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A new nonlinear DNA model

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Abstract

The torsional dynamics of DNA can be described by nonlinear models, predicting soliton open states related to replication and transcription processes. In particular, the Yakushevich model yields soliton solutions with appropriate topological properties to describe those processes. In the present work, we developed a model that combines the dynamical aspects of both Yakushevich and Yomosa models, treating the stacking interaction between adjacent bases in a nonlinear way. By doing so, both transversal and longitudinal interactions are treated on the same foot. Stable soliton solutions, energies and its dynamics were obtained.

Key words: DNA; non linear dynamics; replication; soliton; transcription.

Un nuevo modelo no lineal del ADN

Resumen

La dinámica torsional del ADN puede ser descrita por modelos no lineales, prediciendo la existencia de estados abiertos relacionados con los procesos de replicación y transcripción. En particular, el modelo de Yakushevich proporciona soluciones solitónicas con las propiedades topológicas apropiadas para describir esos procesos. En el presente trabajo se ha desarrollado un modelo que combina los aspectos dinámicos tanto del modelo de Yakushevich como el de Yomosa, tratando la interacción de empaquetamiento entre las bases nucleícas adyacentes en una forma no lineal. De esta manera, tanto las interacciones transversales como longitudinales a través de la doble hélice son tratadas igualmente. Como resultado se obtienen soluciones solitónicas, con su energía y dinámica correspondiente.

Palabras clave: ADN; dinámica no lineal; replicación; solitón; transcripción.

1. Introducción

Nonlinear torsional models have been proposed to describe the dynamics of DNA (1, 2). In such models some of the interactions between the base pairs are taken in a nonlinear way while in others linearly. In the present work, all the interactions are treated on equal foot without discarding any no linearity intrinsically present in the interactions. Two types of interactions are considered: a transversal interaction due to the coupling by hydrogen bonds between adjacent (and complementary) bases and a longitudinal interaction between consecutive bases along the chain, also called the stacking in-

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teraction, and finally, a longitudinal interaction between elements of the backbone of the DNA strand. The helical structure of DNA is not considered in this model and it is not relevant to the soliton nature of the solutions obtained (1, 2).

2. The Model

The stacking and backbone interactions can be written for a single strand as:

$$H_S = S\left[1-\cos\left(\varphi_n - \varphi_{n-1}\right)\right] \qquad [1]$$

which leads to a differential equation term of the type:

$$\sin\left(\varphi_n - \varphi_{n-1}\right) - \sin\left(\varphi_{n+1} - \varphi_n\right) \qquad [2]$$

By performing a Taylor expansion, this term can be written as:

$$-2S\,\sin\left(\frac{1}{2}\left(\frac{\partial^2\varphi}{\partial z^2}\right)_n a^2\right)\cos\left(\left(\frac{\partial\varphi}{\partial z}\right)_n a\right) \qquad [3]$$

The term due to the transversal interaction is taken as in the Yakushevich (2) model.

The Equations

The combination of the two interactions yield the following equations:

$$I_i\varphi_{itt} = -2S\sin\left(\frac{1}{2}a^2\varphi_{izz}\right)\cos\left(a\varphi_{iz}\right)$$
$$-k\frac{\Delta l}{l}\left[\left(2R^2 + Rl_0\right)\sin\varphi_i - R^2\sin\left(\varphi_i + \varphi_j\right)\right] \qquad [4]$$

with:

$$\frac{\Delta l}{l} = 1 - l_0\left[\left(2R + l_0 - R\cos\varphi_1 - R\cos\varphi_2\right)^2\right.$$
$$\left.+\left(R\sin\varphi_1 - R\sin\varphi_2\right)^2\right]^{-\frac{1}{2}} \qquad [5]$$

The stable soliton solutions are very much like those of Yakushevich model (3). Adding a dissipative term to the differential equations introduces a stabilization to the soliton solution, eliminating some nonlinear (but not solitary) waves. In Figure 1 the effect of the dissipative term is evident. Soliton states can be represented as curves connecting critical points in solution space, as shown in the top of Figure 2.

Long range interactions

It has been demonstrated (3) that the Yakushevich model exhibits long range interactions between the solitons, due to the particular structure of the nonlinear term describing the transversal interaction. To check for long range behavior, a step function is supposed as an initial condition and the spreading of it is measured as a function of time. In the case of short range behavior the spreading stabilizes after some time. For the system treated here, the spreading continues endlessly which accounts for a long range behavior. This results are shown in Figure 3. Collision experiments between kink and antikink solutions yield information about the range of the interaction and the internal structure of the solitons. Some of the results are shown in Figure 4.

