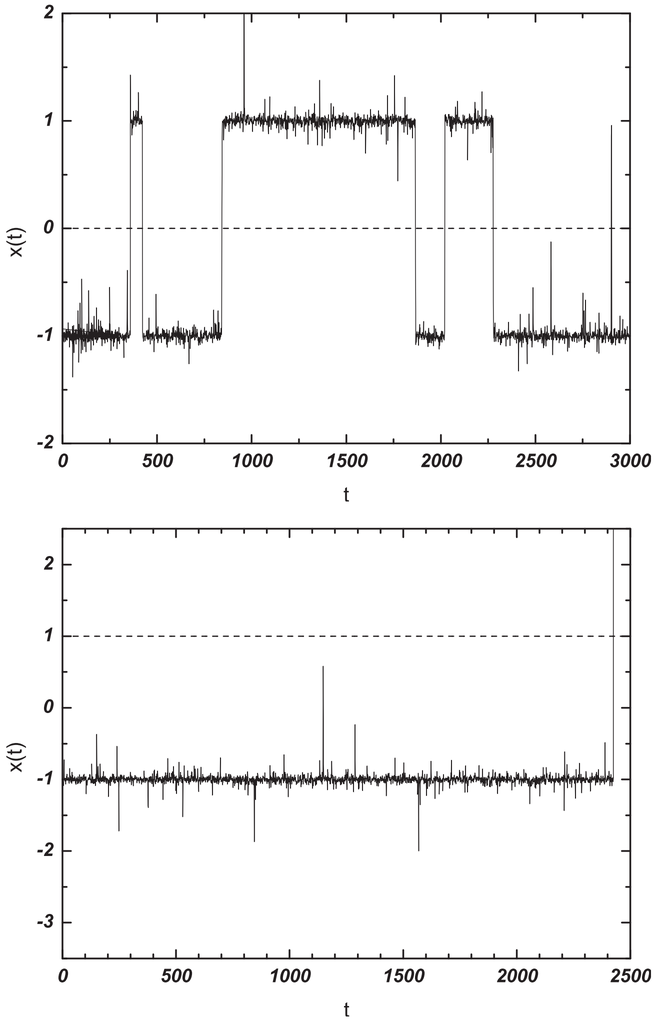


Fig. 2. Lévy motion in the potential profiles of type I (above) and type II (below). The Lévy index $\alpha = 1.5$

The sketches of these potentials are shown in Fig. 1, where $a = b = 1$.

The typical trajectories of a particle immersed in the potentials are presented in Fig. 2. In the figure above, the transition of a particle from one well to another one in a potential of the first type is observed; the figure below demonstrates the particle's single crossing of the metastable potential maximum. For $U_1(x)$, we will be interested in investigating the first *crossing* time problem. That is, we will evaluate the time needed for a particle to cross the potential barrier, not taking into account its possible subsequent retrieval. On the contrast, for the second potential type, we will have the first *escape* time problem, since, after jumping out of the potential well, the particle has a relatively small probability to return back.

Now let us turn to the dimensionless variables in the Langevin equation. To do this, we make the substitutions $x \to xx_0$, $t \to tt_0$,, and $D \to DD_0$:
— for the first potential type, $x_0 = \sqrt{a/b}$, $t_0 = m\gamma/a$, $D_0 = \dfrac{a}{m\gamma}\left(\dfrac{a}{b}\right)^{\alpha/2}$;
— for the second potential type, $x_0 = \sqrt{b/a}$, $t_0 = m\gamma/\sqrt{ab}$, $D_0 = \dfrac{\sqrt{ab}}{m\gamma}\left(\dfrac{b}{a}\right)^{\alpha/2}$.
This procedure is analogous to that described in [9] in detail.

For the dimensionless variables in each case and after the time quantization, we have

