A simple model of DNA dynamics

Giuseppe Gaeta
Centre de Physique Theorique
Ecole Polytechnique, F-91128 Palaiseau (France)

In 1989 professor Yakushevich (of the Institute of Biological Physics of the Academy of Sciences of the URSS) proposed a simple model for DNA (torsion) dynamics [1], from now on called Y model. Further details on this model, as well as on many other "theoretical physics" issues in biology and molecular biology are also contained in the book [2].

This model is schematically illustrated in Figs.1 and 2; the (longitudinal) springs joining discs on the same chain give only a torque, while the (transversal) ones joining discs on different chains work as shown in Fig.2; see [1] for further details. It is quite clear that this model does not take into account the helical structure of DNA.

A consequence of the double helix structure of DNA and a simple way to take this into account is that, even if we consider only next neighbour interactions among the bases, this leads to interaction (also called non-covalent interactions) among bases which are far apart along the bases (as the two which are pointed out schematically in Fig. 4), since they are actually neighbouring in space.

A proposal to modify Yakushevich model in this direction [3], see Fig.3, was indeed presented shortly after the the appearance of [1] (see also [4] for a related discussion on topological features), and leads to qualitatively new phenomena. We refer to [1],[3] for a full discussion of the model, while here we just discuss the aspects which are relevant to the topic of the conference.

In Y model, the degrees of freedom correspond to torsion of the bases, so that to each base is associated a single scalar variable, $\phi_k^i \equiv \phi_k^i(t)$, where $i = \pm 1$ identifies the chain of the double helix to which the base belongs, while k identifies the site along the helix.

The Hamiltonian will be written as

$$\mathcal{H} = T + V^{(\ell)} + V^{(t)} \quad (1)$$

Contribution to the workshop *Nonlinear Coherent Structures in Physics and Biology* (Dijon, 4-6 June 1991)

where T is the kinetic energy,

$$T = \sum_{i,n} \frac{1}{2} I(\dot{\phi}_n^{(i)})^2 \tag{2}$$

and $V^{(\ell)}, V^{(t)}$ are the potential energy terms corresponding to longitudinal and transversal interactions respectively:

$$V^{(l)} = \sum_{i,n} \frac{1}{2} K_L a^2 (\phi_{n+1}^{(i)} - \phi_n^{(i)})^2 \tag{3}$$

$$V^{(t)} = \sum_{n} \frac{1}{2} K_T (\Delta l_n)^2 \tag{4}$$

Here K_L, K_T are "elastic constants"; I is the moment of inertia of the discs, and Δl_n is, after ref. [1],

$$\Delta l_n = [(2r + l_0 - r\cos\phi_n^{(1)} - r\cos\phi_n^{(2)})^2 + (r\sin\phi_n^{(1)} - r\sin\phi_n^{(2)})^2\ ]^{1/2} - l_0 \equiv l_n - l_0 \tag{5}$$

where a is the distance among the bases, and r their radius.

Notice that we have assumed that the discs are all equal, that the coupling constants for interactions of the same type are equal, and that the longitudinal elastic constants along the two chains are equal.

In the "helicoidal" version of Y model [3], from now on referred to as modified Y model, one adds a term

$$V^{(h)} = \sum_{i,n} \frac{1}{2} K_H d^2 (\phi_{n+h}^{(i)} - \phi_n^{(-i)})^2 \tag{6}$$

in the Hamiltonian, with K_H another elastic constant and d the distance in space among bases interacting via the $V^{(h)}$ term, to take into account the helicoidal (i.e. non-covalent) interaction of the kind illustrated in Fig.4; the original Y model corresponds then to $K_H = 0$.

In the continuum limit, we have z the coordinate along the chains, and we are left with two scalar fields $\phi^i \equiv \phi^i(z,t)$, $i = \pm 1$.

We want to consider the case $\ell_0 \simeq 0$, i.e. $\Delta\ell_n \simeq \ell_n$; moreover we are interested in long wavelenght solutions, which justifies passing to the continuum limit. When all these approximations are made, one is left with the equations

$$I\phi_{tt}^{(i)} = K_L a^4 \phi_{zz}^{(i)} - K_T r^2 [2\sin\phi^{(i)} - \sin(\phi^{(i)} + \phi^{(-i)})] + K_H d^2 [2(\phi^{(-i)} - \phi^{(i)}) + \phi_{zz}^{(i)} w^2] \tag{7}$$

where w is the lenght of an half-wind of the helix in the z coordinate (i.e. along the helix itself).