Chaos

If these equations are perturbed by periodic forces and dissipation, the dynamical behavior will be in some sense similar to that of the cubic Duffing equation, which is well known to have a chaotic attractor. Phase space maps for different values of the dissipation are shown in Figure 5.

Conclusions

The proposed model, which is completely non linear, have soliton solutions of the same type and stability properties as those

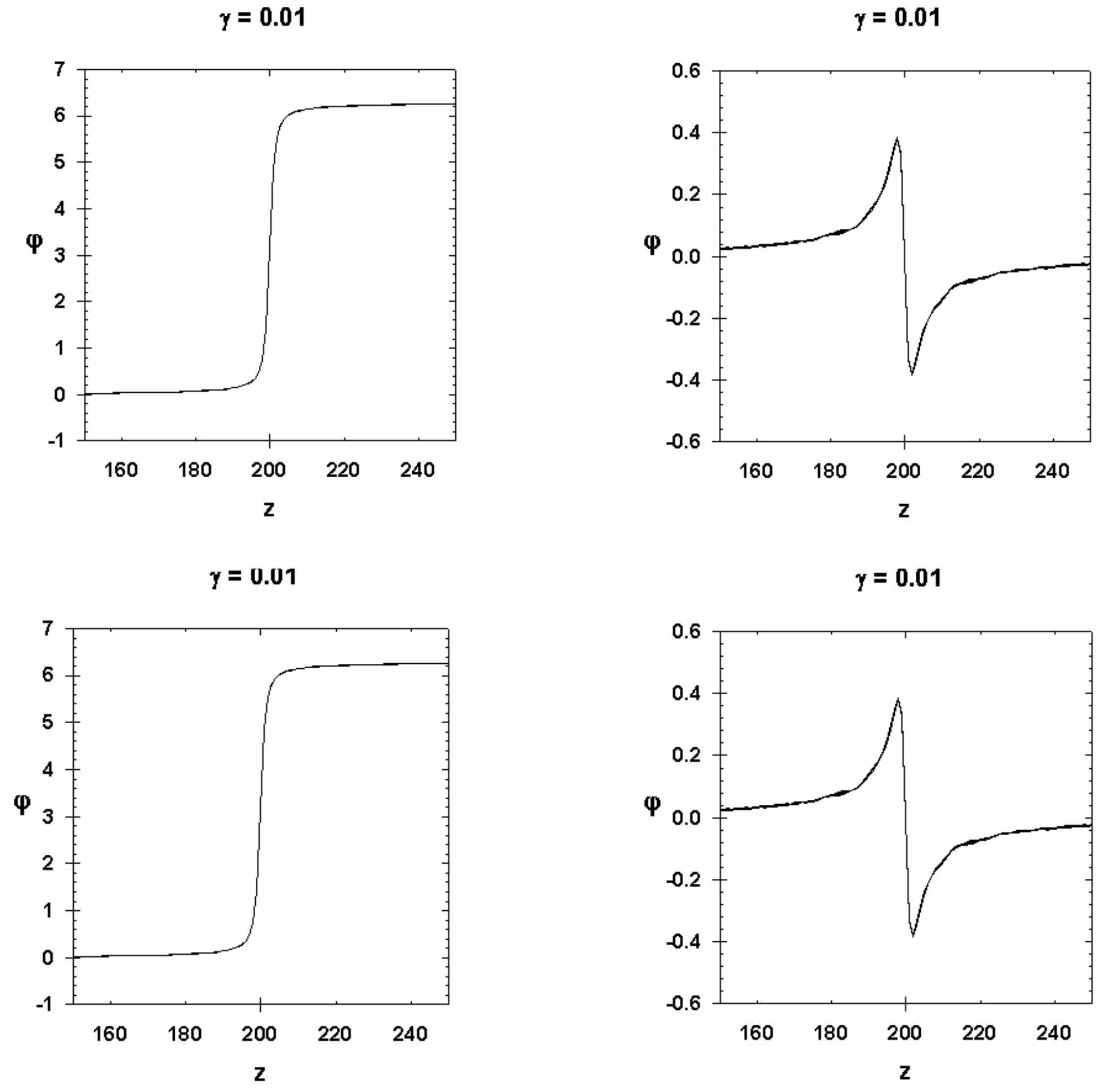

Figura 1. Soliton solutions for different magnitudes of the dissipative term. On top, low dissipation causes the solution to exhibit some superposition of soliton and nonlinear waves. Below, the increment of the dissipative term stabilizes the solution to a pure soliton, eliminating some nonlinear (but not solitary) waves.

of the Yakushevich model. This means that the relevant term that accounts for the general properties of the solutions is the transversal one, i.e., the interaction between the nucleotide bases, which in turn causes the long range and chaotic behaviors, as previously stated[3]. The non linearity in the stacking interaction contributes to the generation of non linear waves, possibly introducing some modifications of the interaction between solitons, the way they propagate and their long range properties. For non homogeneous DNA chains, not discussed in this work, the non linear term could be of relevance in describing some issues related to transcription and replication processes.