$$U_1(x): \quad x_{n+1} - x_n = \left(x_n - x_n^3\right)\delta t +$$

$$+(D\delta t)^{\frac{1}{\alpha}}\xi_\alpha(t_n)\,; \tag{4}$$

$$U_2(x): \quad x_{n+1}-x_n=\left(x_n^2-1\right)\delta t+$$

$$+(D\delta t)^{\frac{1}{\alpha}}\xi_\alpha(t_n)\,. \tag{5}$$

For the simulations, we use a Lévy noise generator described in [10]. For a potential of type I, the computational modeling is conducted in such a way: a "particle" is placed at the point $x = -1$, then the iterations start. When the "particle" reaches the point $x = 0$, the iterations stop, and the event of barrier crossing and the respective time instant are determined. For a potential of type II, the "particle" again starts its motion from the point $x = -1$, but, in contrast with the previous case, the iterations stop, when the "particle" reaches $x = 10$. The mean time is evaluated by averaging $10,000$ such events. The simulation was performed in two ways: we used, firstly, the programming language *Borland C++ Builder 6* and, secondly, the mathematical package *Mathematica 5*. The time step was taken to be equal to 0.01 in *Borland C++ Builder* program and 0.1 in the simulation with *Mathematica*. The calculations made on *Borland C++ Builder* and *Mathematica* gave the same results (the accuracy was better than 0.7 percent). It was also proved that the simulation scheme is independent of the time quantization parameter (the inaccuracy did not exceed the error for the usual scheme of integrating an ordinary differential equation of the first order by using the method of rectangles).

3. Mean Crossing/Escape Time

First, we are interested in evaluating the mean crossing/escape time of a particle from the potential well. The simulation shows that, as in the classical case of a Gaussian random force, the Lévy particle's mean crossing/escape time does not depend much on the form of the potential profile but on the barrier's height. Indeed, Fig. 3 representing such a dependence proves this aspect due to the obvious similarity between the top and bottom images.

At first, we note that the curves for $\alpha = 2$ are in a good agreement with classical results for the Kramers'

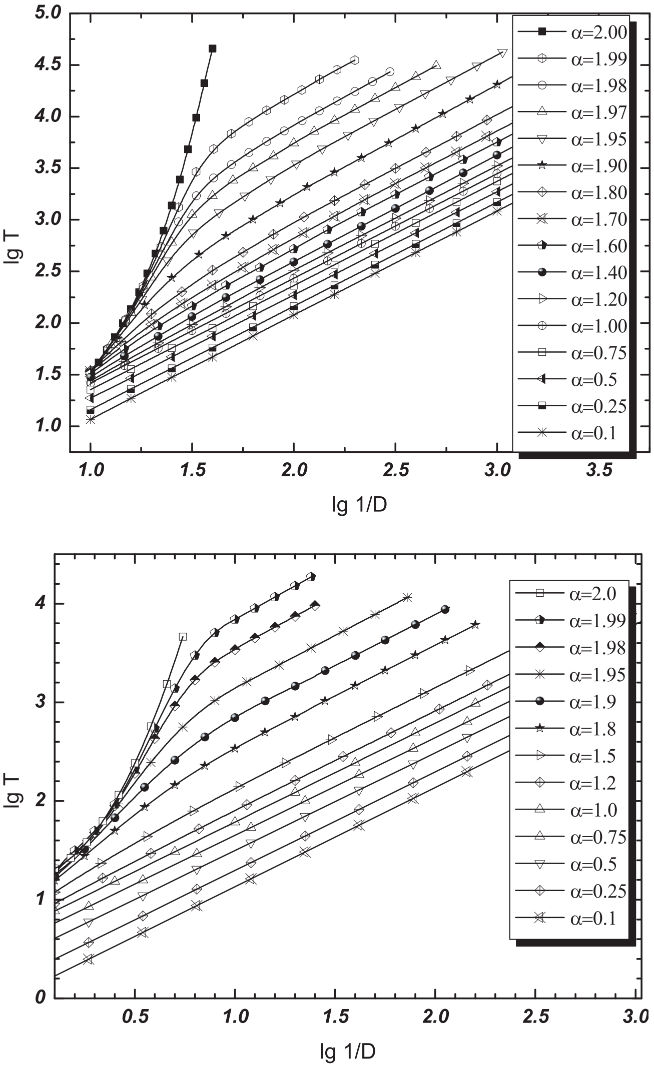


Fig. 3. Mean crossing time for profile I (above) and the mean escape time for profile II (below) versus the reciprocal noise intensity

problem, demonstrating the exponential dependence on the reciprocal noise intensity [11]:

$$U_1(x): \quad T \approx \frac{\pi}{\sqrt{2}}e^{1/(4D)}; \tag{6}$$

$$U_2(x): \quad T \approx \frac{3\pi}{2}e^{4/(3D)}. \tag{7}$$

Now let us turn to cases $\alpha < 2$. As seen from Fig. 3, the mean time versus D has power-law asymptotics for D small enough. Furthermore, if we construct the quantity $\mu(\alpha)$ such that

