Simple Models of DNA Dynamics

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Summary

In this note I briefly discuss the possibility of considering meaningful *simple* models describing DNA nonlinear dynamics; the focus is mainly on base opening dynamics - which is easily accessible to experimental observation - and by simple I mean models which have only one or two degrees of freedom per segment (i.e. nucleoside plus base) of the double helix. After discussing the feature such a model is required to have, I consider two models (Y and PB models) recently introduced, and show that despite their semplicity (relative, since they are not solvable), they succeed to grasp some essential feature of DNA dynamics, and exhibit good agreement with experimental observation. A more complete version of the discussion and results presented here will be given in the review paper [6].

1. Structure of DNA

The molecule of DNA is both extremely complicate and big; although there are attempts of "ab initio" molecular computations of such an intricate system, we will just set for an attempt to identify the (few) degrees of freedom relevant to the processes we want to study, which are essentially the *transcription* of DNA sequence by (Y model) and the *spontaneous denaturation* of DNA (PB model), and in general relevant at body temperature, and build an effective model for the evolution of these. Indeed, as we will see in the following, such an approach can be quite successfull.

The chemical structure of DNA is well known and will not be described here; for informations on the structure and properties of DNA, the reader is referred to [1]. We just recall that the distance between successive sites of the double helix, i.e. the lenght of each segment, is about 3.4 Angstrom, and the pitch of the helix is usually of 10 sites. In order to form the DNA molecule, two such helices couple, by hydrogen bonds linking bases at corresponding sites on the two helices; bases linked by H bonds are said to form a pair.

It should be immediately remarked - and stressed - that atoms between which the H bonds exist are not at all isolated: they are part of a very complicate molecule, which moreover behaves in a way strongly dependent on the physico-chemical environment it lives in: this is to say that (although it is tempting to do this, and sometimes we will actually do it for the sake of simplicity) one is not justified in modelling the H bonds between bases as if they were between isolated atoms.

A similar remark holds also for the other interactions between atoms of the molecule; anyway, as we will remark in a moment, the excitation energy of many degrees of freedom is well above body temperature, so that it seems quite safe to consider these degrees of freedom as frozen.

2. Interactions in DNA

The chemical (covalent) bonds between atoms of the DNA molecule have actually, as just mentioned, for the greater part of cases excitation energies well above the temperature at which DNA lives. In these conditions, we should consider the backbone as rigid, with no "small oscillations" possible: although we are going to discuss classical mechanics models for the degrees of freedom of interest, we should not forget that the molecule obeys quantum mechanics, so that even in classical modelling it would be physically *wrong* to allow for motions of these "hard" degrees of freedom.

Let us look more closely at the structure of DNA, with special attention to "soft" degrees of freedom, i.e. to degrees of freedom excited at body temperature. These are of three kinds:

a) the H bonds between pairing bases;

b) the bases are essentially free to rotate around the N-C bond linking them to the nucleoside[1] (free with respect to covalent interactions; interactions of other nature - e.g. electrostatic - with the other atoms in the molecule give a restoring torque, as we will see later);

c) the sugar ring in the nucleoside has nearly degenerate equilibrium positions, separated by a potential barrer, and can tunnel between the equilibrium positions on the two sides of the plane. This is known as *sugar puckering*, and the excitation energy of such sugar puckering modes is similar to that of the H bonds. Sugar puckering affects the geometry of the double helix, and one of its effects is to take apart bases in a H bonded pair, i.e. to move radially (with respect to the axis of the double helix) the base attached to the sugar affected by puckering.

The identification of these degrees of freedom as the only ones which should actually be affected by body-temperature dynamics is actually enough to introduce and justify the models we want to discuss. Indeed, due to the great complexity of the molecule, the models (and the parameters appearing in them) should be regarded as effective ones for the models of these selected degrees of freedom, i.e. we should not try to deduce details of the models and value of the parameters from first principles and the structure of the molecule, but just find a model which describes coherently with experimental observations the motion of these degrees of freedom.

We will anyway mention some other details on interactions in DNA, before determining the models; this will permit to fix terminology.

Usually, the interactions between bases are divided into *pairing* and *stacking* ones; the former are essentially due to H bonds, while the latter are due to a number of effects in the molecule, and their net effect is to keep stacked one over the other the bases on each helix. The stacking interactions also greatly influence the pairing. The energy of H bond pairing also greatly differs for the pairs (A-T) and (G-C): indeed, this is no surprise, since in one case the bases are couples by three H bonds, while in the other one by two H bonds.

The stacking interactions can be thought as responsible for the restoring forces trying to keep the bases in their equilibrium positions independently of the H bonds, i.e. the forces opposing the "rotational" and "vibrational" movements of points *b)* and *c)* above.

Indeed, one observes experimentally that once three consecutive pairs of bases are bridged by H bonds, stacking forces to continue the closing of the double helix; this also gives a brute extimate of 1/3 for the ratio between pairing effects due to stacking and direct pairing forces due to H bonds.

3. Local openings of the double helix

The local openings of the double helix, i.e. the breakings of the H bonds between pairing bases, are accessible to experimental observation. This is usually done through study of absorption of UV rays; see e.g. [1] for details. From our point of view, the base pairs openings will be the central object of our study.

It should be ramarked, in relation to the above discussion of accessible degrees of freedom, that the H bonds can be broken either by increasing the distance between pairing bases (e.g. by the geometrical effect related to sugar puckering, as described above), either by rotation of the bases around the N-C bond connecting them to the relative nucleoside. Indeed, H bonds are often strongly directional, so that a change in direction of the bases, although comporting only a small variation in the relative distance, can be quite effective in breaking the H bonds.

[1] From now on this will be "the" N-C bond, for ease of notation.

As already remarked, the great complexity of the molecule suggests to keep the above considerations at a very qualitative level, as the H bonds have no apriori reason to behave like those between isolated atoms.

4. Models for DNA dynamics

¿From the above short discussion, it follows that our simple models for DNA dynamics should have several features:

a) Consider only the two degrees of freedom per helix segment, i.e. per base, considered above; from now on we will cal "vibrational" the dynamics associated to sugar puckering and rectilinear (radial with respect to the axis of the double helix) separation of the bases in a pair, and "torsional" the dynamics associated to rotations of the bases around the C-N bond linking them to the sugar ring in the nucleoside.

b) Consider direct pairing and stacking forces.

c) Not depend on details of the forces between bases, but only on qualitative features. On the other side, and always due to our lack of understanding of such a complex molecule, the constants (coupling constants and parameters) appearing in the model should be seen as effective ones, i.e. we have some freedom in their choice.

We will moreover choose to describe the dynamics we are interested in in terms of classical mechanics rather than in quantum terms (but, as explained before, the restriction to the degrees of freedom we actually consider is justified by quantum mechanical considerations); this is admittedly a matter of preference, and other approaches would be possible, considering quantum mechanical models or even looking at the double helix as an Ising system (the two states of the "spin" at a site would correspond then to "closed" or "open" H bonds between bases at the site), see e.g. [2] and [3].

Although a model having these features would already be extremely simplified (we are in fact considering by now only two degrees of freedom per base), we want to operate a further simplification. Namely, we want to consider separately models for the vibrational dynamics alone and for the torsional dynamics alone (vibrational and torsional in the sense explained above), so to have only *one* degree of freedom per base. We will moreover introduce still another further severe simplification: we will assume that all the bases are equal: i.e. they have the same mass and moment of inertia, and all couplings of the same type are equal. (We will moreover assume the double helix to be of infinite lenght, as we suppose side effects to be inessential).

