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Exact traveling wave solutions in the coupled plane-base rotator model of DNA

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ABSTRACT

The internal dynamics of the DNA base pairs is studied starting from the generalized coupled plane base-rotator model of DNA, obtained by Yomosa and later improved by Takeno and Homma. We conceive the double-stranded DNA as an anisotropically coupled spin chain simple model. The generalized Hamiltonian expressed in terms of quasi-spin operators is averaged over the generalized coherent states in the Perelomov sense, in order to obtain the classical non-linear evolution equations of this molecular system where the inhomogeneity has not been considered. This approach provides the equations of motion, which could be reduced to a nonlinear Schrödinger equation with a saturable nonlinearity. This non-linear equation, under certain restrictions in the parametric space, supports traveling periodic triangular, bell, bubble and kink like solutions.

1. Introduction

Despite the complex nature of the DNA, its internal dynamics have been studied using theoretical models. Broadly, these models take into account the fundamental structural aspects of DNA and the degrees of freedom most likely to dominate conformational changes. These simplified models are based on longitudinal and transverse motions, bending, stretching and rotations [1–6]. In many cases the theoretical results produced by these models not only give a good understanding of the biological processes studied, but also match experimental data. As an example let us mention the model proposed by Peyrard and Bishop [7,8], in which the main contribution to the double helix melting process is given by the stretching of the hydrogen bonding, leading to the bases opening. Instead of the rotational motion of bases, this model includes two different internal motions, which means that the bases are displaced with respect to their equilibrium positions along the direction of the hydrogen bonding. The potential for the hydrogen bonding is modeled by a Morse potential and the anharmonic coupling due to the stacking between the neighboring bases is added. The same process was studied by Christiansen et al. [9] including the transversal motions, longitudinal motions, and torsional motions. Other non-linear models implemented are: the dynamical mechanisms of transitions between different DNA forms [10], regulation of transcription [11], protein synthesis (insulin production) [12], carcinogenesis [13], among others. The base pairs play a fundamental role, since the genetic information is encoded in them. The rotational motion of the bases contributes more towards the opening of bases. This opening happens in most of the biological processes, such as conformational changes, denaturation, transcription and replication. This opening of bases causes non-linear molecular excitations along the DNA double helix. A model based on the rotational motion of bases was developed by Yomosa (the plane-base rotator model) [14], being a generalization of the Frenkel–Kontrova model [15]. This model takes into account the main agents responsible for keeping the internal structure of this molecule: the hydrogen bond energy, the stacking energy, and the features of the base pairs. These coupled base pairs are allowed to rotate in planes perpendicular to the helical axis. This plane-base rotator model was improved and generalized to a coupled three-dimensional rotators model by Takeno and Homma [16,17]. This has been refined and extended in [18–20].

On the other hand, the generalized coherent states approach has been employed widely in many branches of physics: astrophysics, orbital magnetism of two-dimensional electrons, nuclear physics, mathematical physics, bio-physics, quantum optics, see for example [21–25] just to mention a few. One method for treating such models, in semi-classical fashion, is to choose the trial state based on the symmetry of the analyzed model. Thus, the generalized coherent states approach is commonly used in the case of spin or quasi-spin models.

In this paper, we study the pure dynamics of DNA concerning the existence, among others, of the soliton-like excitations. For the sake of simplicity we confine ourselves to considering the Takeno–Homa model [16,17] whose Hamiltonian is expressed in terms of

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quasi-spin operators. The following section is devoted to briefly explain the plane-base rotator model. Consequently, in the third section we will apply the generalized coherent states to average the generalized Hamiltonian, we shall pass from a quasi-quantum problem to a classical one. From the Hamiltonian we can obtain the classical equations of motion. These equations are treated in the third and the fourth section and reduced to a non-linear Schrödinger equation with saturable non-linearity, that finally shows the appearance of different types of analytical solutions. Finally, in the last section we present some numerical results and several remarks.

2. The mathematical plane-base rotator model

We follow the reasoning made by Takeno and Homma [17]. Three fundamental considerations were employed for studying the structure and dynamics of DNA: (i) the main dynamical contributions can be obtained by paying attention to the bases in the double strands. (ii) The fluctuations of positions are produced by the rotational motion of the bases at the points where these are attached to the strand. (iii) The fluctuation of positions under certain circumstances leads to breaking of the hydrogen bonds, inducing the unzipping of the double strands of DNA.

We consider the conventional B-form of DNA with helical axis along, for say, the z direction. The double strands of DNA are represented by the S and S' ribbons wound around each other, respectively. The base attached to the strand is represented by an arrow, the base attached to its complementary strand is represented by a conjugate arrow. The strands of DNA stay together by hydrogen bonds that occur between complementary nucleotide base pairs. The conformation and stability of the DNA double helix is mainly determined by the stacking energy between adjacent bases or intrastrand energy, the energy of hydrogen bonding between the complementary bases or interstrand energy, among other energies. The interstrand energy is given by the distance between the tips of the *nth* base (Q_n) and its complementary base (Q_n') and it can be written as,

$$L_n^2 = 2 + 4r^2 + 2[S_n^x S_n^{x\prime} + S_n^y S_n^{y\prime} - S_n^z S_n^{z\prime}] - 4r[S_n^x + S_n^{x\prime}] \tag{1}$$

