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The Investigation of the External Influence on the Motion Regimes of Nanoparticles

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On the basis of self-consistent Lorenz system, taking into account the dispersion of the characteristic time of the average velocity variation the motion regimes of nanoparticles were investigated within the rigid mechanism of the self-organization. The influence of the environment was taken into account by means of a stochastic source in the equation describing the evolution of the control parameter. As a result, the Fokker-Planck equation has been obtained and has been solved in the steady state, the phase diagram of the system and the dependence of the average velocity of nanoparticles have been constructed and analyzed.

Keywords: Lorenz system, Le Chatelier principle, Fokker-Planck equation, Ornstein-Uhlenbeck process.

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1. INTRODUCTION

Nowadays the nanotechnology is considered to be one of the most progressive directions of the modern science development. The development of it provides an opportunity to create a variety of technical devices in all branches of science and engineering and especially in biology and medicine. Interesting is the fact, that distinctive feature of nanoscale biological objects is ability to the self-organization. This feature is actively used now in the modeling of complex systems behavior. That's why one of the actual problems nowadays is a consideration of nanoparticle's collective behavior.

In this regard, in recent years to describe the motion of nanoparticles the theory of Brownian motion is used [1-4]. Despite the fact that the theoretical basis of the motion of Brownian particles were investigated by Albert Einstein more than a century ago, some of the nuances of his theory could be explained only now. They are based on a study of the so-called "hot" Brownian motion [1,4]. The last differs from the usual Brownian motion in that the metal particles (for example gold nanoparticles) are heated by a focused laser beam, and so that each particle has a reserve of internal energy, which is converted into mechanical energy.

It turns out that between the motion regimes of the gold nanoparticles [1-4] and biological nanoobjects, such as bacteria [5,6], we can find a sufficiently close analogy. Thus the three types of motion regimes (directional motion with different velocities, rotational motion and interrupted motion) are observed. The last mode is similar to the stick-slip motion in condensed matter physics [7]. And as is well known the study of analogies between living and nonliving systems is of great practical interest nowadays.

As a result the aim of our work is to consider a stochastic dynamics of the motion of active nanoparticles within the model of Brownian motion. In addition, to account the effects arising due to the compensation of the torque of nanoparticles we need to consider the influence of the stochastic sources and to consider the rigid mechanism of the system self-organization.

2. MAIN STATEMANTS

Using the example of condensed matter [7-9], the representation of self-organizing system reduces to the description of the time dependencies of three degrees of freedom: the order parameter, the conjugate field, and the control parameter. As the order parameter, which distinguishes motion regimes of nanoparticles, we will take the average velocity v of the active nanoparticles movement. It should be noted that by the 'average velocity' we mean the velocity of directed movement. Thus, in the case of rotational motion, a particle is rotating but the mentioned average velocity is zero.

The interaction between the particles themselves or between the environment can be presented via some kind of field $H(\vec{r},t)$ .Thus, the conjugate field reduces to the long-range force $h \equiv \nabla H(\vec{r},t)$. Since for the directed motion the nanoparticles always have a priority direction, further we will consider only one-dimensional case.

Besides in our consideration we will use the internal parameter ε, which describes internal energy and takes different values. However, this parameter is imposed on restrictions which are defined by the environment.

Considering that for the self-organized systems the order parameter $v(t)$ dominates the behavior of the conjugate field $h(t)$ and the control parameter $\varepsilon(t)$, we take the expression for the average acceleration in the form

$$\dot{v} = -\frac{v}{t_v}\left(1+\frac{\kappa}{1+v^2/v_d^2}\right)+a_v h . \qquad (2.1)$$

Here we have taken into account the relaxation term, linear reaction on the force increasing, and the dependence of the relaxation time t_v on the velocity (κ is a dispersion constant, v_d - dispersion scale, a_v is a positive constant).