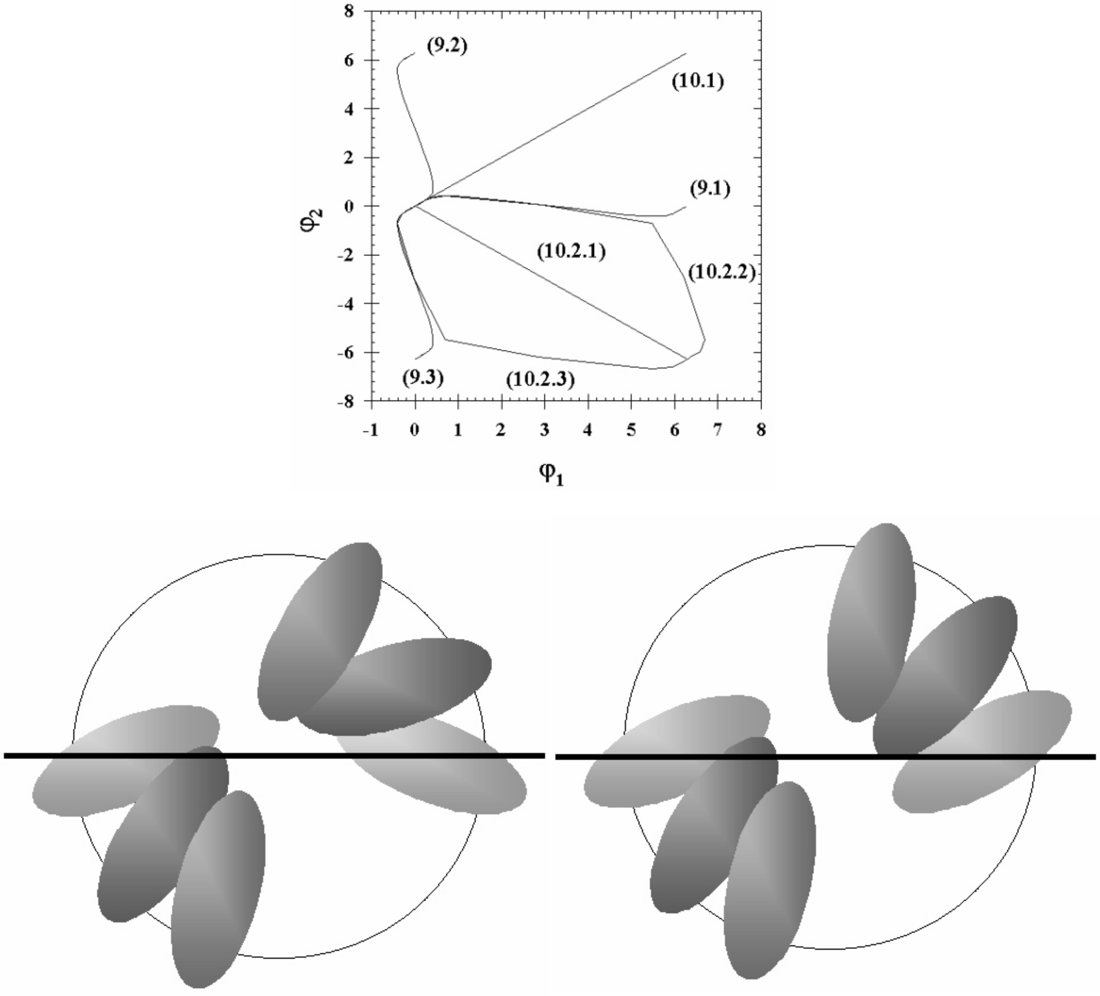

Figura 2. On top, curves representing soliton solutions. The states shown in Figure 1 correspond to either curves (9.1) and (9.2), meanwhile curve (9.3) corresponds to the antisoliton to curve (9.2). Solutions (10.1), (10.2.1), (10.2.2) and (10.2.3) are all kink type, and only (10.2.2) and (10.2.3) are stable. Solution (10.1) is called symmetric and is qualitatively represented bottom left. All other solutions are called asymmetric and represented bottom right.