Such models were introduced by Peyrard and Bishop [4] for the vibrational dynamics, and by Yakushevich [5] for the torsional one; we will sometime refer to them as "planar" ones for reasons to be evident in the following. They will also be indicated, for short, as PB model and Y model respectively.

It must be stressed that while the reduction to two degrees of freedom per base discussed above was well justified physically, the present splitting of the dynamics in two noninteracting parts is admittedly due to an attempt to deal with a manageable problem rather than to physical considerations. We will see anyway that, somehow rather surprisingly, these "one degree of freedom models" are able to capt relevant experimentally observed features of DNA dynamics; this will give a justification *a posteriori* of our splitting.

We will write down the models in term of kinetic (T) plus potential (V) energy. If $\phi_n^{(i)}$ ($i = 1, 2$, $n \in \mathbf{Z}$) is the generalized coordinate describing the base at site n on the i-th chain of the double helix - which we suppose of infinite lenght - the Hamiltonian will be written as

$$H = T(\dot{\phi}) + V(\phi) \tag{1}$$

where we assume

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

with $\widetilde{m}$ the mass or the moment of inertia of the bases, according to the degree of freedom taken in consideration.

As for the potential energy, we will decompose it into three parts: a pairing - or *transverse* - interaction energy V_T, a stacking interaction energy V_S, and a third kind of energy (helicoidal interaction energy) V_H to be discussed later on and which for the moment will just be set to zero. So we will have

$$V = V_T + V_S \tag{3}$$

(models which satisfy (3), i.e. for which no "helicoidal" interaction is present, will be called *planar*), and we assume that

$$V_T = \sum_n U_T(\phi_n^{(1)}, \phi_n^{(2)}) \quad ; \quad V_S = \sum_{i,n} U_S(\phi_{n+1}^{(i)}, \phi_n^{(i)}) \tag{4}$$

We will use coordinates such that $\{\phi_n^{(i)} = 0\}$ correspond to the equilibrium stable configuration.

It should be stressed that, since stacking is considerably stronger[2] than H bonding, the nonlinear effects will appear essentially only in the direct pairing (transverse) interactions, i.e. the dynamic will be such to stretch the stacking interactions much less that the H bonds. These observations suggest to consider the harmonic potential approximation for stacking interactions, which we will indeed adopt. It should be stressed that, as it will be clear in the following, this leads to the appearance of the Laplacian once we pass to the continuum limit.

We pass now to describe two prototypical models of torsional and vibrational DNA dynamics, due respectively to Yakushevich and to Peyrard and Bishop. Earlier proposals of similar models were formulated by several authors, but will not be discussed here.

5. A model of DNA torsion dynamics

In the model proposed by L. Yakushevich [5], the pairing interaction is considered in the approximation of harmonic potential, depending on the distance between the endpoints of the bases, i.e. the atoms bridged by H bonds. Although the force is linear in this distance, when we describe the position of the bases by means of an angle θ of rotation around the N-C bond the force becomes a nonlinear function of such an angle. The details of pairing interactions in such a model are shown in fig.1.

Here the distance ℓ between points p_1 and p_2 satisfies

$$\ell^2 = [d + 2r - r(\cos\theta_1 + \cos\theta_2)]^2 + [r(\sin\theta_1 + \sin\theta_2)]^2 \tag{1}$$

It is then convenient to pass to coordinates

$$\phi_\pm = \frac{\theta_1 \pm \theta_2}{2} \tag{2}$$

in terms of which, by standard trigonometric identities, the distance is written as

$$\ell^2 = d^2 + +4r^2 \left(1 + \cos^2\phi_- - 2\cos\phi_+ \cos\phi_-\right) \tag{3}$$

Yakushevich does also suggest to consider the approximation $d \to 0$.

In other words we are considering the stretchning of H bonds due to small rotations of the bases and extend this to the full range $[0, 2\pi]$ of angular coordinates. Notice that we are trascurating the directionality effects, as only distance is taken into account.

The potential describing the pairing interaction will then be

$$U_T = \frac{1}{2}\alpha[1 + \cos^2\phi_- - 2\cos\phi_+ \cos\phi_-] \tag{4}$$

(notice that this is 2π-periodic in both angular coordinates, as it should); this is sketched in fig.2by level curves.

As for stacking interactions, we will also *a fortiori* keep the harmonic approximation for them; if $\theta_n^{(i)}$ is the angular coordinate relative to the n-th base along the i-th chain ($i = 1, 2$), the stacking interaction potential between bases at sites n and $n+1$ will be

$$U_S = \frac{1}{2}\beta\left[(\theta_{n+1}^{(1)} - \theta_n^{(1)})^2 + (\theta_{n+1}^{(2)} - \theta_n^{(2)})^2\right] \tag{5}$$

[2] It is maybe worth remarking that there is no contradiction with the extimate of 1/3 for the ratio of pairing effects due to stacking to direct pairing forces given above: here we consider the strenght of the stacking interaction themselves, and not just of their pairing effect.

Passing again to the coordinates (2), i.e.

$$\theta_n^{(1)} = \phi_n^{(+)} + \phi_n^{(-)} \quad ; \quad \theta_n^{(2)} = \phi_n^{(+)} - \phi_n^{(-)} \tag{6}$$

the above reads

$$V_S \frac{1}{2}\beta \left[(\phi_{n+1}^{(+)} - \phi_n^{(+)})^2 + (\phi_{n+1}^{(-)} - \phi_n^{(-)})^2 \right] \tag{7}$$

In the following, in order to avoid confusion and to lighten notation, we will prefer to write ψ for ϕ_+ and χ for ϕ_-; with this the planar Yakushevich model is defined by the Hamiltonian

$$H = T + V_S + V_T \tag{8}$$

$$T = \sum_n \frac{1}{2} I \left[(\dot{\theta}_n^{(1)})^2 + (\dot{\theta}_n^{(2)})^2 \right] = \sum_n \frac{1}{2} I \left(\dot{\psi}_n^2 + \dot{\chi}_n^2 \right) \tag{9}$$

$$V_S = \sum_n \frac{1}{2}\beta \left[(\psi_{n+1} - \psi_n)^2 + (\chi_{n+1} - \chi_n)^2 \right] \tag{10}$$

$$V_T = \sum_n \frac{1}{2}\alpha \left[1 + \cos^2 \chi_n - 2\cos\psi_n \cos\chi_n \right] \tag{11}$$

where we introduced the ψ, χ coordinates in the kinetic term T as well. The equilibrium (stable) configuration is represented by $\{(\psi_n, \chi_n) = (0,0)\ \forall n\}$; I is the moment of inertia of the bases around the N-C bond.

The above hamiltonian gives as equations of motion

$$\begin{aligned} I\ddot{\psi}_n =& \beta(\psi_{n+1} - 2\psi_n + \psi_{n-1}) - \alpha \sin\psi_n \cos\chi_n \\ I\ddot{\chi}_n =& \beta(\chi_{n+1} - 2\chi_n + \chi_{n-1}) - \alpha \sin\chi_n (\cos\psi_n - \cos\chi_n) \end{aligned} \tag{12}$$

which for small oscillations reduce to

$$\begin{aligned} I\ddot{\psi}_n =& \beta(\psi_{n+1} - 2\psi_n + \psi_{n-1}) - \alpha\psi_n \\ I\ddot{\chi}_n =& \beta(\chi_{n+1} - 2\chi_n + \chi_{n-1}) \end{aligned} \tag{13}$$

6. The continuum limit of planar Yakushevich model

We do now want to consider the continuum limit of this model: the arrays $\{\psi_n(t)\}$, $\{\chi_n(t)\}$ will then be substituted by fields $\psi(x,t), \chi(x,t)$ which take values in the circle $S^1 = [0, 2\pi]$ and such that

$$\begin{aligned} \psi(n\delta, t) = \psi_n(t) \\ \chi(n\delta, t) = \chi_n(t) \end{aligned} \tag{1}$$

where δ is the unit distance between successive bases along the axis of the double helix, $\delta \simeq 3.4 \mathring{A}$. It should be stressed that in considering the continuum approximation, it makes no sense to consider wavelenght λ shorter than the interbase distance, i.e. than δ.

