Numerical modeling of denaturation of non-uniform DNA

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DNA molecules are considered as structural elements of promising electronic devices [1]. Electronic nanobiochips have several advantages over modern silicon chips. They are miniature, fast and accurate. It is also possible to use DNA molecules in storage and logic devices [1, 2].
The numerical realization of a helical mechanical model of a DNA molecule by the Runge-Kutta method of the fourth order of accuracy with time step having automatically selected value is considered. The model is a further development of the well-known spiral DNA model proposed by M. Barbi and co-authors [3].
The results of calculations for propagation of various types of perturbations along the non-uniform DNA molecule are given. Molecular dynamics simulations for DNA denaturation was carried out on the basis of the proposed mechanical model. Agreement of the numerical denaturation temperature with the experimental values was obtained.

[1] Lakhno V D and Vinnikov A V 2018 *Keldysh Institute Preprints* 1–26
[2] Goldhaber-Gordon D, Montemerlo M, Love J, Opiteck G and Ellenbogen J 1997 *Proceedings of the IEEE* **85** 521–540
[3] Barbi M, Cocco S and Peyrard M 1999 *Physics Letters A* **253** 358–369