УДК 581.17 + 581.84

O.I. Pundyak
L'viv Cooperative College of Economy and Low, Clepariv Str., 11, L'viv 79000 Ukraine
e-mail: knyshoi@ukr.net

UNCERTAINTY OF SPATIAL DISTRIBUTION OF INHOMOGENEOUS PARTICLES IN LIMITED VOLUME

The motion of inhomogeneous non spherical particle in viscous medium under the influence of potential field in limited volume has been considered. Spatial distribution of such a particle is uncertain when whole free volume is small. Such an uncertainty is possible for cell organelles within a cell and also for spatial distribution of segments of polypeptide chain of a protein macromolecule or other molecules adsorbed on the segments.

Keywords: potential field, spatial distribution, viscosity, friction coefficient, cell organelles, protein macromolecules, segment of polypeptide chain.

Introduction

As it has been shown earlier [1], the distribution of distances between two bounded particles with different shapes and dimensions in viscous medium is determined unambiguously by their interaction potential and macroscopic parameters. It is a consequence of dissipative processes, which differently depend on directions of the particles movement. Do other variants of analogical uncertainties exist? An attempt was here done to present more simple model of such a dissipative anisotropy.

Consideration of the model

Let us consider the movement of inhomogeneous non spherical particle in viscous medium under the influence of gravity [2]. The particle freely moves in limited volume, which has the shape of cube. Such a movement can be described as:

$$m\ddot{x} + h\dot{x} + (m - m_m)g + F_x = A_x(t), \tag{1}$$

$$m\ddot{y} + h\dot{y} + F_y = A_y(t), \tag{2}$$

$$m\ddot{z} + h\dot{z} + F_z = A_z(t), \tag{3}$$

where m and m_m are correspondingly the particle mass and the mass of the medium of the same volume; h is friction coefficient of the particle depending on its orientation toward the movement direction; x, y, z are coordinates of mass centrum of the particle; g is gravity centrifugation; $A_x(t)$, $A_y(t)$, $A_z(t)$ are projections of fluctuation force on coordinate axes; $F_x(x)$, $F_y(x)$, $F_z(x)$ are the projections of the potential force allowing the particle to be only within the limited volume. For the sake of simplicity let $F_x = F_y = F_z = 0$ if $0{,}5d < x < b$; $0{,}5d < y < b$; $0{,}5d < z < b$; $b \equiv a - 0{,}5d$, where a is dimension of the cubic free volume; d is averaged diameter of the particle.

Let us integrate (1) with respect to x. According to the law of equipartition and the symmetry of movement laws under a time reversal transformation we will obtain:

$$S + 2\delta E_p = 2I, \tag{4}$$

where $S \equiv (\bar{h}_1 - \bar{h}_2)\int_{x_1}^{x_2} \bar{\dot{x}}dx;\quad I \equiv \int_{x_1}^{x_2} \bar{A}\,dx;$ $\bar{h}_1$ and $\bar{h}_2$ are averaged friction coefficients for a particle which moves correspondingly from coordinate surface x_1 to the surface x_2 and back; $\bar{\dot{x}}$ is averaged velocity of the particle; δE_p is the difference of potential energies of the particle on the surfaces x_1 and x_2: $\delta E_p = g(m - m_m)(x_2 - x_1)$.

As it is known, the spatial distribution depends on averaged value of energy given from the heat bath to the system (or in other words it depends on averaged work should be done by fluctuation force) for replacement of the particle from one coordinate surface to the other [3]. Therefore the spatial distribution can be written as:

$$P(x_2)/P(x_1) = \exp(-\mathrm{I}/kT), \qquad (5)$$

where *P(x)* is probability of location of the particle on surface *x*. According to (4) and (5) the spatial distribution of symmetrical particles (for them $\bar{h}_1 = \bar{h}_2$) is always a function of their potential energy.

A potential field can orient unsymmetrical particle. So these particles are differently oriented toward the direction of their movement during their direct and back transition. Therefore $\bar{h}_1 \neq \bar{h}_2$ for them and *S* in (4) depends on $\bar{\dot{x}}$. We can average velocities of the particle by two different ways: 1) with the respect to the ensemble of all identical systems containing only the particles which move from one coordinate surface to the other ($\bar{\dot{x}}_{all}$); 2) with the respect to the ensemble of the systems, containing only the particles which move from one coordinate surface to the other being not returned to previous location during this transition ($\bar{\dot{x}}_{dir}$). These $\bar{\dot{x}}_{all}$ and $\bar{\dot{x}}_{dir}$ are the results of averaging of all possible corresponding trajectories of the particle: some of them get back or almost get back and some of them get to the other coordinate surface. Averaged velocity of the firsts equals zero or are near zero; averaged velocity of the lasts (if the mean free path of the particle is much less then its averaged diameter *d*) is independent from coordinate and equals to D/d (it is the velocity of brownian translocation of the particle on the distance equal to its dimension), where D is coefficient of diffusion of the particle: D = k_bT/$\bar{h}$, $\bar{h}$ is averaged friction coefficient. If the particle volume V_{par} is near whole free volume V_{whole}, then:

$$\bar{\dot{x}}_{all} \approx \frac{k_b T}{d\bar{h}} \frac{V_{par}}{V_{whole}}\,;\ \bar{\dot{x}}_{dir} \approx \frac{k_b T}{d\bar{h}} \frac{V_{par}}{V_{dir}}, \qquad (6)$$

where V_{dir} is the volume located between the surfaces x_1 and x_2. According to (4), (5) and (6):

$$\frac{P(x_2)}{P(x_1)} \approx \exp\left[(x_2 - x_1)\left(\frac{\chi\gamma}{2d} + \frac{g(m - m_m)}{k_b T} \right)\right], \qquad (7)$$

where $V_{par}/V_{whole} \leq \chi \leq V_{par}/V_{dir}$; $\gamma \equiv (\bar{h}_1 - \bar{h}_2)/\bar{h}$. In common macroscopic systems $\chi \to 0$. But if V_{par} is not very small comparatively to V_{whole}, then distribution (7) is uncertain.

Spatial orientation of the particles

If unsymmetrical particles consist of only two spherical departments with different densities, they can be oriented in gravity field. The relation of probabilities to be the department 1 under the department 2 (P_{12}) and the department 2 to be under the department 1 (P_{21}) can be written as:

$$\frac{P_{12}}{P_{21}} = \exp\left[\mathrm{gl} \frac{(\mu_2 - \mu_{2o}) - (\mu_1 - \mu_{1o})}{kT} \right], \qquad (8)$$

where μ_1 and μ_2 are correspondingly masses of the departments; μ_{1o} and μ_{2o} are correspondingly the masses of the medium of the same volume with the departments 1 and 2; *l* is the distance between the centers of the departments. According to formula (8) the particles are considerably oriented in gravity field when:

$$gl\left|\ (\mu_1 - \mu_{1o}) - (\mu_2 - \mu_{2o})\ \right| \gg kT. \qquad (9)$$

The density of biological systems has the order of 10^3 kg/m^3. It is the same with the density of water. If the departments have not very differing dimensions and approach one another, then *l* has the same order with their radiuses and $l = r_1 + r_2$. At the room temperature condition (9) can be rewritten as:

$$\frac{4\pi lg(r_1^3(\rho_1 - \rho_w) - r_2^3(\rho_2 - \rho_w))}{3 \cdot 10^{-21}} \gg 1, \qquad (10)$$

where ρ_1, ρ_2, ρ_w are correspondingly densities of the departments 1, 2 and of water; r_1 and r_2 are correspondingly radiuses of the departments. According to (10): $l \sim 10^{-6}$ m or bigger. That is the dimensions of biological cells or their big organelles.

Anisotropy of friction coefficients

Let us elucidate the difference $(\bar{h}_1 - \bar{h}_2)$ in formula (4). According to Stocks' formula, friction coefficient of a spherical particle equals $h = 6\pi\eta r$, where *r* is the particle radius; η is the medium viscosity. In the case, when the particle consists of two rigidly bounded spherical departments of different radiuses, the friction coefficient of the particle equals

$$h = 6\pi\eta(\varepsilon_{12} r_1 + \varepsilon_{21} r_2), \qquad (11)$$

where ε_{12} and ε_{21} are coefficients of the influence of the moving departments on neighboring local medium. $0 < \varepsilon_{12}$ (or ε_{21}) ≤ 1. ε_{12} and ε_{21} depend on the departments radiuses (r_1 and r_2) and on the orientation toward the movement direction (α): $\varepsilon_{12} = \varepsilon_{12}(r_1;\, r_2;\, \alpha)$; $\varepsilon_{21} = \varepsilon_{21}(r_1;\, r_2;\, \alpha)$. The function $\varepsilon_{12}(r_1;\, r_2;\, \alpha)$ increases when r_1 increases or r_2 decreases. $\varepsilon_{12} = 1$ when department 2 moves just behind department 1 ($\alpha = 0$). ε_{12} has its minimal value when $\alpha = 180°$ (it means that the department 1 moves just behind department 2). The function $\varepsilon_{21}(r_1;\, r_2;\, \alpha)$ increases when r_2 increases or r_1 decreases. $\varepsilon_{21} = 1$ when department 1 moves just behind department 2 ($\alpha = 180°$). ε_{21} has its minimal value when $\alpha = 0°$ (it means that the department 2 moves just behind department 1).

Under the conditions (9) the difference $(\bar{h}_1 - \bar{h}_2)$ in formula (4) equals the difference between the friction coefficients of the particle moving with the department 1 in front and back:

$$(\bar{h}_1 - \bar{h}_2) = 6\pi\eta(r_1 + r_2\varepsilon_{21} - r_1\varepsilon_{12} - r_2). \qquad (12)$$

Biological applying

1. Let us consider big amyloplasts which serve as gravity receptors in gravisensitive plant cells, for example germinating moss spores [4]. The amyloplasts are able to interact with less thick vacuoles [5] creating inhomogeneous non spherical couples similar with the particles considered above. They can not penetrate through cell wall. Thus for them free volume is limited. Diameter of the cells equals approximately 6 micrometers and diameter of the organelles is equivalent to 1 micrometer. Under these conditions at the room temperature χ in formula (7) according to (12) is within $10^{-1} \leq \chi < 1$. Thus distribution of amyloplasts in germinating moss spores is uncertain. It can be confirmed by our visual observation of the amyloplasts distribution within germinating *Funaria hygrometrica* spores. Considerable percentage of the spores (approximately 9%) had all amyloplasts shifted upwards [4].