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The equation for the conjugate field

$$\dot{h} = -\frac{h}{t_h} + a_h v\varepsilon \,, \tag{2.2}$$

has taken into account the relaxation term with relaxation time t_h and the positive feedback that provides the system self-organization (a_v is a positive constant).

The last evolution equation of the system

$$\dot{\varepsilon} = \frac{\left(\varepsilon_e - \varepsilon\right)}{t_\varepsilon} - a_\varepsilon vh + \zeta\left(t\right), \tag{2.3}$$

describes the relaxation of the internal parameter to the final value of ε_e, which is given by an external influence (t_ε – the corresponding relaxation time). At the same time negative feedback (the constant $a_\varepsilon > 0$) of the conjugate field and velocity with the rate of change of the internal state parameter leads, in accordance with Le Chatelier's principle, to a decrease of this parameter. Besides, the stochastic influence of the environment is represented by the source of the noise of the control parameter $\zeta(t)$, which is defined by the Ornstein-Uhlenbeck process.

$$\left\langle \zeta\left(t\right)\right\rangle = 0, \left\langle \zeta\left(t\right), \zeta\left(t'\right)\right\rangle = \frac{I}{\tau}\exp\left(-\frac{\left|\left(t-t'\right)\right|}{\tau}\right). \tag{2.4}$$

Here I is the intensity of fluctuations, and τ - corresponding relaxation time.

According to Ref. [10], the system of synergetic equations (2.2) – (2.4) is the simplest field scheme that presents the effects of the self-organization. For the analysis of this system is convenient to use dimensionless variables, relating the time t, the velocity v, the conjugate field h, the internal parameterε, and the fluctuations intensity I to the scales

$$t_s \equiv t_v, v_s = \left(a_h a_\varepsilon t_h t_\varepsilon\right)^{-1/2}, h_s = \left(a_v^2 t_v^2 a_h a_\varepsilon t_h t_\varepsilon\right)^{-1/2},$$
$$\varepsilon_s = \left(a_h t_h a_v t_v\right)^{-1}, I_s = \left(t_\varepsilon a_h t_h a_v t_v\right)^{-2}.$$

Then the behavior of active Brownian particles is represented by dimensionless system

$$\dot{v} = -v\left(1 + \frac{\kappa}{1 + v^2/v_d^2}\right) + h\,, \tag{2.5}$$

$$\sigma^{-1}\dot{h} = -h + v\varepsilon\,, \tag{2.6}$$

$$\delta^{-1}\dot{\varepsilon} = \left(\varepsilon_e - \varepsilon\right) - vh + \zeta\left(t\right), \tag{2.7}$$

where $\sigma^{-1} \equiv t_h/t_v, \delta^{-1} \equiv t_\varepsilon/t_v$.

In general, the system does not have an analytical solution, so we will take into account that during the evolution the internal state parameter ε coordinates the changes of the velocity and field. This leads to the following approximation

$$t_v \gg t_\varepsilon, t_v \approx t_h \quad (\delta^{-1} \ll 1, \sigma \approx 1)\,. \tag{2.8}$$

As a result, we finally obtain the differential equation of the second order in the canonical form of the motion equation for the nonlinear stochastic oscillator

$$\ddot{v} + \gamma\left(v\right)\dot{v} = f\left(v\right) + g\left(v\right)\zeta\left(t\right), \tag{2.9}$$

where

$$\gamma\left(v\right) = 1 + \sigma\left(1 + v^2\right) + \kappa\frac{1 - v^2/v_d^2}{\left(1 + v^2/v_d^2\right)^2},$$
$$f\left(v\right) = \sigma\left(\varepsilon_e - 1\right)v - \sigma v^3 - \sigma\kappa\frac{v\left(1 + v^2\right)}{1 + v^2/v_d^2}, \tag{2.10}$$
$$g\left(v\right) = \sigma v.$$