We can now rewrite the various terms of the hamiltonian in the field formulation; we get

$$T = \frac{1}{\delta} \int \frac{1}{2} I(\psi_t^2 + \chi_t^2) \mathrm{d}x \tag{2}$$

$$V_T = \frac{1}{\delta} \int \frac{1}{2}\alpha [1 + \cos^2\chi - 2\cos\psi\cos\chi] \mathrm{d}x \tag{3}$$

$$V_S = \frac{1}{\delta} \int \frac{1}{2}\delta^2 \beta \left[(\nabla\psi)^2 + (\nabla\chi)^2 \right] + O(\delta^4) \mathrm{d}x \tag{4}$$

where $\nabla \equiv \partial / \partial x$ and the $(1/\delta)$ factors are only for normalization purposes, i.e. to keep the normalization of the field hamiltonian equal to that of the discrete one.

The evolution equations for the fields ψ, χ issuing from this hamiltonian (or, equivalently, the continuum limit of the equations of motion for ψ_n, χ_n) are

$$\begin{aligned} I\psi_{tt} =&\beta\delta^2\triangle\psi - \alpha\sin\psi\cos\chi + O(\delta^4) \\ I\chi_{tt} =&\beta\delta^2\triangle\chi - \alpha\sin\chi(\cos\psi - \cos\chi) + O(\delta^4) \end{aligned} \tag{5}$$

where $\triangle$ is the spatial Laplacian, $\triangle \equiv \partial^2/\partial x^2$

We stress that here δ is a physical parameter, fixed by nature, so that we cannot simply consider the limit $\delta \to 0$ in order to get rid of the $0(\delta^4)$ terms. We will not discuss this point in detail here (see [6] for a discussion), but just state that if λ_0 is the shorter wavelenght appearing in the Fourier decomposition of ψ, we have to ask not only $\lambda_0 > \delta$, but

$$\lambda_0 >> 2\delta \tag{6}$$

7. Solitons in planar Yakushevich model

We want now to focus our attention on soliton solutions for the Yakushevich model. The soliton solutions propagate without changing their form, i.e. we have

$$\begin{aligned} \psi(x,t) =&\psi(x - vt) \equiv \psi(z) \\ \chi(x,t) =&\chi(x - vt) \equiv \chi(z) \end{aligned} \tag{1}$$

This ansatz, once used into the field evolution equations, produces the *equations for Yakushevich solitons*:

$$\begin{aligned} (v^2 - \kappa)\psi_{zz} =& -\frac{\partial W}{\partial \psi} \equiv -\sin\psi\cos\chi \\ (v^2 - \kappa)\chi_{zz} =& -\frac{\partial W}{\partial \chi} \equiv -\sin\chi(\cos\psi - \cos\chi) \end{aligned} \tag{2}$$

Corresponding, the hamiltonian and lagrangian for Yakushevich solitons read

$$H_S = \frac{I}{\delta}\int \frac{1}{2}(v^2 + \kappa)\left[(\nabla\psi)^2 + (\nabla\chi)^2\right] + W(\psi,\chi)\mathrm{d}x \tag{8}$$

$$L_S = \frac{I}{\delta}\int \frac{1}{2}(v^2 - \kappa)\left[(\nabla\psi)^2 + (\nabla\chi)^2\right] - W(\psi,\chi)\mathrm{d}x \tag{9}$$

where now $\nabla \equiv \partial/\partial z$.

On physical grounds, we would require that for $z \to \pm\infty$ the fields go to the equilibrium (zero-energy) configuration; due to the 2π periodicity of W in both ψ and χ, this means

$$\begin{aligned} &\psi_z(\pm\infty) = \chi_z(\pm\infty) = 0 \\ &\psi(\pm\infty) = 2\pi n_\pm \quad ; \quad \chi(\pm\infty) = 2\pi m_\pm \end{aligned} \tag{10}$$

With no loss of generality we can assume

$$n_- = m_- = 0 \tag{11}$$

so that the finite energy solutions are classified by $(n_+, m_+) \equiv (n, m)$ alone, i.e. by two integers. This corresponds indeed to the topological classification of solitons $\mathbf{R} \to S^1 \times S^1$, as n and m are *rotation numbers* for the fields ψ and χ. Solitons in the (n,m) class will be topologically stable, and we can look for them by minimizing the energy with prescribed boundary conditions. We will not, anyway, use the topological theory of solitons [7], and keep the discussion at a simple level.

By interpreting z as a time, and $\widetilde{\mu} \equiv (v^2 - \kappa)$ as an effective mass, (7) aquires the meaning of a mechanical (Newton) equation for a particle of mass $\widetilde{\mu}$ moving in the two dimensional plane (with coordinates ψ, χ) under the effects of the potential W. The boundary conditions given above fix then the total energy to be

$E=0$; it is then immediate to see that nontrivial solutions can exist only if the effective mass is negative; this also gives an upper bound on the speed of solitons:

$$\begin{aligned} \widetilde{\mu} &= v^2 - \kappa < 0 \\ |v| &< \sqrt{\kappa} = v_{\max} \end{aligned} \tag{12}$$

which in turn implies

$$\mu \equiv -\widetilde{\mu} \leq \kappa = \mu_{\max} \tag{13}$$

¿From now on we will use $\mu = -\widetilde{\mu} = \kappa - v^2$; notice that in terms of this effective mass, the effective potential will be $-W$. Equations (7) are now

$$\begin{aligned} \mu\psi_{zz} =& \frac{\partial W}{\partial \psi} \\ \mu\chi_{zz} =& \frac{\partial W}{\partial \chi} \end{aligned} \tag{14}$$

Multiplying the first one by ψ_z and the second one by χ_z, we get

$$\frac{1}{2}\mu\frac{\mathrm{d}}{\mathrm{d}z}\left(\psi_z^2 + \chi_z^2\right) = \frac{\mathrm{d}}{\mathrm{d}z}W(\psi,\chi) \tag{15}$$

so that integrating - and using the boundary conditions (10), which sets the integration constant to zero - we get

$$\frac{1}{2}\mu\left[(\nabla\psi)^2 + (\nabla\chi)^2\right] = W(\psi,\chi) \tag{16}$$

This relation is satisfied by soliton solutions $(\bar{\psi},\bar{\chi})$; using it in (8), and writing $\nu = \kappa + v^2$, we have for the energy of such a solution

$$\begin{aligned} E =& \frac{1}{2}\frac{I}{\delta}\int (\nu+\mu)\left[(\nabla\bar{\psi})^2 + (\nabla\bar{\chi})^2\right]\mathrm{d}z \\ E =& \frac{I\kappa}{\delta}\int \left[(\nabla\bar{\psi})^2 + (\nabla\bar{\chi})^2\right]\mathrm{d}z \end{aligned} \tag{17}$$

8. Explicit soliton solutions

In the simplest cases, i.e. for the $(1,0)$ and the $(0,1)$ soliton solutions (see the discussion of boundary conditions in the previous section), it is actually possible to give an analytic expression for the soliton solutions.