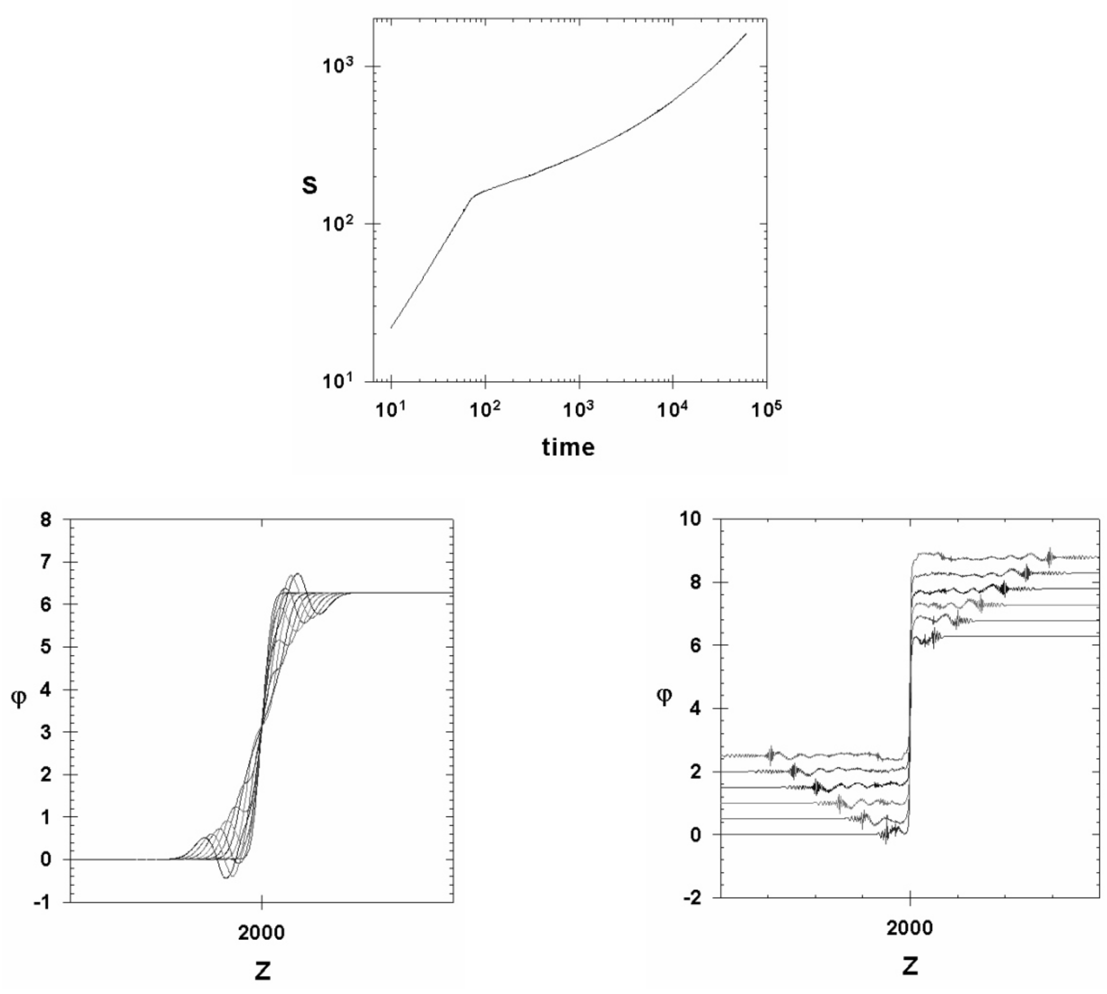

Figura 3. On top, spread of a step function as it evolves in time. Notice that there are clearly two regimes. On the left below it is represented the general behavior for the regime at short times as the solution evolves from the initial step function to a solution of the kink type and nonlinear oscillations appear. On the right it is shown the regime at larger times. Notice how nonlinear oscillations propagate at both sides of the kink soliton.

