Long-range interactions and wave patterns in a DNA model

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Abstract. We propose a spin-like model of DNA nonlinear dynamics with long-range interactions between adjacent base pairs. We show that the model equation is a modified sine-Gordon equation. We perform the linear stability analysis of a plane wave, which predicts high-amplitude and extended oscillating waves for high values of the long-range parameter. This is confirmed numerically and biological implications of the obtained patterns are suggested.

1 Introduction

The complexity and role of DNA make it the most important molecule in nature. Describing its dynamics therefore remains a fascinating task for modern physicists and biophysicists alike, because it is nowadays accepted that DNA undergoes dynamical features that are not yet fully unmasked. There have been many attempts to describe that complicated dynamics using appropriate models. The first nonlinear model was suggested by Englander et al. [1]. Later, Yomosa proposed a further theory based on a dynamic plane base-rotor model [2,3]. Along the same line, Takeno and Homma [4,5] developed that idea and proposed a general spin-like model, and showed its efficiency in describing open states in DNA. Further modifications of the same model have recently been introduced by Daniel and Vasumathi [6] and Tabi et al. [7] who showed the importance of helicity in DNA spin-like models. In this paper, we further modify the same model and point out the importance of long-range dispersive interactions of the Kac-Backer type [8,9] in describing hydrogen bonds oscillations. The importance of long-range interactions is due to the presence of phosphate groups along the strands [10]. Those phosphate groups are shielded by the counter-ions supplied by the medium. The long-range interaction therefore allows to take into account the screening of the interactions or an indirect coupling between base pairs (e.g. via water filaments). This has been justified in the paper of Shafraevskaya et al. [11] who studied experimentally the diffusion of charge in DNA and demonstrated the importance of long-range excitation migration in DNA. Also experimentally, the evidence for long-range attractive hydration forces was studied by Rau and Parsegian [12]. Besides, there are the results of some recent measurements indicating that moderate long-range repulsive interactions are suitable to describe the long-range communication in DNA [13]. This qualitative discrepancy is also shared by theoretical findings so that the real long-range force to be adopted for DNA dynamics remains unclear. Along the same line, Rau and Parsegian [12] also emphasized that many other forces could be responsible for long-range interactions in DNA, a conclusion which motivated the present work. In the rest of this paper we perform the linear stability analysis of a planar wave, the solution of a modified sine-Gordon (sG) equation, and predict the appearance of highly localized soliton-like structures in the presence of long-range interactions. Numerical simulations further confirm our analytical predictions and bring out the presence of extended breather-like structures.

2 Model

In this work, we consider the so-called B-form of the DNA molecule as presented in fig. 1(a) (S and S’ represent the two strands of the molecule). Since in this model we intend to introduce the DNA spin-like model with long-range interactions, we can assimilate that model to the Heisenberg
one by writing the Hamiltonian of the anisotropic model as

$$H_0 = \sum_n \left( -\sum_{j \neq n} J g_{nj} (S_n \cdot S_j) + A (S_n^z)^2 \right), \quad (1)$$

where the summation is over the $N$ base pairs of the DNA lattice. In the above equation, $S_n = (S_n^x, S_n^y, S_n^z)$ represents the spin vector at the $n$-th base pair, and the terms proportional to $J g_{nj}$ and $A$ stand for the ferromagnetic spin-spin exchange long-range interaction and uniaxial magnetocrystalline anisotropy with the easy axis along the $z$-axis. The long-range interaction constant $g_{nj}$ is given by [8,9]

$$g_{nj} = \frac{f(1-\nu)}{\nu} n^{-|n-j|}, \quad \text{with} \quad \sum_n g_{nj} = 2f, \quad (2)$$