This is due to the fact that in this case only one of the fields is nonzero, so that we are reduced to a one-dimensional mechanical problem; a short look at the effective potential $-W$, either in its analytic form either in fig.2, suffices to get convinced that $(n,0)$ and $(0,n)$ soliton solutions with $|n|>1$ require *both* fields to be not identically zero[3], so that we can not reduce to a one dimensional motion.

We will not give here the details of the (standard) computation of these explicit solutions, but just their final form; the reader is referred to [6,8] for details.

In the case of the (1,0) soliton, we have with $A=\sqrt{2\alpha/\mu}$ the explicit solution

$$\psi(z) = \arccos\left[\frac{\sinh^2(Ax)-1}{\sinh^2(Ax)+1}\right] \tag{1}$$

For the (0,1) soliton, we have with $B = 2\sqrt{\alpha/\mu}$,

$$\chi(z) = \arccos\left[\frac{B^2z^2-1}{B^2z^2+1}\right] \tag{2}$$

[3] Obviously, this is *a fortiori* true if both the soliton numbers (n,m) are not zero.

It should be remarked that both (1) and (2) obey simple scaling relations under changes of α, μ and of the lenght scale for z; this is not a fortuitous case, but indeed corresponds to general scaling properties of soliton solutions for the *planar* Yakushevich model, as discussed elsewhere [6,8].

9. A model of DNA vibration dynamics

We pass now to consider the "vibrational" dynamics of DNA, associated to sugar puckering modes; as recalled before, this corresponds to radial motion of the bases with respect to the axis of the double helix; the coordinate $x_n^{(i)}$ describing the position of the base will then be its distance from the axis of the double helix, or better - in order to keep $\{x_n^{(i)} = 0\}$ as the equilibrium configuration - this distance minus the distance corresponding to the equilibrium position.

Such a model was proposed by Peyrard and Bishop [4], who suggested to use as pairing potential the Morse potential; namely, if $x_n^{(i)}$ is the coordinate defined above for the n-th base on the i-th chain, we have

$$U_T = D\left[e^{-\alpha(x^{(1)}+x^{(2)})/2} - 1\right]^2 \tag{1}$$

or, passing again to the coordinates

$$\phi_\pm = \frac{x^{(1)} \pm x^{(2)}}{2} \quad ; \quad \phi_+ \equiv \psi \ , \ \phi_- \equiv \chi \tag{2}$$

we rewrite this as

$$U_T = D\left[e^{-\alpha\psi} - 1\right]^2 \tag{3}$$

As for stacking interactions, we keep to the harmonic potential approximation, which gives

$$U_S = \frac{1}{2}\beta\left[\left(x_{n+1}^{(1)} - x_n^{(1)}\right)^2 + \left(x_{n+1}^{(2)} - x_n^{(2)}\right)^2\right] \tag{4}$$

or, passing to the ψ, χ coordinates,

$$U_S = \frac{1}{2}\beta\left[(\psi_{n+1} - \psi_n)^2 + (\chi_{n+1} - \chi_n)^2\right] \tag{5}$$

Finally, the hamiltonian for this (Peyrad-Bishop, or PB) model will be

$$H = T + V_S + V_T \tag{6}$$

$$T = \sum_{i,n} \frac{1}{2}m\left(x_n^{(i)}\right)^2 = \sum_n \frac{1}{2}m\left(\dot\psi_n^2 + \dot\chi_n^2\right) \tag{7}$$

$$V_S = \sum_n \frac{1}{2}\beta\left[(\psi_{n+1} - \psi_n)^2 + (\chi_{n+1} - \chi_n)^2\right] \tag{8}$$

$$V_T = \sum_n \frac{1}{2}D\left[e^{-\alpha\psi_n} - 1\right]^2 \tag{9}$$

Here m is the mass of the bases; the parameters α, β are *not* the same as in the Yakushevich model.

In discussing small oscillations around the equilibrium configuration $\psi_n = \chi_n = 0$, we need the quadratic part of V_T; this is simply

$$V_T^{(2)} = \sum_n \frac{1}{2}(D\alpha^2)\psi_n^2 \tag{10}$$

The above hamiltonian gives as equations of motion

$$\begin{aligned} m\ddot\psi_n &= \beta(\psi_{n+1} - 2\psi_n + \psi_{n-1}) - \alpha D\left[e^{-\alpha\psi_n} - 1\right] \\ m\ddot\chi_n &= \beta(\chi_{n+1} - 2\chi_n + \chi_{n-1}) \end{aligned} \tag{11}$$

which for small oscillations reduce to

$$
\begin{aligned}
m\ddot{\psi}_n =& \beta(\psi_{n+1} - 2\psi_n + \psi_{n-1}) - \alpha^2 D\psi_n \\
m\ddot{\chi}_n =& \beta(\chi_{n+1} - 2\chi_n + \chi_{n-1})
\end{aligned}
\tag{12}
$$

10. The continuum limit of planar Peyrard-Bishop model

In order to pass to the continuum limit of this model, we proceed similarly to the case of the Yakushevich model; i.e., the arrays $\psi_n(t), \chi_n(t)$ are substituted by fields $\psi(x,t), \chi(x,t)$ such that

$$
\begin{aligned}
\psi(n\delta, t) =& \psi_n(t) \\
\chi(n\delta, t) =& \chi_n(t)
\end{aligned}
\tag{1}
$$

with δ the distance between successive bases along the axis of the double helix, $\delta \simeq 3.4\mathring{A}$. Notice that χ takes value on the whole real line $\mathbf{R}$, while for ψ the physical range is $\psi \geq -2d_0$, where d_0 is the distance of the bases from the axis of the double helix at equilibrium. Actually, for both ψ and χ it makes no sense to consider too big absolute values; th erelevant point here for later discussion is that, contrary to the Yakushevich case, the topology of the target space is trivial (this means in particular that we have no topological solitons).

With the same remarks as in the Yakushevich case, we can write the hamiltonian in the field formulation as

$$
H = T + V_T + V_S \tag{2}
$$

$$
T =\frac{1}{\delta} \int \frac{1}{2} m \left(\psi_t^2 + \chi_t^2\right) \mathrm{d}x \tag{3}
$$

$$
V_T =\frac{1}{\delta} \int \frac{1}{2} D \left(e^{-\alpha\psi} - 1\right)^2 \mathrm{d}x \tag{4}
$$

$$
V_S =\frac{1}{\delta} \int \frac{1}{2} \delta^2 \beta \left[(\nabla\psi)^2 + (\nabla\chi)^2\right] \mathrm{d}x \tag{5}
$$

and the corresponding field evolution equations are

$$
\begin{aligned}
m\psi_{tt} =& \beta\delta^2 \triangle\psi + \alpha D \left(e^{-\alpha\psi} - 1\right) \\
m\chi_{tt} =& \beta\delta^2 \triangle\chi
\end{aligned}
\tag{6}
$$

We recall that these are valid if and only if the solutions have wavelenghts large compared to δ.

11. Helical geometry and helicoidal DNA models

The models discussed up to now have been at several reprises qualified as *planar*; this is due to the fact that they can be schematized as in fig.3, which also means that they don't take into account the peculiar geometry of the double helix.

It turns out that taking this into account, even in a "minimal" way, produces qualitative changes in the dynamics, quite relevant also in relation with "observable" properties of the model (especially in the case of the PB model).

