MULTILEVEL COLLECTIVE SELF-ORGANIZATION OF BIOLOGICAL PARTICLES

I.A. Denisov*, *A.A. Zimin*, *P.I. Belobrov

MOLPIT, Siberian Federal University, Institute of Fundamental Biology and Biotechnology, Institute of Biophysics SB RAS: Svobodny79, Krasnoyarsk, 660041, Russia

E-mail: d.ivan.krsk@gmail.com; reyenka@gmail.com; peter.belobrov@gmail.com

In order to understand hierarchical organization of complex biomolecules in condensed phases new approaches able to treat collective effects arising from many-body interactions in cells have to be developed, e.g. blot and droplet terms are introduced in [1] to consider bioparticle interactions. We present three-level collective self-organization model based on introduction of five distinct interaction potentials. This model is realized in the "Multilevel organization model" GPL-licensed application [2]. The most essential difference between the proposed model and traditional hybrid potentials lies into treatment of pairwise potentials between organization levels, which includes interaction of given bioparticle with more complex "higher" and more primitive "lower" levels of bioparticles [3].

Our approach could be formulated in Hamilton formalism if we introduce the following Hamiltonian using simplified multi-index (bold-emphasized) notation:

$$H = \sum p^2/2m + \sum_{\mathbf{L}} U^{\mathbf{L}} + \sum_{\mathbf{L+1\backslash D}} U^{\mathbf{L+1}} + \sum_{\mathbf{L-1\backslash P}} U^{\mathbf{L-1}} + \sum_{\mathbf{P}} U^{\mathbf{P}} + \sum_{\mathbf{D}} U^{\mathbf{D}}, \qquad (1)$$

where **p** is the quasimomentum, U is the interaction potential between current level particles and: $U^{\mathbf{L}}$ — themselves, $U^{\mathbf{L+1}}$ — particles at higher level, $U^{\mathbf{L-1}}$ — particles at lower level, $U^{\mathbf{P}}$ — "parent" particles at lower level, $U^{\mathbf{D}}$ — "child" particles at higher level; **P** — denotes group of "parents", **D** — of "children", **L** — group of particles at current level, **L–1** — group of particles at lower level, **L+1** — group of particles at higher level.

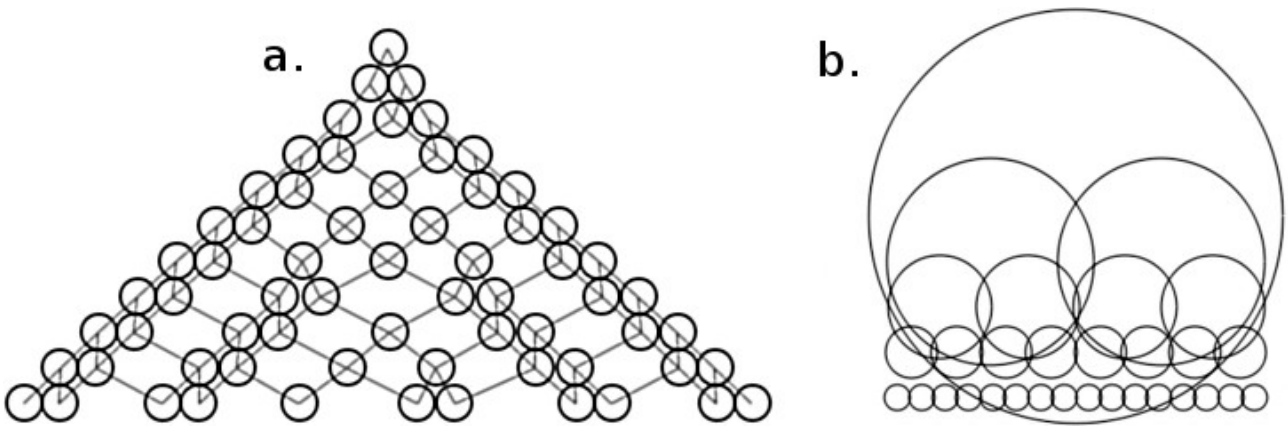

Fig. 1. Multilevel self-organized systems with (**a**) repulsion from upper level L+1, (**b**) recursive inheritance of radius with radius increment.

Various combinations of these five potentials give explosive number of collective dynamics and lead to different patterns of self-organization in a multilevel space (Figs. 1 and 2). Introduction of higher-level particles allow taking into account new properties arising from collective interactions.

