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Solitons in planar and helicoidal Yakushevich model of DNA dynamics

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We study the soliton solutions for the Yakushevich model of DNA torsion dynamics, with special attention to the dependence of their energy on speed and to their scaling properties. We give explicit solutions in the simpler case, and a numerical approach for more complicated ones.

1. Introduction

In the Yakushevich model [1] of DNA torsion dynamics, one considers two discrete chains, $i=\pm 1$, whose sites are denoted by an integer $n \in \mathbb{Z}$; to each site is associated an angular variable $\phi_n^{(i)}$ (with $\phi_n^{(i)}=0\ \forall i, n$ corresponding to equilibrium configuration), and the dynamics of the model is given by the Newton equations

$$I\ddot{\phi}_n^{(i)} = -\frac{\partial V}{\partial \phi_n^{(i)}}, \tag{1}$$

where the potential V splits into two parts V_{T} and V_{S} representing respectively the "transverse" interaction among corresponding sites of the two chains and the first neighbour interaction along the same chain; these correspond physically to hydrogen bonding and stacking [2].

Since stacking is quite stronger than hydrogen bonding, one considers a harmonic potential for V_{S}; the form of V_{T} is discussed by Yakushevich [1] (see also ref. [3] for the present choice of coordinates); if the same orientation is chosen for the two chains we have

$$V_{\mathrm{S}} = \sum_{i=\pm 1} \sum_n \tfrac{1}{2}\tilde{K}_s[\phi_{n+1}^{(i)} - \phi_n^{(i)}]^2,$$

$$V_{\mathrm{T}} = \sum_n \tilde{\alpha}\{[\sin(\phi_n^{(1)}) + \sin(\phi_n^{(-1)})]^2 + [2-\cos(\phi_n^{(1)}) - \cos(\phi_n^{(-1)})]^2\}. \tag{2}$$

In ref. [4], I proposed to introduce an "helicoidal" interaction, taking care of the helical geometry (see refs. [4] and [5] for motivation and discussion); this introduces a third, "nonlocal" term V_{H} in V (this is called nonlocal since it concerns interactions among bases which are not contiguous along the helix; anyway the source of the interaction lies in the fact that the bases are near in the three-dimensional space). This connects bases which are h bases away, where h is the half-pitch of the helix measured in sites; i.e. $h=5$ for standard DNA geometry. If the ϕ's remain small, we can take it to be

$$V_{\mathrm{H}} = \sum_{i,n} \tfrac{1}{2}\tilde{K}_{\mathrm{H}}(\phi_{n+h}^{(\epsilon(i))} - \phi_n^{(i)})^2,$$

but if the ϕ's vary over 2π we should preserve the 2π periodicity of the angular variables, e.g. [3] by assuming

$$V_{\mathrm{H}} = \sum_{i,n} \tilde{K}_{\mathrm{H}}[1-\cos(\phi_{n+h}^{(\epsilon(i))} - \phi_n^{(i)})], \tag{3}$$

which will be our choice.

In this note, we want to discuss full nonlinear solutions to (1) with

$$V = V_{\mathrm{T}} + V_{\mathrm{S}} + V_{\mathrm{H}}.$$

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Such a model will be called a helicoidal Yakushevich model (hY for short); the linearized dynamics for it (and related models) around the equilibrium position has already been discussed elsewhere [1,3–5]), so here we discuss only soliton solutions.

In particular, the helicoidal interaction introduces a preferred length scale besides the lattice size in the model; in the case of soliton solutions a preferred length scale is also a preferred speed scale, so that one could wonder it this can help to explain the selection of size and speed for the would-be solitons occurring in DNA processes; having in mind such a motivation, we want to discuss the dependence of soliton energy on the soliton speed.

Our interest in the problem is mainly due to the hypothesis that solitonic excitations play a major role in DNA transcription, as first suggested by Englander et al. [6] (they were also able to assign a definite size to such would-be solitons, that turned out to be of order $2h$ in site units). It should be stressed that these should be solitons in both the topological and the dynamic meaning of the term: this ensures topological stability and complies with the geometry of DNA transcription on the one hand, and ensures propagation of the excitation with no energy dissipation on the other. In other terms, according to Englander et al.'s idea we should concentrate on kink-like solitons rather than on pulse-like ones; we will indeed proceed in this way.