The modification we consider here was first proposed in the context of the Yakushevich model, and then applied also to the Peyrard- Bishop one [9,10]; the models modified in this way will be qualified as *helicoidal*. In the following, we will write hY for "helicoidal Yakushevich", and hPB for "helicoidal Peyrard- Bishop".

In a double helix (with pitch of the helix $2h$ in base units) it happens that bases which are half-wind of the helix apart, i.e. h sites away, come to be spatially near, so that they can interact; this fact is shown schematically in fig.4. It should be stressed that such an interaction is actually present in real DNA, where it is realized by bridging water filaments between the concerned bases.

¿From the point of view of our models, and referring to the notation previously employed, this means that the hamiltonian will now be of the form

$$H = T + V_T + V_S + V_H \tag{1}$$

where V_H represents these new or - as they will be called - *helicoidal* interactions. These will appear through terms of the form, referring again to section * for notation,

$$U_H = k\left(\phi_n^{(1)}, \phi_{n+h}^{(2)}\right) + k\left(\phi_n^{(2)}, \phi_{n+h}^{(1)}\right) \tag{2}$$

It should be remarked that helical geometry poses some constraint on the choice of coordinates for helicoidal models (the present author was actually responsible for introducing a wrong choice of coordinates). The choice of coordinates made above for both models we consider took this problem into account, and is therefore correct.

As mentioned above, the helicoidal interaction is due in real DNA to bridged water filaments; given that the distance between bases coupled by these is $5h \simeq 17.0\mathring{A}$, from the geometry of water molecules and the size of O-H-O bonds one can estimate these filaments to be made up of ~ 8 H_2O molecules; stretching the filament amounts to stretching ~ 9 H bonds; this also means that the corresponding elastic constant should be $\sim 1/9$ of that assumed for single H bonds. Due to this, these bonds will be stretched much less than the H bonds pairing bases at corresponding sites on different helices (i.e. than the H bonds entering in V_T). We are therefore perfectly justified in considering the harmonic approximation for V_H, which we will indeed do in the following.

As it is the case for all the interactions in our simple models, also the V_H introduced here should be seen as an effective one; therefore one should be most careful in extending the above discussion, which justified the harmonic approximation, to quantitative matters, i.e. to an extimation for the ratio of the coupling constants relative to V_T and V_H (this should be ~ 9 by the above argument). Indeed, e.g; in the context of the hPB model Dauxois gave quite different estimates in order to fit experimantal findings [10].

We will leave the coupling constant for V_H, as already done for the other constants appearing in the model, as an effecive constant to be adjusted. We als stress that, given the relatively long range of this effective interaction, it is potentially even more sensitive than the other ones to the effect of the complicate interactions in the molecule and with its environment.

12. Introduction of helicoidal terms in the Peyrard- Bishop model

We will begin by shortly considering the effect of introducing "helicoidal" terms in the PB model, as was first done by Dauxois [10].

We add to the PB hamiltonian a term V_H which, coherently with the discussion of the previous section, is simply an harmonic potential:

$$U_H = \frac{1}{2}\gamma\left[\left(x_{n+h}^{(1)} - x_n^{(2)}\right)^2 + \left(x_{n+h}^{(2)} - x_n^{(1)}\right)^2\right] \tag{1}$$

Upon introduction of the ψ, χ coordinates, so that

$$x_n^{(1)} = \psi_n + \chi_n \quad ; \quad x_n^{(2)} = \psi_n - \chi_n \tag{2}$$

the interaction energy reads, with straightforward algebra,

$$U_H = \frac{1}{2}\gamma\left[(\psi_{n+h} - \psi_n)^2 + (\chi_{n+h} + \chi_n)^2\right] \tag{3}$$

Notice the different signs in the ψ and χ parts of this.

The total hamiltonian of the helicoidal Peyrard- Bishop (hPB) model reads therefore

$$H = T + V_S + V_T + V_H \tag{4}$$

with T, V_S, V_T as in the PB model and

$$V_H = \sum_n \frac{1}{2}\gamma \left[(\psi_{n+h} - \psi_n)^2 + (\chi_{n+h} + \chi_n)^2 \right] \tag{5}$$

with h the half-pitch of the helix in base units (i.e. $h = 5$ for ordinary DNA).

The hPB hamiltonian gives as equations of motion

$$\begin{aligned} m\ddot{\psi}_n =& \beta(\psi_{n+1} - 2\psi_n + \psi_{n-1}) + \gamma(\psi_{n+h} - 2\psi_n + \psi_{n-h}) - \alpha D \left[e^{-\alpha\psi_n} - 1 \right] \\ m\ddot{\chi}_n =& \beta(\psi_{n+1} - 2\psi_n + \psi_{n-1}) - \gamma(\psi_{n+h} - 2\psi_n + \psi_{n-h}) \end{aligned} \tag{6}$$

which for small oscillations reduce to

$$\begin{aligned} m\ddot{\psi}_n =& \beta(\psi_{n+1} - 2\psi_n + \psi_{n-1}) + \gamma(\psi_{n+h} - 2\psi_n + \psi_{n-h}) - \alpha^2 D\psi_n \\ m\ddot{\chi}_n =& \beta(\chi_{n+1} - 2\chi_n + \chi_{n-1}) - \gamma(\psi_{n+h} - 2\psi_n + \psi_{n-h}) \end{aligned} \tag{7}$$

Let us now consider the continuum limit of this model. Clearly the helicoidal interaction leads to the appearance of nonlocal (in x, the coordinate along the axis of the double helix) terms; the field evolution equations will be, understanding that $\psi \equiv \psi(x,t)$, $\chi \equiv \chi(x,t)$ unless otherways indicated, and writing $w = h\delta$,

$$\begin{aligned} m\psi_{tt} =& \beta\delta^2 \triangle\psi + \gamma\mathcal{W}_+(\psi) + \alpha D \left(e^{-\alpha\psi} - 1 \right) \\ m\chi_{tt} =& \beta\delta^2 \triangle\chi - \gamma\mathcal{W}_-(\chi) \end{aligned} \tag{8}$$

with $\mathcal{W}_\pm$ defined as

$$\mathcal{W}_\pm(\phi) = \phi(x+w,t) \mp 2\phi(x,t) + \phi(x-w,t) \tag{9}$$

13. Dispersion relations for the helicoidal Peyrard- Bishop model

We set

$$\kappa = \beta\delta^2/m \quad , \quad \sigma = D\alpha^2/m \quad , \quad \rho = \gamma/m \ ;$$

with these the equations for small oscillations in the hPB model are

$$\begin{aligned} \psi_{tt} =& \kappa\triangle\psi + \rho\mathcal{W}_+(\psi) - \sigma\psi \\ \chi_{tt} =& \kappa\triangle\chi - \rho\mathcal{W}_-(\chi) \end{aligned} \tag{1}$$

Passing to Fourier components, i.e. to

$$\begin{aligned} \psi(x,t) =& F_{q,\omega} e^{iqx} e^{i\omega t} \equiv F_{q,\omega} |q,\omega> \\ \chi(x,t) =& G_{q,\omega} e^{iqx} e^{i\omega t} \equiv G_{q,\omega} |q,\omega> \end{aligned} \tag{2}$$

we have to take care of the action of the nonlocal operators $\mathcal{W}_\pm$ on $|q,\omega>$: this is

$$\mathcal{W}_\pm \left(|q,\omega> \right) = \left(e^{iqw} \mp 2 + e^{-iqw} \right) |q,\omega> = 2 \left[\cos(qw) \mp 1 \right] |q,\omega> \tag{3}$$

With this, the dispersion relations are immediately seen to be

$$\begin{aligned} \omega_\psi^2 =& \kappa q^2 + 2\rho \left[1 - \cos(qw) \right] + \sigma \\ \omega_\chi^2 =& \kappa q^2 + 2\rho \left[1 + \cos(qw) \right] \end{aligned} \tag{4}$$

It is maybe preferable to use standard trigonometric formulas and reexpress the above as

$$\begin{aligned} \omega_\psi^2 =& \kappa q^2 + 4\rho \sin^2 \left(\frac{qw}{2} \right) + \sigma \\ \omega_\chi^2 =& \kappa q^2 + 4\rho \cos^2 \left(\frac{qw}{2} \right) \end{aligned} \tag{5}$$

The dispersion relations (4),(5) are plotted in fig.5(with values of the parameters following the estimates given by [10]). It is immediately clear, by comparing with the dispersion relations of the planar PB model, that the introduction of helicoidal terms has drastically changed the (small oscillations) dynamics.