3. THE STATIONARY SOLUTION OF THE FOKKER-PLANCK EQUATION

To find the distribution function of the system in the phase space, we arrive at the Fokker-Planck equation [11], using the method of Shapiro [12]

$$\frac{\partial P\left(v,t\right)}{\partial t} = -\frac{\partial}{\partial v}\left[D_1(v)P(v,t)\right] + \frac{\partial^2}{\partial v^2}\left[D_2(v)P(v,t)\right], \tag{3.1}$$

where $P\left(v,t\right)$ is the probability density of the velocity distribution,

$$D_1\left(v\right) = \frac{1}{\gamma\left(v\right)}\left[f\left(v\right) - M_0\frac{g^2\left(v\right)}{\gamma^2\left(v\right)}\frac{\partial\gamma\left(v\right)}{\partial v} + M_1 g\left(v\right)\frac{\partial g\left(v\right)}{\partial v}\right],$$
$$D_2\left(v\right) = M_0\frac{g^2\left(v\right)}{\gamma^2\left(v\right)},$$

Are the drift and the diffusion coefficients, respectively, and $M_0 = I$, $M_1 = I\tau$.

Equation (3.1) can be represented as the continuity equation for the probability distribution $P(v,t)$

$$\frac{\partial P\left(v,t\right)}{\partial t} + \frac{\partial S\left(v,t\right)}{\partial v} = 0\,, \tag{3.2}$$

where $S(v,t)$ – the probability current

$$S\left(v,t\right) = D_1\left(v\right)P\left(v,t\right) - \frac{\partial}{\partial v}\left[D_2(v)P(v,t)\right]. \tag{3.3}$$

In the stationary case with the zero probability current S the Eq. (3.2) reduces to the expression

$$D_1\left(v\right) - \frac{\partial}{\partial v}D_2\left(v\right) = 0\,. \tag{3.4}$$

As a result of solving the equation (3.4), we arrive at the expression (3.5) which gives an implicit dependence of steady-state velocity on the internal state parameter given by the external environment. The corresponding phase diagram, defining the existence regions of different values of a stationary velocity, is shown in Fig. 1a.

$$\varepsilon_e - 1 - \upsilon^2 + I\tau\sigma - \kappa\frac{1+\upsilon^2}{1+\upsilon^2/\upsilon_d^2} - \frac{2I\sigma\left[1+\sigma+\kappa\left(3\upsilon^2/\upsilon_d^2 - 2\upsilon^4/\upsilon_d^4 + 1\right)\Big/\left(1+\upsilon^2/\upsilon_d^2\right)^3\right]}{\left[1+\sigma\left(1+\upsilon^2\right)+\kappa\left(1-\upsilon^2/\upsilon_d^2\right)\Big/\left(1+\upsilon^2/\upsilon_d^2\right)^2\right]^2} = 0. \quad (3.5)$$