which is known as the Kac-Baker potential, where $|n-j|$ measures the absolute distance between the two sites $n$ and $j$ and the parameters $f$ and $\nu$ are, respectively, the range of the interactions, with $0 \leq \nu < 1$, and the elastic constant of strands. For a given $\nu$, $g_{nj}$ decreases when $j$ increases. Experimentally, one can relate the parameter $\nu$ to the number of neighboring interactions. Note that the limit $\nu \to 0$ reduces to the nearest-neighbor problem and the limit $\nu \to 1$ (possible only for $N \to \infty$) defines the infinite-range problem [8,9]. The above Hamiltonian is considered for one strand, therefore similar considerations can be made for the second strand $S'$ by replacing $S_n$ by $S'_n$. The whole Hamiltonian for the DNA molecule can then be written, after reformulating $S_n = (S_n^x, S_n^y, S_n^z) = (\sin \theta_n \cos \phi_n, \sin \theta_n \sin \phi_n, \cos \theta_n)$ and $S'_n = (S'_n^x, S'_n^y, S'_n^z) = (\sin \theta'_n \cos \phi'_n, \sin \theta'_n \sin \phi'_n, \cos \theta'_n)$, as

$$H_0 = \sum_n \left[ -\sum_{j \neq n} J g_{nj} \left( \sin \theta_n \sin \theta_j (\cos \phi_n - \phi_j) ight. ight.$$

$$+ \sin \theta'_n \sin \theta'_j (\cos \phi'_n - \phi'_j) + \cos \theta_n \cos \theta_j 
+ \cos \theta'_n \cos \theta'_j + A \cos^2 \theta_n + A \cos^2 \theta'_n \right]. \quad (3)$$

In figs. 1(b) and (c), we show the horizontal projection of the $n$-th base pair in the $xy$ and $xz$ planes, respectively. In these figures, $Q_n$ and $Q'_n$ denote the tips of the $n$-th bases belonging to the strands $S$ and $S'$, $P_n$ and $P'_n$ represent the points where the bases in the $n$-th base pair are attached to the strands $S$ and $S'$, respectively.

It has been shown that interstrand base-base interactions or hydrogen bonding energy deeply depend on the distance between the two complementary bases [4,5]. Thus, from figs. 1(b), (c), the square of the distance between the edges of the arrows $(Q_nQ'_n)^2$ is written as [4,5,7]

$$(Q_nQ'_n)^2 = 2 + 4r^2 + (z_n - z'_n)^2 + 2(z_n - z'_n) \times (\cos \theta_n - \cos \theta'_n) - 4r \sin \theta_n \cos \phi_n + \sin \theta'_n \cos \phi'_n + \sin \phi_n \sin \phi'_n)$$

$$- \cos \theta_n \cos \theta'_n, \quad (4)$$

where $r$ is the radius of the circle. The corresponding base-base distance can be obtained in terms of $S_n$ and $S'_n$ as follows:

$$(Q_nQ'_n)^2 = 2 + 4r^2 + 2 \left( S_n^x S'_n^x + S_n^y S'_n^y - S_n^z S'_n^z \right)$$

$$- 4r \left( S_n^x + S'_n^x \right), \quad (5)$$

and the hydrogen bond interaction can be described by the potential

$$H_1 = \sum_n \eta \left( \sin \theta_n \sin \theta'_n (\cos \phi_n - \phi'_n) - \cos \theta_n \cos \theta'_n \right), \quad (6)$$

where $\eta$ represents a measure of the interstrand interactions. In eq. (5), the longitudinal compression along the direction of the helical axis has been neglected and we have assumed $z_n = z'_n$ [4,5]. The total Hamiltonian is finally given in terms of the variables $(\theta_n, \phi_n)$ and $(\theta'_n, \phi'_n)$ by

$$H = \sum_n \left[ -\sum_{j \neq n} J g_{nj} \left( \sin \theta_n \sin \theta_j (\cos \phi_n - \phi_j) ight. ight.$$

$$+ \sin \theta'_n \sin \theta'_j (\cos \phi'_n - \phi'_j) + \cos \theta_n \cos \theta_j 
+ \cos \theta'_n \cos \theta'_j + \eta \left( \sin \theta_n \sin \theta'_n (\cos \phi_n - \phi'_n) 
- \cos \theta_n \cos \theta'_n \right) + A \cos^2 \theta_n + A \cos^2 \theta'_n \right]. \quad (7)$$

The equations of motion for the corresponding quasi-spin model in the limit $A \gg J, \eta$ [4,5] lead to the system $\dot{\phi}_n = 2A \cos \theta_n$ and $\dot{\phi}'_n = 2A \cos \theta'_n$, where the overdot represents the time derivative. With such considerations,