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Transformation of the Internal Energy of the Active Nanoparicles under Canonical Representation

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The kinetics of the active nanoparticles within the framework of the canonical representation was investigated. On the basis of the phase portraits method the behavior of the system was studied for the case of the anharmonic oscillator under the transformation of the internal energy of the particles into the total mechanic energy of motion.

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1. INTRODUCTION

Starting with the famous lecture "there's Plenty of Room at the Bottom" by Richard Feynman, presented on the eve of 1960 at the annual meeting of the American Physical Society, the interest in nanoscale system and their technology application has been increasing. Especially in recent years the interest has grown to the so-called Janus nanoparticles (gold-capped colloidal spheres), which perform an active Brownian motion when heated by light [1-3]. In this case it means that the particle can make not only the energy of the motion, as a result an active Brownian motion arises [4]. Especially Feynman highlighted the unusual properties of biological nanosystems, which on the one hand have an enormous amount of information; on the other hand they can perform variety actions: recycle some substances into the energy, make various types of motion, change their shape, etc. Therefore the active nanoparticles are presented as a model of self-propelled motion in biology [4].

Although it is worth noting that the active Brownian particles (or self-phoretic colloids) and so-called run-and-tumble particles (motile bacteria) are not always equivalent. The paper [5] discusses the relationship of these two concepts, where the criterion of equivalence $a \leftrightarrow (d\text{-}1)D_r$ are obtained (a is a tumble rate, D_r – the rotational diffusivity, d - dimension).

It is well known from the thermodynamics of irreversible processes that systems can exhibit a rich variety of complex behavior if there is a supercritical influx of free energy. Among the prominent examples that can be observed in biological systems there are processes of pattern formation, morphogenesis, and different types of collective motion, such as swarming. It is worth noting the problem of the types of the active nanoparticles motion, which are often reduced to three types: translational, rotational and amoebae-like (run-and tumble) motion. At the same time a description of the collective motion is often reduced to the one-body problem [4].

It turns out that the analysis techniques of such system behavior is not limited by the Langevin equation [4], but also based on a Hamiltonian system [6],

the numerical Monte Carlo simulation, etc. So the problem of modeling the processes, occurring in nonlinear biological systems (especially the biological motion), is one of the topical in recent years.

We consider the kinetics of the active Brownian particle motion using Hamiltonian system complemented with the internal energy dependence and feedbacks.

2. BASIC EQUATIONS

The properties of the dynamical systems can be conveniently studied using the concept of phase space [7]. In this case the particle state is given by a point in the phase space $(\mathbf{q}, \mathbf{p})$ of n-dimensional vectors $\mathbf{q} = q_1, q_2, \ldots, q_n$ and $\mathbf{p} = p_1, p_2, \ldots, p_n$. The change in the system state over time t leads to the displacement of a point $(\mathbf{q}, \mathbf{p})$ in the phase space, resulting in a so-called phase trajectory.

Usually [7], the phase flow is defined by the differential equations of the motion

$$\dot{\mathbf{q}} = Q(\mathbf{q}, \mathbf{p}, t),$$
$$\dot{\mathbf{p}} = P(\mathbf{q}, \mathbf{p}, t), \qquad (2.1)$$

the solution of which is the particles trajectory in the phase space (the dot denotes differentiation with respect to time t). An important feature of the physical systems is an existence of the certain symmetry properties of the motion that express the corresponding conservation laws. The condition of the conservation of the phase volume determines the class of Hamiltonian systems, for which the motion equations

$$\dot{\mathbf{q}} = \frac{\partial H}{\partial \mathbf{p}},$$
$$\dot{\mathbf{p}} = \frac{\partial H}{\partial \mathbf{q}}, \qquad (2.2)$$

are given by the so-called Hamiltonian or Hamilton function

$$H(\mathbf{q}, \mathbf{p}, t) = K(\mathbf{p}, t) + P(\mathbf{q}, t), \qquad (2.3)$$

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which represent the total mechanical energy of the system, i.e. the sum of kinetic K and potential P energy. It is know, that according to the Liouville theorem for the Hamiltonian systems the possibility of the existence of asymptotically stable equilibrium state and asymptotically stale limit cycle is eliminated. However, for biological systems a great variety of states (including asymptotically stable) can be observed [8].

