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A non homogeneous composite model for propagation of twist solitons in real DNA chains

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Abstract

We report our numerical investigations concerning the propagation of solitons in a real DNA chain (the Human Adenovirus C) using a realistic model of DNA torsional dynamics that takes fully into account the inhomogeneities in the nitrogen bases pair necessary for the codification of the genetic information. We find that twist solitons of diameter about 50 base pairs (*bps*) propagate in the DNA chain for distances about $2-10$ times their diameters before stopping owing to dissipative effects. Our results show that twist solitons may play a crucial role in the replication process of real DNA chains. On a more general level our results demonstrate that solitonic propagations take also place in highly inhomogeneous media. This is possible if the geometric and dynamical properties of the medium are such that the soliton does not develop high sensibility to the presence of inhomogeneities. The latter just play the role of a dissipative effect on the soliton motion.

Solitonic excitations are very common in nonlinear dynamical systems. In particular it has been proposed that they may play an important role also for functional process of the DNA double chain such as transcription and denaturation. Since the original proposal by Englander, several simplified models for dynamics of the DNA chain have been proposed that should take into account the (nonlinear) dynamics of the radial and/or torsional relevant degrees of freedom of the chain. Most of these models allow for solitonic solution describing stretching and/or twisting exitation of the DNA chain.

Some examples of solitons propagation in inhomogeneous media have been subject of investigation both in the framework of non linear DNA dynamics and generic solitonic propagation. However, these investigation either refer to homogeneous chains, or localized inhomogeneities - in the form of e.g discontinuities, potential barriers , delta potentials etc. - or even the inhomogeneities are parametrized by particular ad hoc rules.

Our starting point is the inhomogeneous version of the composite model for DNA torsional dynamics, described in detail in Ref. [1, 2, 3]. Our composite model for DNA is a double chain of some large but finite number N of coupled double pendulums. It is a natural generalization of the well known model by

Yakushevich where, at every node of each chain, the whole group base-sugar-phosphate is represented by a single disc centered at the chain's backbone axis.

In our model we split the group in two components represented in concrete by two discs: one again centered about the backbone axis and representing the sugar-phosphate group and the other, representing the nitrogen base, which can rotate about a fixed point on the sugar. Note that the genetic information encoded in DNA's molecule is entirely contained in the sequence of bases while the sugar-phosphate backbone is homogeneous. This separation of degrees of freedom allows us to treat separately the homogeneous and inhomogeneous components of the chain.

Our numerical investigation about the propagation of twist solitons in a real DNA chain show that solitons of size of about 50 bps can propagate in the DNA chain till 10 times the soliton size [4]. Considering the fact that we use a very simplified mechanical model of DNA, which does not take into account effects that may enhance the soliton performance (such as the presence of the DNA polymerase), our result give a strong indication that twist solitons may indeed explain replication of real DNA chains.

Moreover ur numerical investigation has shown that soliton propagation is also possible in highly inhomogeneous media. This possibility can be traced back to two different (and independent) features of the mechanical system under consideration. The first is the presence in the molecular chain of both a homogeneous part that supports the topological soliton (the sugar-phosphate ring) and an inhomogeneous part (the bases) that encodes the genetic information and acts as dissipative. The second is the feature of the Morse potential that localizes the interaction of the inhomogeneous part of the chain essentially near the potential minimum. Far away from this minimum the interaction becomes very weak. Again, this weakens the soliton sensibility to inhomogeneities in the chain.

References

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