Notice that in the PB and hPB models the ψ and χ fields do exactly decouple, so that we are actually in presence of separate dynamics; we stress that this is true not only for small oscillations, but at the full nonlinear level as well.

Let us briefly comment on these dispersion relations by remarking some features of theirs.

a) Now there is no mode with $\omega(q) = 0$ for $q \to 0$; this means that we have a threshold for creation of excitations of given (small) amplitude.

b) The crossing of the two branches[4], and their relative ordering for $q = 0$, are controlled by the sign of the quantity

$$s = 1 - \frac{\alpha}{2\gamma}$$

c) the ψ branch has absolute minimum at $q = 0$, while the χ branch has an absolute minimum at $q_0 \neq 0$ ($q_0 \simeq 4\pi/w$, which corresponds to a wavelenght $\lambda_0 \simeq w/2$). This latter fact is an obvious consequence of the introduction of the helicoidal interaction and of the signs in the χ part of V_H: χ waves with $\chi_{n+h} = -\chi_n$ cost less energy.

14. Nondispersive waves and breather modes in the helicoidal Peyrard-Bishop model

The waves corresponding to extremal points of the dispersion relations have zero group velocity; i.e., they are *standing waves* or, in other words, correspond to *breather modes*: there are oscillatory local openings of the double helix which remain localized without spreading or travelling.

The PB model is aimed at describing the denaturation of DNA; this process arises indeed by local opening of "bubbles" in the double helix, i.e. opening of consecutive pairs of bases.

The experiments tell us that the size of the bubbles is of a few base units, and the time frequencies involved are of the order of picoseconds; it is hoped that the breather modes of the hPB model can indeed model this process.

We discuss here numerical findings[5] based on parameter estimates given in [10]. It turns out that the hPB model is rather well compatible with experimental findings.

Notice also that, due to the virial theorem, the energy of waves of amplitude A and obeying the dispersion relation $\omega = \omega(q)$ is just

$$E = A^2 m \omega^2(q) \tag{1}$$

Let us now write for ease of notation

$$\xi = \frac{qw}{2} \tag{2}$$

and rewrite the dispersion relatons, in terms of the physical coupling parameters, as

$$\begin{aligned} \Omega_\psi(\xi) &\equiv m\omega_\psi^2(q(\xi)) = 4\gamma\left[B\xi^2 + C + \sin^2(\xi)\right] \\ \Omega_\chi(\xi) &\equiv m\omega_\chi^2(q(\xi)) = 4\gamma\left[B\xi^2 + \cos^2(\xi)\right] \end{aligned} \tag{3}$$

where the parameters B, C are given by

$$B = \frac{\beta}{h^2\gamma} \quad ; \quad C = \frac{\alpha D}{4\gamma} \tag{4}$$

The extremal points $\xi = \xi_0$ of these are obtained by solving $\partial\Omega/\partial\xi = 0$, namely

$$2B\xi \mp \sin(2\xi) = 0 \tag{5}$$

[4] As already mentioned, in the PB model the two branches are non interacting, so that the crossing points have no physical meaning; the situation will be different in the context of the Y model.

[5] More complete and refined numerical simulations of this model are being performed by Peyrard and collaborators; these also concern estimates of parameters.

with the minus sign for the ψ branch and the plus one for the χ branch. Notice that necessarily $\xi_0 \leq 1/B = h^2\gamma/\beta$.

The wavelenght corresponding to ξ_0 is simply given by

$$\lambda(\xi_0) = \frac{2\pi}{q(\xi_0)} = \frac{\pi h}{\xi_0}\delta \tag{6}$$

(Notice that the above bound on ξ_0 ensures then $\lambda_0 \geq [(\pi\beta)/(h\gamma)]\delta$; with the value of β/γ considered in this section, this also ensures $\lambda_0 >> \delta$, as required for the validity of our continuum approximation).

The time frequency ω and period T corresponding to ξ_0 are

$$\omega(\xi_0) = \sqrt{\frac{\Omega(\xi_0)}{m}} \tag{7}$$

$$T(\xi_0) = \frac{2\pi}{\omega(\xi_0)} \tag{8}$$

¿From (1), and expecting each field mode to have an average energy $< E >= \frac{1}{2}kT$, we have ($T \simeq 37\ ^0C$) the expected amplitude of oscillations corresponding to ξ_0:

$$A(\xi_0) = \sqrt{\frac{kT/2}{\Omega(\xi_0)}} \tag{9}$$

As for the parameters α, β, γ, m, we stick to the estimates given by Dauxois [10]; adapting the notation to our present one, these are given in table I (we report $\alpha^2 D$ rather than α since the former is the coefficent of the linear term in the equations of motion). The corresponding numerical results are reported, for the ψ and χ branches, respectively in tables II and III. As anticipated, the orders of magnitude that we obtain in this way for λ and T are in good agreement with experimental observations (notice that opening of the double helix correspond to the ψ mode).

α	$\simeq$	0.8 eV/Å^2	$\simeq$	$1.3 \cdot 10^4$ erg/cm^2
β	$\simeq$	1.5 eV/Å^2	$\simeq$	$2.4 \cdot 10^4$ erg/cm^2
γ	$\simeq$	0.5 eV/Å^2	$\simeq$	$8.0 \cdot 10^3$ erg/cm^2
m	$\simeq$	300 m.u.	$\simeq$	$5 \cdot 10^{-22}$ g

Table I - Parameter choice for hPB model

ξ	1.4	3.7	4.0	0.
$\Omega(\xi_0)$	8.5 10^3	1.5 10^4	2.2 10^4	3.2 10^4
$\omega(q_0)$	4.1 10^{12}	5.5 10^{12}	6.6 10^{12}	8.0 10^{12}
$T(q_0)$	1.5 ps	1.1 ps	0.9 ps	0.8 ps
$A(q_0)$	0.16$\AA$	0.12$\AA$	0.10$\AA$	0.08$\AA$
$\lambda(q_0)$	11.2 δ	4.2 δ	3.9 δ	∞

Table II - Physical quantities (χ branch, hPB model)

ξ	1.8	2.8	0
$\Omega(q_0)$	6.8 10^4	5.9 10^4	2.6 10^4
$\omega(q_0)$	1.2 10^{13}	1.1 10^{13}	7.2 10^{12}
$T(q_0)$	0.5 ps	0.6 ps	0.9 ps
$A(q_0)$	5.6 $10^{-2}\AA$	6.0 $10^{-2}\AA$	9.0 $10^{-2}\AA$
$\lambda(q_0)$	8.7 δ	5.6 δ	∞