In [6] a general theory of canonical dissipative systems was developed including the couplings of the internal energy with the kinetic energy and with the total mechanical energy of the system.

Further we consider the motion of active nanoparticles in a medium with liquid friction. For this purpose in (2.2) it is necessary to consider the additional term, which represents the Stokes formula ($\dot{\mathbf{p}} \propto -\gamma \mathbf{p}$). The latter determines the friction force of a solid sphere in the liquid/gas medium at low Reynolds number [4]. Here $\gamma = 6\pi R \eta_m / m$ is a liquid friction coefficient (m, R are the mass and the size of the particle and η_m is the viscosity of the medium).

In addition, for a description of the active motion the internal energy ε of the system and its transformation into total mechanical energy must be considered.

As a result on the basis of the canonical system of we obtain

$$\dot{\mathbf{q}} = \frac{\partial H}{\partial \mathbf{p}}, \qquad (2.4)$$

$$\dot{\mathbf{p}} = -\frac{\partial H}{\partial \mathbf{q}} - \gamma \frac{\partial H}{\partial \mathbf{p}} + \beta \varepsilon f_1(H), \qquad (2.5)$$

$$\dot{q} = \frac{p}{m},$$

$$\dot{p} = -m\omega^2 q - 3\alpha_1 q^2 - 4\beta_1 q^3 - \frac{p}{m}(\gamma + \beta\varepsilon) + \alpha\varepsilon\left[m\omega^2 q + 3\alpha_1 q^2 + 4\beta_1 q^3\right], \qquad (3.2)$$

$$\dot{\varepsilon} = \frac{\varepsilon_e - \varepsilon}{\tau} - \mu\varepsilon \frac{p^2}{m} - 2\lambda\varepsilon\left[\frac{1}{2}m\omega^2 q^2 + \alpha_1 q^2 + \beta_1 q^3\right].$$

Using the scales

$$t_s \equiv \frac{m}{\gamma}, \ q_s \equiv \left(\frac{m}{\mu\tau\gamma^2}\right)^{1/2}, \ p_s \equiv \left(\frac{m}{\mu\tau}\right)^{1/2}, \ \varepsilon \equiv \frac{\gamma}{\beta}.$$

For the time, coordinate, momentum and internal energy, as well as introducing the additional dimensionless parameters

$$\chi \equiv t_s^2 \omega^2, \ \delta \equiv \frac{\tau}{t_s}, \ \kappa \equiv \frac{3\alpha_1}{\gamma} t_s q_s, \ \eta \equiv \frac{4\beta_1}{\gamma} t_s q_s^2.$$

Instead of (3.2) we have

$$\dot{q} = p,$$

$$\dot{p} = -\chi q - \kappa q^2 - \eta q^3 - p + \varepsilon p + \varphi\chi\varepsilon q + \varphi\varepsilon\left(\kappa q^2 + \eta q^3\right),$$

$$\delta\dot{\varepsilon} = \varepsilon_e - \varepsilon - \varepsilon p^2 - \psi\chi\varepsilon q^2 - \psi\varepsilon q^3\left(\frac{2}{3}\kappa + \frac{1}{2}\eta q\right). \qquad (3.3)$$

Using the adiabatic approximation $\tau \ll t_s$, $\delta \ll 1$, we obtain the dependence of the internal energy

$$\dot{\varepsilon} = \frac{\varepsilon_e - \varepsilon}{\tau} - 2\mu\varepsilon f_2(H). \qquad (2.6)$$

In the equation (2.6) it is taken into account the relaxation term, which describes the decrease of the internal energy in stand – alone mode to the value ε_e, defined by external conditions (τ is the corresponding relaxation time); and the dissipation term, which describes the decrease of the internal energy after its transformation into total mechanical energy. At the same the corresponding transformation brings a positive contribution in the second equation of the system (2.2). The function f_1 and f_2 are defined by the transformation into the concrete form of the energy; β and 2μ are the positive coupling constants.