For the nth base in the S and S' strands, respectively. We choose $z_n = z_n'$, z_n and z_n' being the positions of the nth-base in the S strand and in the complementary S' strand with respect to the helical axis, to neglect the longitudinal compression waves along the direction of the helical axis and r is the radius of the circle depicted in Fig. 1. In the equation of the interstrand energy (1) we have used the set of relations between the quasi-spin operators $\vec{S}_n = (S_n^x, S_n^y, S_n^z)$ and $\vec{S}_n' = (S_n'^x, S_n'^y, S_n'^z)$ and the rotational angles θ, φ as usual $S_n^x = \sin\theta_n \cos\varphi_n$, $S_n^y = \sin\theta_n \sin\varphi_n$, $S_n^z = \cos\theta_n$ $S_n'^x = \sin\theta_n' \cos\varphi_n'$, $S_n'^y = \sin\theta_n' \sin\varphi_n'$, $S_n'^z = \cos\theta_n'$

Thus, we conceive the double-stranded DNA as an anisotropically coupled spin chain model, as seen in Fig. 2 where the base–base interaction is restricted to the nearest neighbors interaction, that is, the nth base(spin) interacts with the $(n-1)$th base (spin) and the $(n+1)$th base (spin).

By considering the relevance of inter-strand energy Takeno and Homma proposed the study of the following Hamiltonian:

$$\begin{aligned} H = \sum_n \Big[& -J_n\left(S_{n+1}^x S_n^x + S_{n+1}^y S_n^y\right) - K_n S_{n+1}^z S_n^z \\ & - J_n'\left(S_{n+1}'^x S_n'^x + S_{n+1}'^y S_n'^y\right) - K_n' S_{n+1}'^z S_n'^z + \lambda_n\left(S_n^x S_n'^x + S_n^y S_n'^y\right) \\ & - \mu_n S_n^z S_n'^z - h_n\left(S_n^x + S_n'^x\right) + A_n (S_n^z)^2 + A_n' (S_n'^z)^2 \Big] \end{aligned} \tag{2}$$

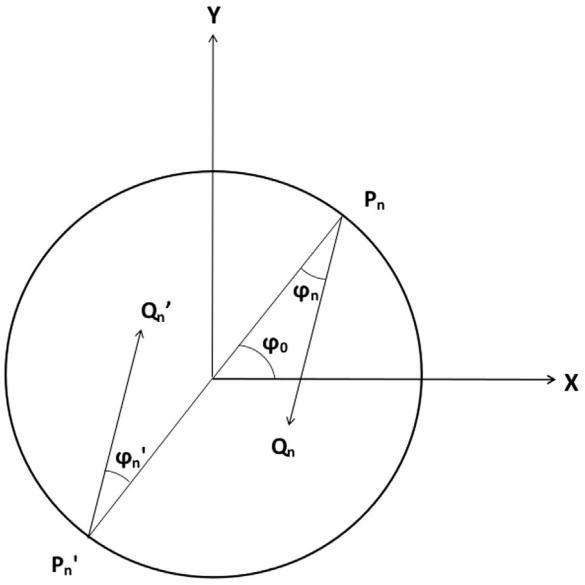

Fig. 1. Projection of the nth base pair in a plane.

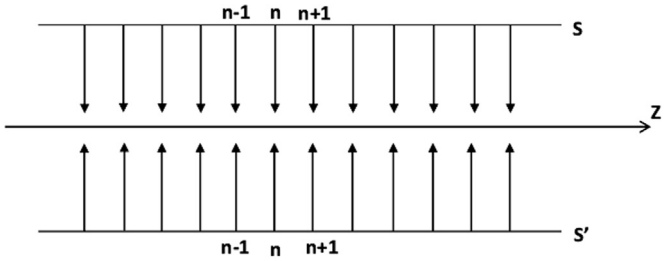

Fig. 2. DNA as an anisotropically coupled spin chain.

The first term of (2) represents the stacking energy between the nth base and its nearest neighbors in the plane normal to the helical axis, J_n and J_n' correspond to the intrastrand constant for the S and the S' strand. When K_n and K_n' are not equal to J_n and J_n', respectively, an anisotropy is introduced in the intrastrand interaction. For the quasi-spin lattices corresponding to the strands S and S', J_n and J_n' represent ferromagnetic exchange integrals due to spin–spin interaction. Next, the contribution of the inter-strand energy is taken into account and λ_n and μ_n represent measures of the interstrand interactions between the opposite bases in both strands. The local field energy of the base and the complementary base or the local field energy of the spin in both sites is measured by the coupling constant h_n. Finally, A_n and A_n' represent the uniaxial anisotropic coefficients (with positive values) due to the magneto crystalline anisotropy in the ferromagnetic spin system, causing the rotation of bases in a plane normal to the helical axis of the DNA. The inhomogeneity of the DNA strand is not considered in the Hamiltonian (2). From the Hamiltonian (2) expressed in terms of quasi-spin operators we proceed to obtain the classical equations of motion by applying the so-called reduction procedure.

3. Classical equations of motion

Since the Hamiltonian (2) is expressed in terms of generators of the $SU(2)$ group and due to the symmetry of the problem we use the Perelomov generalization [26,27] in the construction of coherent states. In order to study quasi-spin Hamiltonian the main