From our point of view here, this model presents two remarkable features:

Soliton solutions

There are special ansatzes which lead to well known equations and in turn to soliton solutions. Indeed, for $\phi^{\mu} = 0, \phi^{(1)} \equiv \phi$, we get

$$I\phi_{tt} = K_L a^4 \phi_{zz} - K_T r^2 \sin\phi - K_H d^2 \phi \tag{8}$$

Similarly, for $\phi^{(-1)} = -\phi^{(1)} \equiv \phi$, we get

$$I\phi_{tt} = (K_L a^4 - K_H d^2 w^2)\phi_{zz} - 2K_T r^2 \sin\phi - 4K_H d^2 \phi \tag{9}$$

I.e., we get sine-Gordon type equations; the K_H coupling is responsible for the appearance of a mass term.

As for the $\phi^{(-1)} = \phi^{(1)} \equiv \phi$ case, we have no qualitative difference due to the introduction of the helicoidal interaction: indeed, we get

$$I\phi_{tt} = (K_L a^4 + K_H d^2 w^2)\phi_{zz} - 2K_T r^2 \sin\phi + K_T r^2 \sin 2\phi \tag{10}$$

We remark that this kind of ansatzes fits well in the framework of "conditional symmetries" [5,6] in the group theoretical approach to differential equations [7,8,9]

Dispersion relations

By linearizing eq. (7), we get

$$I\phi_{tt}^{(i)} = K_L a^4 \phi_{zz}^{(i)} - K_T r^2[\phi^{(i)} - \phi^{(-i)}] + K_H d^2[2(\phi^{(-i)} - \phi^{(i)}) + \phi_{zz}^{(i)} w^2] \tag{11}$$

If now we look at travelling wave solutions,

$$\begin{aligned} \phi^{(1)}(z,t) &= \alpha e^{i(qz-\omega t)} \\ \phi^{(-1)}(z,t) &= \beta e^{i(qz-\omega t)} \end{aligned} \tag{12}$$

we get the relation

$$(\sigma - I\omega^2)^2 = \mu^2 \tag{13}$$

where

$$\sigma = q^2(K_L a^4) + (K_T r^2 + 2K_H d^2) \tag{13'}$$

$$\mu = K_T r^2 + 2K_H d^2(1 - w^2 q^2) \tag{13"}$$

so that the spectrum of the model consists of an acoustical and an optical branch,

$$\omega^2 = \frac{\sigma \pm \mu}{I} \tag{14}$$

given explicitely by

$$\begin{aligned} I\omega_a^2 &= (K_L a^4 + K_H d^2 w^2) q^2 \\ I\omega_o^2 &= (K_L a^4 - K_H d^2 w^2) q^2 + (2K_T R^2 + 4K_H d^2) \end{aligned} \tag{15}$$

In this case, the introduction of an helicoidal coupling is responsible for quite relevant qualitative changes in the behavious of the model.

Indeed, for $K_H = 0$, the two branches are at constant distance (see Fig.5),

$$\omega_0^2 - \omega_a^2 = \frac{2K_T}{I} r^2 \tag{16}$$

while for $K_H \neq 0$ they can cross, as depicted in Fig.6. The corresponding wavelenght λ_{cr} is given by

$$\frac{\lambda_{cr}}{w} = 2\pi \left(\frac{K_H}{K_T r^2 + 2K_H d^2} \right)^{1/2} \equiv 2\pi \left(\frac{1}{2+\chi} \right)^{1/2} \tag{17}$$

Conditions for such a crossing are shortly discussed in [3]; here we notice that a similar crossing of bands in the spectrum of (simple) molecules is well known in laser spectroscopy, and usually corresponds to the appearance of complex phenomena (also called "quantum bifurcations") [10,11,12]; it can be considered, from our point of view, as the signal of appearance of a complicate, possibly chaotic, dynamics.

References

[1] L.V. Yakushevich; *Phys. Lett. A* **136** (1989), 413

[1] L.V. Yakushevich; "Methods of theoretical physics and their applications to biopolymer sciences" (in russian - english translation to appear), Pushchino 1990

[3] G. Gaeta; *Phys. Lett. A* **143** (1990), 227

[4] G. Gaeta; *Phys. Lett. A* **151** (1990), 62

[5] D. Levi and P. Winternitz; *J. Phys. A* **22** (1989), 2915

[6] G. Gaeta; *J. Phys. A* **23** (1990), 3643

[7] P.J. Olver; "Applications of Lie groups to differential equations"; Springer (N.Y.) 1986

[8] G.W. Bluman and S. Kumei; "Symmetries and differential equations", Springer (N.Y.) 1989