$$T(\alpha, D) = \frac{C(\alpha)}{D^{\mu(\alpha)}}, \tag{8}$$

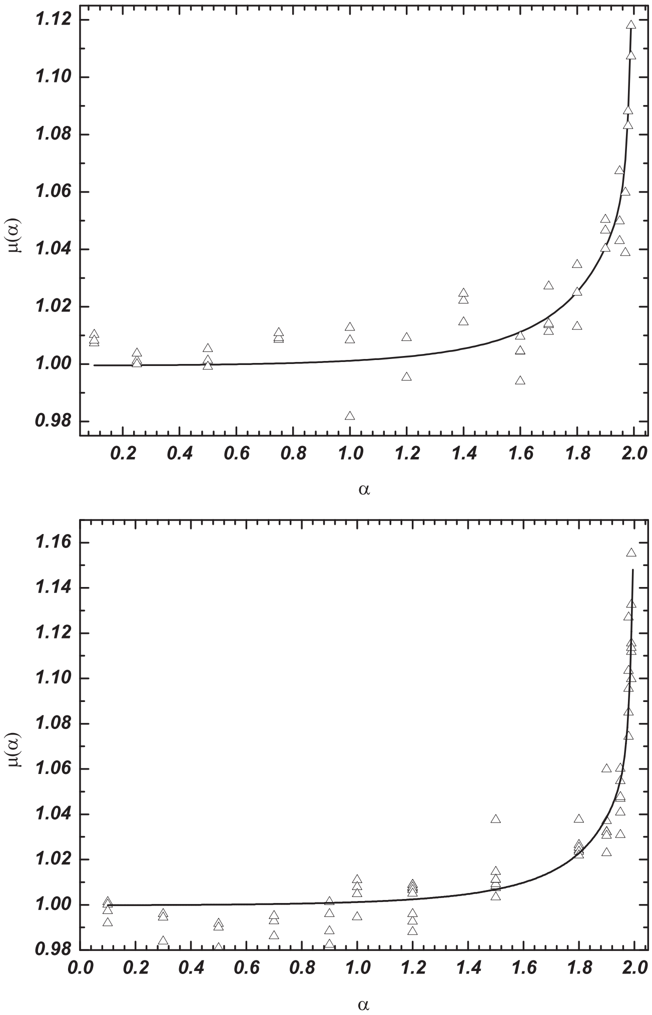


Fig. 4. Power-law asymptotics for potentials of type I (above) and type II (below)

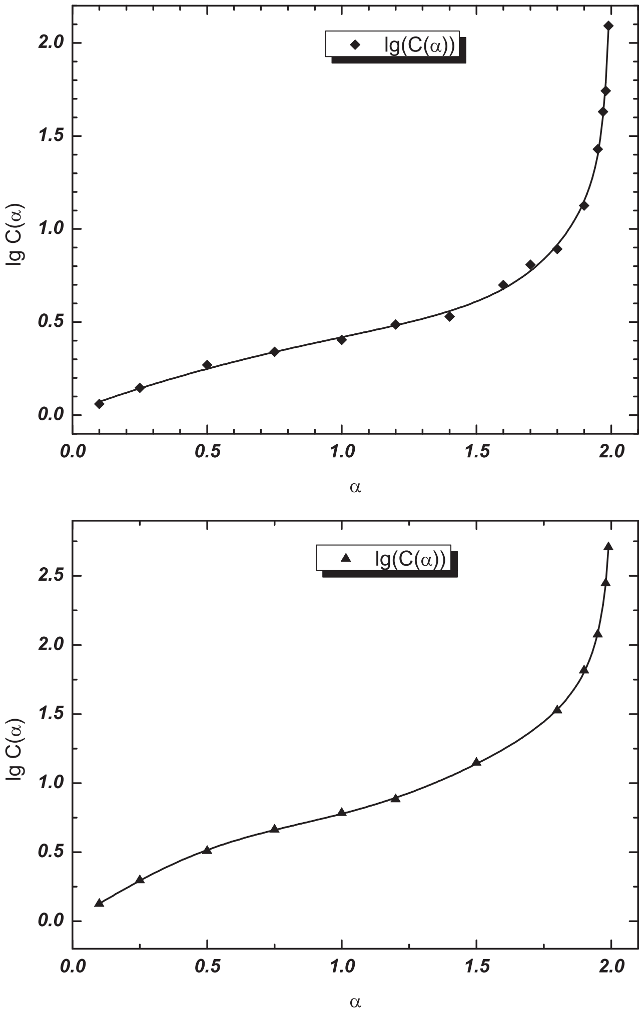


Fig. 5. Obtained values for $\lg C(\alpha)$ for potentials of type I (above) and type II (below)