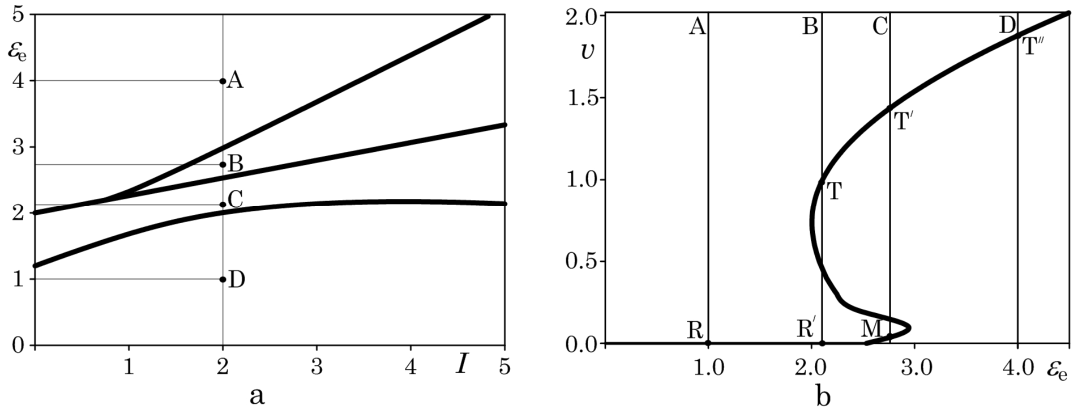

Fig. 1 – State diagram of the system for $\tau = 0.4$, $\upsilon_d = 0.1$ (a) and steady-state dependence of the average velocity for $I = 2$, $\tau = 0.4$, $\upsilon_d = 0.1$

This figure demonstrates that four regions of the diagram correspond to the four states of the system, each of which is indicated by the corresponding letter. In order to visualize the state of the system, which is realized, Fig. 1b shows the dependence of steady-state values of the nanoparticles velocity on the internal state parameter, given by the an external influence, for the noise intensity $I = 2$. Here the rays A, B, C, D correspond to the relevant regions of the phase diagram. For the ray A only rotational motion regime with average velocity $\upsilon = 0$ is realized (the point R in Fig. 1b). The ray B is characterized by the presence of two velocities $\upsilon = 0$ (the point R' in Fig. 1b) and $\upsilon \neq 0$ (the point T in Fig. 1b). This situation corresponds to the interrupted motion regime, when rotational and directional types of motion are alternating consequentially. A several types of the motion coexist for the ray C. However, in this case only directional motion with different velocities v (in Fig. 1b point M corresponds to the motion with low velocity, point T' – to the motion with high velocity) is realized. For the region of the phase diagram, corresponding to the ray D, only one type of the directed motion is realized (the point T'' in Fig. 1b).

4. CONCLUSION

Nowadays for many experiments in nanotechnology for exact control of the corresponding technique, for example, optical tweezers, it is necessary to understand the motion features of nanoparticles. In our paper the evolution equation, which allows us to describe the motion of nanoparticles in liquid, was considered. Taking as a basis a synergistic scheme and accounting the stochastic source, we were able to describe the transition between different motion regimes of the nanoparticles. In addition, the parameters, which define the behavior of the system, were determined, and corresponding values of the stationary velocity were analyzed. Thus, for the investigation of both living and nonliving systems these results may provide additional information and different ideas. Note that the alternative theory advanced with respect to accounting different interactions will monitor and control the nanoparticles motion in the liquid. The subsequent application of this theory is quite promising for the medical and technical research.

REFERENCES

1. D. Rings, R. Schachoff, M. Selmke, F. Cichos, K. Kroy, *Phys. Rev. Lett.* **105**, 090604 (2010).
2. P. Radtke, L. Schimansky-Geier, *Phys. Rev. E* **85**, 051110 (2012).
3. L. Joly, S. Merabia, J.-L. Barrat, *EPL* **94**, 50007 (2011).
4. O. Yushchenko, A. Badalyan, *Phys. Rev. E* **85**, 051127 (2012).
5. G. Ivanitskii, A. Medvinskii, M. Tsyganov, *Phys. Usp.* **37**, 961 (1994).
6. G. Ivanitskii, A. Medvinskii, M. Tsyganov, *Phys. Usp.* **34**, 289 (1991).
7. A.I. Olemskoi, O.V. *Yushchenko, Tech. Phys.* **48**, 1233 (2003).
8. A. Olemskoi, O. Yushchenko, T. Zhilenko, *Phys. Solid State* **53**, 845 (2011).
9. A. Olemskoi, O. Yushchenko, V. Borisyuk, T. Zhilenko, Yu. Kosminska, V. Perekrestov, *Physica A* **391**, 3277 (2012).
10. H. Haken, *Synergetics* (Berlin: Springer: 1978).
11. H. Risken, *The Fokker-Planck equation* (Berlin: Springer: 1989).
12. V. Shapiro, *Phys. Rev. E* **48**, 109 (1993).