3. TRANSFORMATION OF THE INTERNAL ENERGY INTO THE TOTAL MECHANIC ENERGY

We consider the most complicated case when the internal energy is transformed into the total mechanical energy for the anharmonic oscillator, whose Hamiltonian is given by

$$H = \frac{p^2}{2m} + \frac{m\omega^2 q^2}{2} + \alpha_1 q^3 + \beta_1 q^4. \qquad (3.1)$$

Here α_1 and β_1 are the coefficients of the amendments of the third and fourth degree respectively to the Hamiltonian.

Then, we obtain the system

$$\varepsilon = \frac{\varepsilon_e}{1 + p^2 + \psi\left(\chi q^2 + \frac{2}{3}\kappa q^3 + \frac{1}{2}\eta q^4\right)}, \qquad (3.4)$$

the form of which is shown in Fig. 1.

As a result we get a system of two differential equations

$$\dot{q} = p, \qquad (3.5)$$

$$\dot{p} = -\chi q - \kappa q^2 - \eta q^3 - p + \frac{\varepsilon_e\left(p + \varphi\chi q + \varphi\kappa q^2 + \varphi\eta q^3\right)}{1 + p^2 + \psi\left(\chi q^2 + \frac{2}{3}\kappa q^3 + \frac{1}{2}\eta q^4\right)} \qquad (3.6)$$

Among the singular points of the system (3.5) - 3.6) we can highlight the points

$$O\left(0;0\right),$$

$$H\left(-\frac{\kappa - \sqrt{\kappa^2 - 4\chi\eta}}{2\eta};0\right),$$

$$G\left(\frac{\kappa + \sqrt{\kappa^2 - 4\chi\eta}}{2\eta};0\right).$$

the latter two of which exist under the condition

$$\chi < \frac{\kappa^2}{4\eta}. \qquad (3.7)$$

The remaining singular points are determined by the solution of the fourth degree equation

$$q^4 + \frac{4\kappa}{3\eta}q^3 + \frac{2\chi}{\eta}q^2 + \frac{2\left(1 - \varepsilon_e\varphi\right)}{\psi\eta} = 0 \qquad (3.8)$$

