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Conformational perturbation in the DNA molecule of the Muto model

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Modeling of conformational excitations in a DNA molecule makes it possible to advance the study of fundamental patterns and mechanisms of biological functioning of living systems at the cellular level. Conformational excitations in the DNA molecule are involved in such important processes as transcription, translation, denaturation and replication.
In particular, the course of the replication process is accompanied by a rupture of the hydrogen bond.
Such gaps are called an open state. W. Englander in his model connects the concept of an open state with such a mathematical object as a soliton.
In the framework of this work, the physical model of the DNA molecule
formulated by V. Muto, which is formed by the Todd potential and the Lennard-Jones potential, will be investigated. Although this model is two-dimensional, it retains the main features of dynamics
inherent in volumetric models of conformational excitations of the DNA molecule. The study of a two-dimensional model is significantly simplified, which opens up the possibility of using new mathematical methods for its analysis.
The purpose of the study is to find an open state, the mathematical image of which is - soliton. The methods of wavelet analysis will be used as the tools used.

The authors set the following tasks:
1. Implementation of the dynamics of the Todd-Lennard-Jones model.
2. The use of discrete wavelet transform (DWT) for noise filtering.
3. The use of continuous wavelet transform (CWT) to identify solitons.
4. Estimation of the propagation velocity of the open state.
5. Evaluation of algorithmic complexity.
The presence/absence of solitons in the dynamics of this model will allow us to assess the limits of its applicability in further research.

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