Table III - Physical quantities (ψ branch, hPB model)

15. Introduction of helicoidal terms in the Yakushevich model

Let us now consider the effects of introducing helicoidal interactions in the Yakushevich model; here again we add to the Yakushevich hamiltonian an harmonic potential modelling the helicoidal interaction; i.e. we have

$$U_H = \frac{1}{2}\gamma \left[\left(\theta^{(1)}_{n+h} - \theta^{(2)}_n \right)^2 + \left(\theta^{(2)}_{n+h} - \theta^{(1)}_n \right)^2 \right] \tag{1}$$

Here again we pass to normal coordinates ψ, χ, with

$$\theta^{(1)}_n = \psi_n + \chi_n \ \ ; \ \ \theta^{(2)}_n = \psi_n - \chi_n \tag{2}$$

in terms of which (1) reads

$$U_H = \frac{1}{2}\gamma \left[(\psi_{n+h} - \psi_n)^2 + (\chi_{n+h} + \chi_n)^2 \right] \tag{3}$$

Notice here as well the different signs with which ψ and χ enter in this interaction.

The total hamiltonian of the helicoidal Yakushevich (or hY) model reads therefore

$$H = T + V_S + V_T + V_H \tag{4}$$

where T, V_S, V_T are as in the Y model and

$$V_H = \sum_n \frac{1}{2}\gamma \left[(\psi_{n+h} - \psi_n)^2 + (\chi_{n+h} + \chi_n)^2 \right] \tag{5}$$

with h the half-pitch of the helix in base units ($h = 5$).

This hamiltonian gives as equations of motion

$$\begin{aligned} I\ddot{\psi}_n =& \beta(\psi_{n+1} - 2\psi_n + \psi_{n-1}) + \gamma(\psi_{n+h} - 2\psi_n + \psi_{n-h}) - \alpha \sin\psi_n \cos\chi_n \\ I\ddot{\chi}_n =& \beta(\psi_{n+1} - 2\psi_n + \psi_{n-1}) - \gamma(\psi_{n+h} - 2\psi_n + \psi_{n-h}) - \alpha \sin\chi_n (\cos\psi_n - \cos\chi_n) \end{aligned} \tag{6}$$

and small oscillations are described by the equations

$$\begin{aligned} I\ddot{\psi}_n =& \beta(\psi_{n+1} - 2\psi_n + \psi_{n-1}) + \gamma(\psi_{n+h} - 2\psi_n + \psi_{n-h}) - \alpha\psi_n \\ m\ddot{\chi}_n =& \beta(\chi_{n+1} - 2\chi_n + \chi_{n-1}) - \gamma(\psi_{n+h} - 2\psi_n + \psi_{n-h}) \end{aligned} \tag{7}$$

In order to consider the continuum limit of these, we introduce again the nonlocal (linear) operators $\mathcal{W}_\pm$,

$$\mathcal{W}_\pm(\phi) = \phi(x+w,t) \mp 2\phi(x,t) + \phi(x-w,t) \tag{8}$$

and write the full equations as

$$\begin{aligned} \psi_{tt} =& \kappa\triangle\psi + \rho\mathcal{W}_+(\psi) - \sigma \sin\psi \cos\chi \\ \chi_{tt} =& \kappa\triangle\chi - \rho\mathcal{W}_-(\chi) - \sigma \sin\chi (\cos\psi - \cos\chi) \end{aligned} \tag{9}$$

where we have used

$$\kappa \equiv \beta\delta^2/I \ \ , \ \ \rho \equiv \gamma/I \ \ ; \ \ \sigma = \alpha/I \ \ ; \ \ w = h\delta \tag{10}$$

with δ the distance between consecutive bases along the axis of the double helix ($\delta \simeq 3.4 \mathring{A}$).

As for the small oscillation equations, with the same notations these are given simply by

$$\begin{aligned} \psi_{tt} =& \kappa\triangle\psi + \rho\mathcal{W}_+(\psi) - \sigma\psi \\ \chi_{tt} =& \kappa\triangle\chi - \rho\mathcal{W}_-(\chi) \end{aligned} \tag{11}$$

Notice that these are formally analogous to the one obtained for the hPB model, so that we will not discuss the dispersion relations for the hY model, but just refer to the corresponding discussion of the hPB model.

We stress that in the case of the Y and hY models the fields ψ, χ are decoupled at the level of small oscillations (so that we can still call these "normal coordinates"), but are instead coupled through nonlinear terms, contrary to what happens in PB and hPB models. Since the ψ and χ fields are now interacting through nonlinear terms, the "crossing points" (i.e. the points at which the two branches meet) do have physical meaning, corresponding to resonances between the two fields [6,13].

16. Solitons in the helicoidal Yakushevich model

As already recalled, the Yakushevich and helicoidal Yakushevich models have been primarily developed to describe travelling solitons, which are supposed to play a central role in the transcription of DNA [11].

Therefore, we will concentrate on solitons, and not consider standing nondispersive waves in the hY model. These are waves corresponding to the extremal points of the dispersion relations, and their physical interpretation is again as breather modes giving local pulsating and nonpropagating openings of the double helix, i.e. breaking of the H bonds pairing bases at same site on different helices. The numerical computations, presented elsewhere [12], show that indeed experimental data on spontaneous denaturation of DNA are best fitted by the hPB model.

The full field equations for the hY model were obtained to be

$$\begin{aligned} \psi_{tt} =& \kappa \Delta \psi + \rho \mathcal{W}_+(\psi) - \sigma \sin\psi \cos\chi \\ \chi_{tt} =& \kappa \Delta \chi - \rho \mathcal{W}_-(\chi) - \sigma \sin\chi (\cos\psi - \cos\chi) \end{aligned} \tag{1}$$

to which correspondhamiltonian H and lagrangian L given by

$$\begin{aligned} L =& \frac{I}{\delta} \int \frac{1}{2} \left(\psi_t^2 + \chi_t^2\right) - \frac{1}{2}\kappa \left[(\nabla\psi)^2 + (\nabla\chi)^2\right] - W(\psi,\chi) \mathrm{d}x \\ H =& \frac{I}{\delta} \int \frac{1}{2} \left(\psi_t^2 + \chi_t^2\right) + \frac{1}{2}\kappa \left[(\nabla\psi)^2 + (\nabla\chi)^2\right] + W(\psi,\chi) \mathrm{d}x \end{aligned} \tag{2}$$

where now $W(\psi, \chi)$ is made up of a local and a nonlocal ($\mathcal{N}$) part:

$$\begin{aligned} W(\psi,\chi) =& \frac{1}{2}\sigma \left[1 + \cos^2\chi - 2\cos\psi\cos\chi\right] + \mathcal{N}(\psi,\chi) \\ \mathcal{N}(\psi,\chi) =& \frac{1}{2}\rho \left[\left[\psi(x+w) - \psi(x)\right]^2 + \left[\chi(x+w) + \chi(x)\right]^2\right] \end{aligned} \tag{3}$$

The appearance of nonlocal terms in (1),(2) is the main new qualitative feature encountered in the helicoidal version of the model. Physically, this correspond to the introduction of a second lenght scale in the model: beside the lattice spaceing δ, we now also have introduced the (half) pitch of the helix, by the scale $w = h\delta$.