$$\mu(\alpha) = \frac{d \lg T}{d \lg 1/D}, \tag{9}$$

it will tend to 1 for all $\alpha < 1$, see Fig. 4. This fact may have the following explanation. It is a well-known property of the Lévy noise that the less is the parameter α, the longer become the so-called Lévy flights: the outliers, or sudden and sharp high peaks in the noise which arise due to the steep power-law asymptotics of the Levy stable PDFs (for illustrations, see, e.g., [12]). So there may occur the relation between a sudden force's value and the barrier's height such that the particle will jump out of the well in several steps. That is why the particle behaves in the way as there is no potential barrier at all. The calculated values for the quantity $C(\alpha)$ are shown in Fig. 5. In both cases, we detect a weak inflection of the curves at the intermediate α values. Also the value $C(\alpha)$ tends to 1 at small α's.

4. PDF for the First Crossing/Escape Problem

Now let us obtain the probability density function of a particle to escape the well as the function of walking time. The simulation of this problem is conducted in a way much common with the previous one. The numerical integration of the overdamped Langevin equation is held for a fixed value of D (the noise intensity) and stops each time as the "particle" reaches the point $x = 0$ for the potential $U_1(x)$ and $x = 10$ for the potential $U_2(x)$. The obtained times are not averaged, and, after a certain number of such events, they are handled with a simple routine (written on *Mathematica*) that calculates the probability density function (normalizing it by 1). The following calculations were done using again *Borland C++ Builder 6* and *Mathematica* (the latter – to obtain the distribution function). The values of the parameters are as follows:

1. for $U_1(x)$, $\delta t = 0.01$; statistics $= 200,000$ events; $D = 10^{-2.0}$; $x_0 = -1$; $\alpha = 0.1, 0.5, 1.0, 1.5$;

2. for $U_2(x)$, $\delta t = 0.01$; statistics $= 200,000$ events; $D = 10^{-1.4}$; $x_0 = -1$; $\alpha = 0.1, 0.5, 0.9, 1.0, 1.5$.

For both potential profiles and for the whole set of Lévy indices, it possesses an exponential law (see Fig. 6).

As easily seen, it is possible to evaluate the mean crossing/escape times by using these distributions. Indeed, if $p(t) = \nu e^{-\nu t}$ is our probability density function, then

$$\langle T \rangle = \frac{1}{\nu} = e^{-\ln p(0)} \equiv \tau_1, \quad (10)$$

where $\langle T \rangle$ is the mean crossing/escape time. Another way to evaluate it by means of these probability density functions is the following:

$$\langle T \rangle = -\left(\frac{d \ln p(t)}{dt}\right)^{-1} \equiv \tau_2. \quad (11)$$

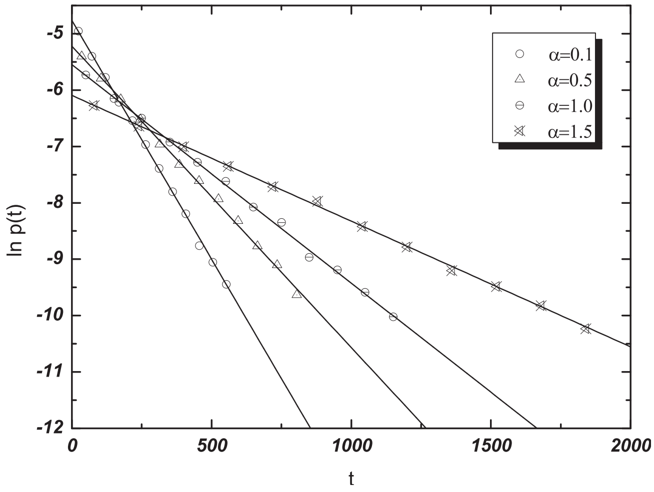
The carried out calculations give the coincidences between crossing/escape times obtained in such ways and those calculated in Section 2 with accuracy better than 1.5 percent (Table).

5. Conclusion

In this paper, the mean first crossing/escape times have been evaluated for two types of potentials using three separate methods, all are based on the numerical integration of the overdamped Langevin equation. It was shown that the mean crossing/escape time of a Lévy particle obeys a different law comparing to that of the classical Brownian particle. Indeed, instead of the exponential law at $\alpha = 2$, it possesses a power-law asymptotics at small values of the noise intensity.

