TRAJECTORIES OF THE DNA KINKS IN THE SEQUENCES CONTAINING CDS REGIONS

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Motivation and Aim: In our previous works [1-2] to model the DNA kinks, we used a simple model based on the sine-Gordon equation with parameters that were averaged over all length of the gene sequence. However, this approach does not allow us to take into account the effect of the internal structure of the DNA sequence, and, in particular, the presence of the CDS regions, on the DNA kinks dynamics. In this paper, we just consider this problem and solve it for the gene encoding interferon alpha 17, the sequence of which consists of three regions: the coding (CDS) region (50..619) and the two regions (1..49 and 620..980) with unknown functional significance.

Methods and Algorithms: To solve the problem, we use several methods: the method of McLaughlin and Scott, the average field approximation and the block method where the parameters of the model equation are averaged separately for each of the three regions. To analyze the DNA kinks dynamics, we use the physical approach which includes the calculation of the energy profile of the sequence and the construction of the trajectory of the movement of the DNA kink in the potential with this profile.

Results: We have obtained the energy profile of the sequence of the gene coding interferon-alpha 17. It was shown that the CDS region corresponds to the region of the energy barrier. The minimum value of the kink initial velocity required to overcome the barrier was estimated. The trajectories with different initial kink velocities were constructed. The trajectories were calculated both with and without dissipative effects. It was shown that with the increasing of the initial kink velocity the trajectories became more independent on the inhomogeneity of the sequence. We suggest that the proposed approach can be applied to analyze the movement of transcription bubbles through the CDS regions of the DNA sequences.

References:
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2. L.V. Yakushevich, L.A. Krasnobaeva (2016) Forced oscillations of DNA bases, Biophysics, **61:** № 2, 286-296.