We want now to concentrate on solitons, i.e. on solutions of the form

$$\begin{aligned} \psi(x,t) =& \psi(x - vt) \equiv \psi(z) \\ \chi(x,t) =& \chi(x - vt) \equiv \chi(z) \end{aligned} \tag{4}$$

Notice that the discussion of boundary conditions conducted in the planar case does still apply here, as well as the related classification of soliton solutions by topological (or soliton) integer numbers (n, m).

Inserting the ansatz (4) into (2), we get the hamiltonian and the lagrangian for helicoidal Yakushevich solitons, where $\nabla \equiv \partial/\partial z$:

$$\begin{aligned} H =& \frac{I}{\delta} \int \frac{1}{2}(v^2 + \kappa) \left[(\nabla\psi)^2 + (\nabla\chi)^2\right] + W(\psi,\chi) \mathrm{d}z \\ L =& \frac{I}{\delta} \int \frac{1}{2}(v^2 - \kappa) \left[(\nabla\psi)^2 + (\nabla\chi)^2\right] - W(\psi,\chi) \mathrm{d}z \end{aligned} \tag{5}$$

We write again $\widetilde{\mu} = v^2 - \kappa = -\mu$, and the bounds on v, μ given in the planar case also apply here.

The field evolution equations are now[6]

$$\begin{aligned} \mu \psi_{zz} &= \frac{\partial W}{\partial \psi} \\ \mu \chi_{zz} &= \frac{\partial W}{\partial \chi} \end{aligned} \tag{6}$$

By the same procedure as in the planar case, these give

$$\frac{1}{2}\mu \left[(\nabla\psi)^2 + (\nabla\chi)^2 \right] = W(\psi,\chi) \tag{7}$$

which again shows, once used in (5), that the energy of soliton solutions $\bar{\psi}, \bar{\chi}$ is given by

$$E = \frac{I\kappa}{\delta} \int \left[(\nabla\bar{\psi})^2 + (\nabla\bar{\chi})^2 \right] \mathrm{d}z \tag{8}$$

17. Exact solution for the helicoidal (1,0) soliton

The nonlocal terms make it quite difficult to obtain explicit soliton solutions for the hY model; one can nevertheless get some scaling relations obeyed by these solutions, which are also of use in order to obtain the explicit form of the simplest of them.

The idea is to scale down the lenght $w = h\delta$ to δ, which produces an "effective planar lagrangian", and then apply the continuous approximation. The limitation to this approach come from the special sign in the nonlocal interaction of χ field, which prevents from obtaining an effective lagrangian of the Yakushevich type, and would introduce terms of the type $\chi\nabla\chi$ (see the discussion in [6]).

The limitations to work with an "effective planar lagrangian" for the rescaled hY model do not apply if we just consider the (1,0) solitons, due to $\chi \equiv 0$. In this case we can obtain the explicit soliton solution just by the one obtained for the planar Y model, by scaling arguments.

Indeed, by scaling arguments [6,8], one proofs that by redefining once again an effective mass

$$\mu_H \equiv \mu - \rho\delta^2 \equiv (\kappa - \rho)\delta^2 - v^2 \tag{1}$$

the equations are formally analogous to the equation encountered in the planar case; i.e. we get

$$\frac{1}{2}\mu_H (\nabla\psi)^2 = \alpha(1 - \cos\psi) \tag{2}$$

This can be integrated as shown earlier; notice that in these terms the introduction of helicoidal interactions amounts to a rescaling of the constant A appearing in the explicit solution, which is now

$$A = \sqrt{\frac{2\alpha}{\mu_H}} = \sqrt{\frac{2\alpha}{\mu - \rho\delta^2}} \tag{3}$$

The dependence of (1,0) soliton energy on speed is given by

$$E(\lambda,\gamma) = \frac{A'}{B' - \gamma^2} E(\delta, 0) \tag{4}$$

where

$$A' = 1 + \frac{\gamma}{\beta} \quad ; \quad B' = 1 + \frac{\gamma}{h^2\beta} \tag{5}$$

(see [6,8] for details). This means that the scaling of energy with speed is qualitatively analogous to the one obtained for the planar Y model; similar considerations apply to the relation of size versus speed of soliton solutions.

[6] With more precise notation, one should have $\delta W/\delta\psi$, $\delta W/\delta\chi$, as these are now functional derivatives.

It should be stressed that the (1,0) solitons correspond to those whose role in DNA transcription was first suggested by Englander [11], so that the discussion of the present section is of particular relevance, although concerning only one specific soliton solution.

18. Numerical results for solitons in the helicoidal Yakushevich model

For solitons other than the (1,0) ones, we are not able to determine explicit analytical solutions, nor exact scaling laws at fixed λ; we must therefore revert to numerical computations.

We fix the parameters α, β, γ, I appearing in the model, and let μ vary between 0 and $\mu_{\max}$ (i.e. we consider different values of γ; it should be recalled that physically $\gamma \simeq 10^{-8}$). For any given value of μ, one can determine numerically, on a sufficently large discrete lattice, the configuration $\bar{\psi}, \bar{\chi}$ which makes extremal - among those with prescribed boundary conditions - the Yakushevich soliton lagrangian (see eq.(2) of section 22).

Let $S(\mu)$ be this extremal value of the lagrangian,

$$S(\mu) = -\frac{I}{\delta} \int \frac{1}{2}\mu \left[(\nabla\bar{\psi})^2 + (\nabla\bar{\chi})^2 \right] + W(\bar{\psi}, \bar{\chi}) \mathrm{d}z \tag{1}$$

The corresponding energy, by comparing the soliton lagrangian and hamiltonian and recalling that for soliton solutions

$$\frac{1}{2}\mu \left[(\nabla\bar{\psi})^2 + (\nabla\bar{\chi})^2 \right] = W(\bar{\psi}, \bar{\chi}) \tag{2}$$

is given simply by

$$H(\mu) = \frac{\mu_{\max}}{\mu} S(\mu) \tag{3}$$

In terms of γ, this reads

$$H(\gamma) = \frac{1}{1-\gamma^2} S\left(\mu(\gamma)\right) \equiv \frac{1}{1-\gamma^2} S\left((1-\gamma^2)\mu_{\max}\right) \tag{4}$$

The minimization of the lagrangian is performed by a Montecarlo algorithm; the values of the parameters are given in table IV and discussed in [8]; the results of the numerical computations are given in fig.6for the (1,1) soliton (as recalled above, the ψ field is supposed to matter for the solitons we are looking for: we want therefore a nonzero ψ soliton number); here we plot $H(\gamma)$ in terms of γ, together with the best fit by functions of the form

$$H(\gamma) = \frac{A}{B - \gamma^2} \tag{5}$$

This shows good qualitative agreement with the situation seen above for the (1,0) soliton, which is in turn qualitatively equivalent to the one for planar Y solitons.

Conclusions

We have discussed the relevant degrees of freedom in DNA dynamics at body temperature; we have then considered in detail two simple models compatible with our general discussion. These give behaviours which are in quite good agreement with experimental findings; in particular the hPB model correctly predicts the size and time frequency order of magnitude for spontaneous openings of base pairs, while the Y and hY models have soliton solutions as those supposed to play a central role in DNA transcription, the size of these matching the experimental observations.

Acknowledgements

I would like to thank the organizers of the conference for inviting me in St. Petersbourg and for giving me this opportunity to present my views on DNA models. My interest in DNA nonlinear dynamics was raised by papers of, and kept awake by correspondence with, prof. L. Yakushevich, which I would like to thank here. I would also like to thank C. Reiss and M. Peyrard for the discussions we had together and for permit to use part of a preliminary version of our joint work [6] here.

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