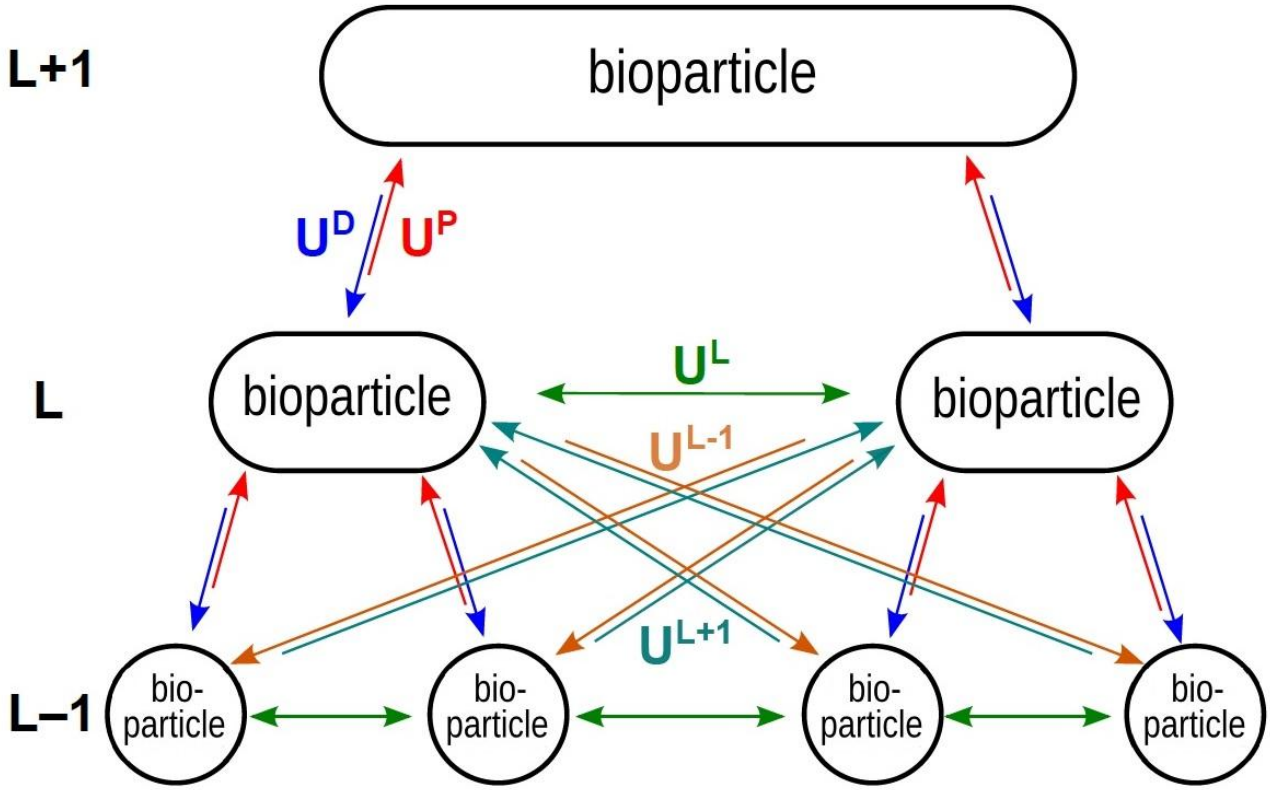

Fig. 2. Three-level system and five potentials for the description multilevel collective self-organization of biological particles. Defined potentials correspond to the formula (1).

The proposed model is ready to handle physical description of multi-level organization of bioparticles, e.g. organization of histones in chromatin, where biologists have already introduced multi-index-like notations (H3.3, H2A.Bbd) for variable histone forms [4].

The research was supported by the Program of the RF Government "Measures to attract leading scientists to Russian educational institutions" (grant no. 11.G34.31.058) and government contract no. 14.A18.21.1911.

1. I.A. Denisov, P.I. Belobrov. Collective excitation at nanodiamond-protein interaction // Nanobiophysics, Kiev (2011), Abstract book, p.46 & 60. URL: http://molpit.com/?page=46

2. I.A. Denisov. Multilevel organization model, URL: http://molpit.com/?page=33

3. J.F.R. Bachega et al. GTKDynamo: A PyMOL plug-in for QC/MM hybrid potential simulations // *J Comp Chem*., Online publ. 19 JUN 2013 DOI: 10.1002/jcc.23346

4. S.V. Razin, A.A. Bystritskiy Chromatin packed genome. – Moscow, BINOM, 2013 (in Russian).