2. Let us consider the movement of a non spherical segment of polypeptide chains or a ligand molecule strongly tided with a protein. In that case we can neglect the influence of gravity. For the sake of simplicity let in formulas (1), (2), (3) $F_y = F_z = 0$ if $0{,}5d < y < b$; $0{,}5d < z < b$; where $b - 0{,}5d$ is protein molecule dimension. Let F_x as intramolecular interaction potential forth is able to rigidly orient the particle alone X-axis. It is confirmed by numeral investigations [6, 7]. V_{par}/V_{whole} of such a system has the order of 1 and therefore uncertainty of (7) can be considerable. It can be approved by the showing of two different stable conformers of complexes of protein apomyoglobin molecules with fluorescent dye bianthryl, which can easy transform one to another. The relation of their concentrations under the same macroscopic parameters was stable and depended on the beginning condition of the complexes initiation [8].

Conclusions

1. If the whole free volume is not very big comparatively to the volume of a non-symmetrical particle orientated by potential field, then spatial distribution of the particle is uncertain. It is a consequence of anisotropy of dissipation of kinetic energy of such a particle.

2. Such an uncertainty is present in distribution of cell organelles of some organisms and also in distribution of segments of polypeptide chains of some proteins.

REFERENCES

1. Pundyak O.I. Estimation of uncertainty of distribution of distances between the particles determined by dissipation of their mechanical energy in viscous medium // Uzhhorod University Scientific Herald. Series Physics – 2001. – Vol. 10. – P. 225 – 228.
2. Pundyak O.I. Int. Conf. Problems of theoretical physics, Electron book of abstracts (L'viv, 2012).

3. Klimontovich Ju.L. Statistical physics, Moscow: Nauka, 1982. – P. 305.
4. Pundyak O.I., Demkiv O.T. Investigation of gravidependent distribution of plastids and vacuoles in germinating moss spores of *Funaria hygrometrica* // Shevchenko Scientific Society Herald. Series Ecology – 2008. – Vol. 23. – P. 156 – 162.
5. Haupt W., Feinleib M. E. Encyclopedia of Plant Physiology, Berlin: Springer-Verlag, 1979. – P. 702.
6. Veitch N.C. Horseradish peroxidase // Advances in Inorganic Chemistry – 2000. – Vol. 51. – P. 107 – 162.
7. Nozue K., Kanegae T. A phytochrome from the fern *Adiantum* with features of the putative photoreceptor NPH1 // Proc. Natl. Acad. Sci. USA – 1998. – Vol. 95. – P. 15826–15830.
8. Pundyak O.I. Conf. 40-th Anniversary of Physics Departmet of Ivan Franko State University, Book of Abstracts (L'viv, 1993), P. 74.

Стаття надійшла до редакції 08.05.2013

О.І. Пундяк
Львівський кооперативний коледж економіки та права,
вул. Клепарівська, 11, 79000, Львів

НЕВИЗНАЧЕНІСТЬ ПРОСТОРОВОГО РОЗПОДІЛУ НЕОДНОРІДНИХ ЧАСТИНОК В ОБМЕЖЕНОМУ ОБ'ЄМІ

Розглянуто рух неоднорідної несферичної частинки у в’язкому середовищі під впливом потенційного поля в обмеженому об’ємі. Просторовий розподіл такої частинки у випадку, коли вільний об’єм малий, є невизначений. Така невизначеність можлива на клітинному рівні щодо розподілу субклітинних структур та на рівні макромолекул щодо розподілу окремих поліпептидних сегментів чи адсорбованих на них молекул.

Ключові слова: потенційне поле, просторовий розподіл, в’язкість, коефіцієнт тертя, клітинні органели, білкові макромолекули, сегменти поліпептидного ланцюга.

О.И. Пундяк
Львовский кооперативный коледж экономики и права
ул. Клепаровская, 11, 79000, Львов

НЕОПРЕДЕЛЕННОСТЬ ПРОСТРАНСТВЕННОГО РАСПРЕДЕЛЕНИЯ НЕОДНОРОДНЫХ ЧАСТИЦ В ОГРАНИЧЕННОМ ОБЪЕМЕ

Рассмотрено движение неоднородной несимметрической частицы в вязкой среде под влиянием потенциального поля. Пространственное распределение такой частицы в случае, когда свободный объем мал, будет неопределенным. Эта неопределенность может быть присуща на клеточном уровне распределению органелл, а также на макромолекулярном уровне - распределению полипептидных сегментов или адсорбированных на них молекул.

Ключевые слова: потенциальное поле, пространственное распределение, вязкость, коэффициент трения, клеточные органеллы, белковые макромолекулы, сегменты полипептидной цепи.