Since subsequent analytical expressions are rather cumbersome, in this section we confine ourselves to the numerical solution of the system (3.5) - (3.6). A few examples of corresponding phase portraits shown in Fig. 2
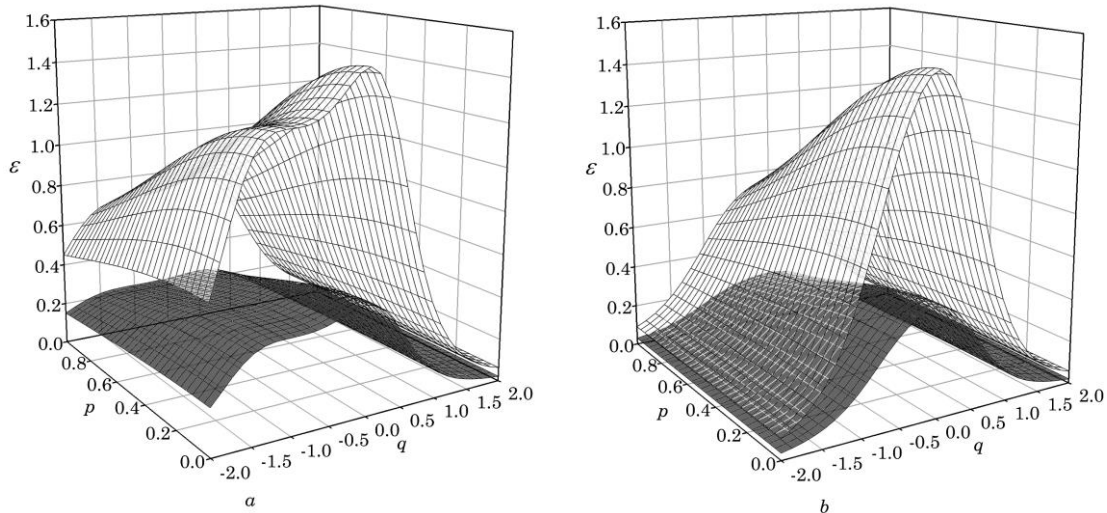
Fig. 1 – Dependence of the internal energy for $\chi = 1$, $\psi = 1$ at *a*) $\kappa = 2$, $\eta = 1$, *b*) $\kappa = 1$, $\eta = 2$. Surface **1** corresponds to the $\varepsilon_e = 0.5$, surface **2** to the $\varepsilon_e = 1.5$.
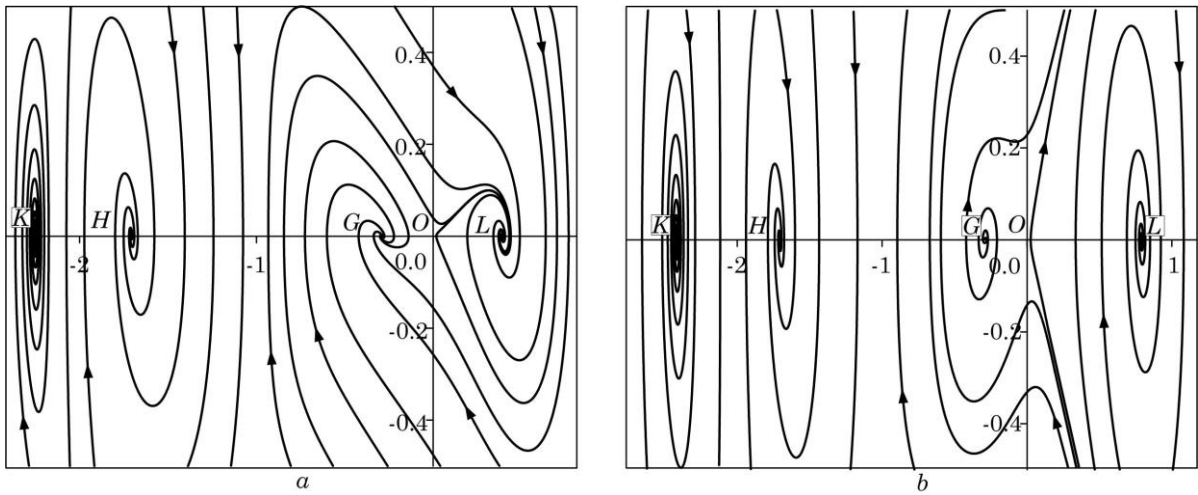
Fig. 2 – Phase portraits of the system (3.5)-(3.6) at $\chi = 0.5$, $\varphi = 3$, $\psi = 3$, $\kappa = 2$, $\eta = 1$ a) $\varepsilon_e = 0.5$, b) $\varepsilon_e = 1.5$.

4. CONCLUSION

As a result of this approach we can conclude about the influence of the medium parameters or character the redistribution of the internal energy on the motion of the active nanoparticles. Analyzing the phase portraits of the system one can consider the stationary states of the system, the transition to the oscillation regime and the total kinetics of the nanoparticles motion.

Thus the understanding of the laws governing the motion of the active nanoparticles can be of great practical application as nanorotors [4], ratchet system to molecular motors [9], etc.

REFERENCES

1. D. Rings et al., *Phys. Rev. Lett*. **105**, 090604 (2010).
2. O.V. Yushchenko, A.Yu. Badalyan, *Phys. Rev. E* **85**, 051127 (2012).
3. O.V. Yushchenko, A.Yu. Badalyan, *J. Nano- Electron. Phys*. **4**, 03009 (2012).
4. P. Romanczuk et al., *Eur. Phys. J*. **202**, 1 (2012).
5. M. Cates, J. Tailleur, *EPL* **101**, 20010 (2013).
6. A. Gluck, H. Huffel, S. Ilijic, *Phys. Rev. E* **83**, 051105 (2011).
7. K. Kreith, *Oscillation Theory. Lecture Notes in Mathematics* (Berlin: Springer-Verlag: 1973).
8. R. May, *Science* **186**, 645 (1974).
9. A. Fiasconaro, W. Ebeling, E. Gudowska-Nowak, *Eur. Phys. J. B* **65**, 403 (2008).