Comparison of mean crossing/escape times obtained in three different ways

	U_1			U_2		
α	simul.	τ_1	τ_2	simul.	τ_1	τ_2
0.1	119.7	117.4	118.1	34.2	33.9	34.1
0.5	187.1	185.1	187.1	78.3	77.8	78.1
1.0	260.8	257.1	258.2	153.7	153.0	153.5
1.5	446.5	443.4	448.4	346.6	342.9	344.9



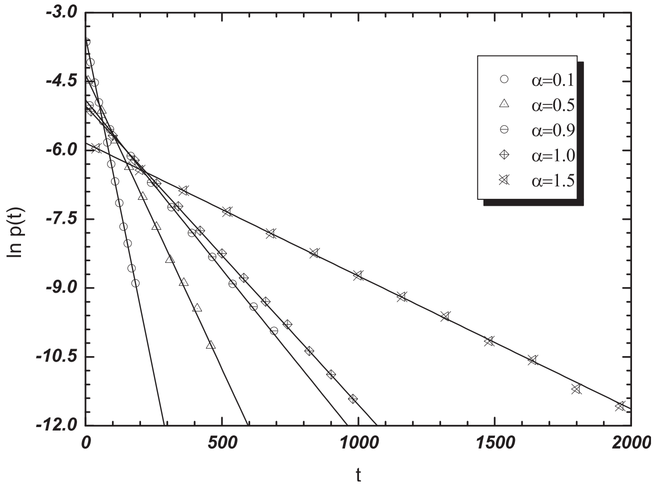


Fig. 6. Crossing/escape probability density functions for both types of potentials (type I above, type II below)

However, the probability density function for the first crossing/escape problem in the domain of Lévy indices ($0 < \alpha < 2$) is proportional to $\exp(-\nu(\alpha)\, t)$, like in the case of the Gaussian probability distribution function of an external random force. The results point clearly to the necessity for creating a consistent kinetic theory which has not been constructed yet.

The author would like to thank A.V. Chechkin for the problem setting and for the discussion of the results and V.Yu. Gonchar for his help in simulations. The helpful comments from J. Klafter and R. Metzler are also appreciated.

1. L.S. Pontryagin, A.A. Andronov, and A.A. Vitt, Zh. Eksp. Teor. Fiz. **3**, 165 (1933).

2. A.V. Chechkin, V.Yu. Gonchar, J. Klafter, and R. Metzler, Adv. Chem. Phys. **133B**, (2006).

3. A.V. Chechkin, V.Yu. Gonchar, J. Klafter, and R. Metzler, Phys. Rev. E **72**, 010101(R) (2005).

4. A.V. Chechkin, V.Yu. Gonchar, J. Klafter, and R. Metzler, Europhys. Lett. **72**, 348 (2005).

5. B.V. Gnedenko and A.N. Kolmogorov, *Limiting Distributions for the Sums of Independent Random Values* (Izd. Tekh.-Teor. Lit., Moscow, 1949) (in Russian).

6. P.D. Ditlevsen, Phys. Rev. E **60**, 172 (1999).

7. C. Bustamante, Y.R. Chemla, N.R. Forde, and D. Izhaky, Annu. Rev. Biochem. **73**, 705 (2000).

8. C.L. Nikias and M. Shao, *Signal Processing with Alpha-Stable Distributions and Applications* (Wiley, New York, 1999).

9. A.V. Chechkin, V.Yu. Gonchar, and M. Szydłowsky, Phys. Plasmas **9**, 78 (2002).

10. J.M. Chambers, C.L. Mallows, and B.W. Stuck, J. Amer. Statist. Assoc. **71** 340 (1976).

11. H. Risken, *The Fokker—Planck Equation* (Springer, Berlin, 1989).

12. A.V. Chechkin and V.Yu. Gonchar, Ukr. Fiz. Zh. **48**, 714 (2003).

Received 23.08.06

ДО ПОЛЬОТІВ ЛЕВІ У ПОТЕНЦІАЛЬНІЙ ЯМІ

О.Ю. Слюсаренко

Р е з ю м е

Розглянуто рух передемпфованої частинки Леві (тобто броунівської частинки, що перебуває під дією зовнішньої випадкової сили із законом розподілу Леві) в потенціальній ямі. Нашою метою було отримання методом чисельного інтегрування передемпфованого рівняння Ланжевена середніх часів вильоту частинки з потенціальної ями та функції розподілу цих часів. Було досліджено варіювання цих величин зі зміною вигляду потенціалу та значень параметра Леві випадкової сили.