[9] H. Stephani; "Differential equations. Their solution using symmetries", Cambridge 1989

[10] I.M. Pavlichenkov and B.I. Zhilinskii; *Ann. Phys.* (N.Y.) **184** (1988), 1

[11] V.B. Pavlov-Verevkin, D.A. Sadovskii and B.I. Zhilinskii; *Europhys. Lett.* **6** (1988), 573

[12] G. Pierre, D.A. Sadovskii and B.I. Zhilinskii; *Europhys. Lett.* **10** (1989), 409

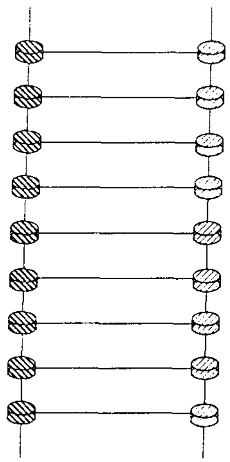

Figure 1 - The Yakushevich model

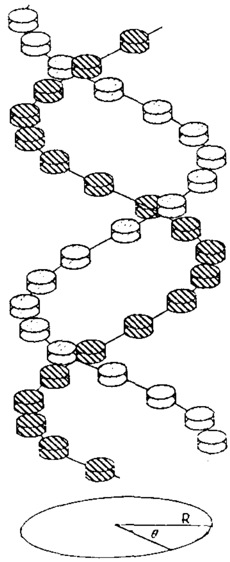

Figure 3 - The modified Y model (interactions are not indicated)

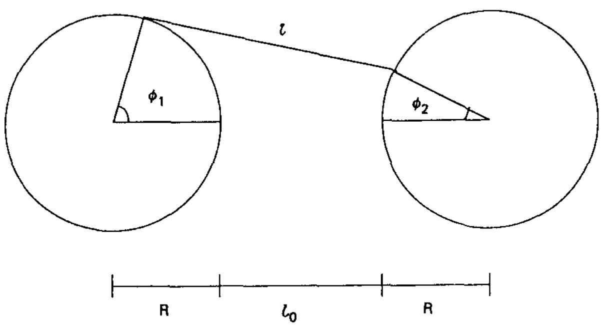

Figure 2 - Detail of the "transversal" interaction in the Y model (from [1])

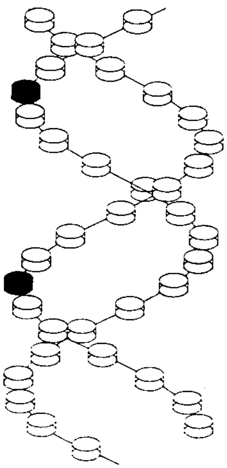

Figure 4 - Two bases interacting
via the "helicoidal" term

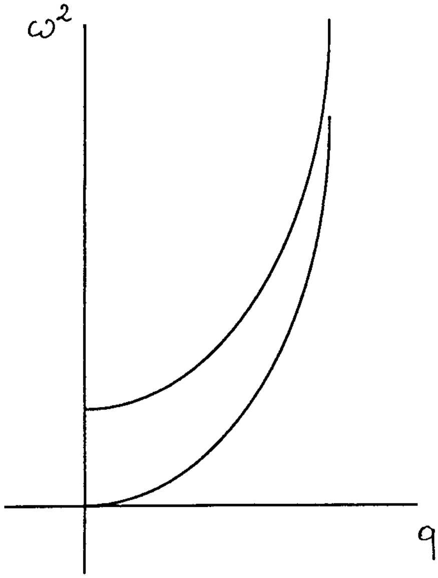

Figure 5 - Dispersion relation
for the Y model

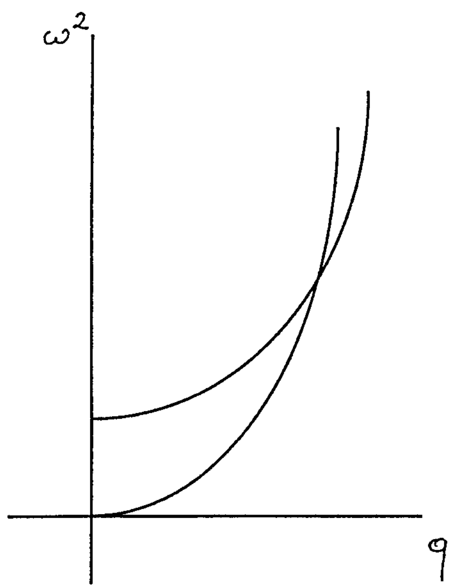

Figure 6 - Dispersion relation
for the modified Y model