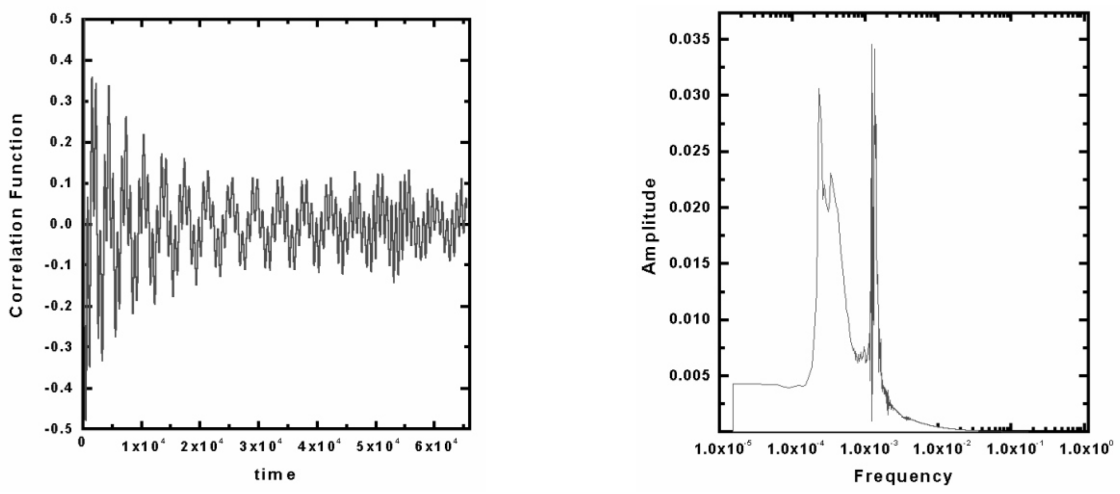

Figura 4. On top, it is shown the time correlation function for an initial separation of 2 base pairs. Bottom, Fourier transform of the correlation function showing well defined peaks corresponding to some of the "products" of the collision. At high frequencies the behavior is 1/f.

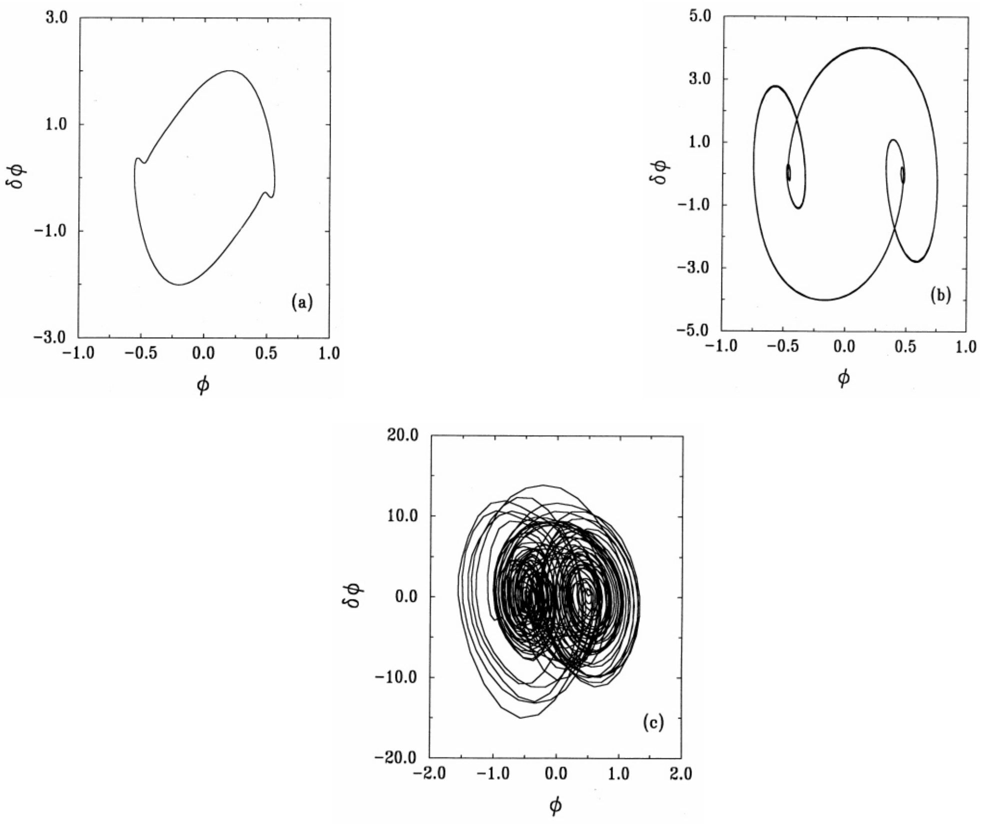

Figura 5. Route to choas. a) = 1, b) γ= 0.2 and c) γ= 0.05

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