A related line of research concerns the DNA denaturation, for which a model sharing many features with the one discussed here has been proposed by Peyrard and Bishop [7] (see also ref. [5]); we will not consider this problem in the present note. It should also be mentioned that other models, similar and/or related to Yakushevich or Peyrard–Bishop models, were proposed by other authors, see refs. [8–10]; we will not consider these here.

2. Change of coordinates

It is convenient to pass to coordinates

$$\psi_n^+ = \tfrac{1}{2}(\phi_n^{(1)} + \phi_n^{(-1)}) ,$$
$$\psi_n^- = \tfrac{1}{2}(\phi_n^{(1)} - \phi_n^{(-1)}) . \tag{4}$$

With some straightforward algebra, we get then

$$V_\mathrm{S} = \sum_n \tfrac{1}{2} K_\mathrm{S} [(\psi_{n+1}^+ - \psi_n^+)^2 + (\psi_{n+1}^- - \psi_n^-)^2] ,$$
$$V_\mathrm{T} = \sum_n \alpha [1 + \cos^2(\psi_n^-) - 2\cos(\psi_n^+)\cos(\psi_n^-)] ,$$
$$V_\mathrm{H} = \sum_n K_\mathrm{H} [1 - \cos(\psi_{n+h}^- + \psi_n^-)\cos(\psi_{n+h}^+ - \psi_n^+)] \tag{5}$$

(notice the different signs in the ψ^+ and ψ^- parts of V_H).

The parameters α, K_S, K_H should be regarded as phenomenological ones; they are related to the previous ones by $\alpha = 4\tilde{\alpha}$, $K_\mathrm{S} = 2\tilde{K}_\mathrm{S}$, $K_\mathrm{H} = \tilde{K}_\mathrm{H}$. Notice that $V = 0$ for $\psi_k^+ = \psi_k^- = 0 \ \forall k$.

3. Field formulation

We can also pass to the continuum approximation; this means considering fields $\psi^+(z, t)$, $\psi^-(z, t)$ with

$$\psi^+(n\delta, t) = \psi_n^+(t) , \quad \psi^-(n\delta, t) = \psi_n^-(t) , \tag{6}$$

with δ the intersite distance along the axis of the double helix. If the fields do not vary too quickly we can then consider

$$(\psi_{n+1}^+ - \psi_n^+) \simeq \delta \partial\psi^+/\partial z = \delta\psi_z^+ ,$$
$$\psi_{n+1}^+ - 2\psi_n^+ + \psi_{n-1}^+ \simeq \delta^2 \psi_{zz}^+ \tag{6'}$$

and the same for ψ^- (here and in the following the z subscripts denote partial derivatives).

Both the continuum approximation and the dropping of terms of higher orders in δ in (6′) are justified if the fields vary slowly on the length scale of the lattice unit; in other words, if in the Fourier decomposition of the fields, only wavelengths large compared with δ are relevant. The solutions we are interested in satisfy indeed this condition, given the above mentioned estimate of Englander et al. [6] of a size of order $2h\delta$ ($h = 5$) for the solitons in real DNA.

In this approximation, eqs. (1), (5) read

$$I\psi_{tt}^\pm = K_\mathrm{S}\delta^2\psi_{zz}^\pm - \frac{\partial W(\lambda)}{\partial\psi^\pm} , \tag{7}$$

with $W = V_\mathrm{T} + V_\mathrm{H}$ and $\lambda = h\delta$; we have introduced the explicit dependence of W on λ in (7) for future discussion.

Equations (7) correspond to a Lagrangian and Hamiltonian given by

$$L=\frac{1}{\delta}\int_{-\infty}^{\infty}\{\tfrac{1}{2}I[(\psi_t^+)^2+(\psi_t^-)^2]$$
$$-\tfrac{1}{2}K_S\delta^2[(\psi_z^+)^2+(\psi_z^-)^2]-W(\psi^+,\psi^-;\lambda)\}\,dz\,, \tag{8}$$

$$H=\frac{1}{\delta}\int_{-\infty}^{\infty}\{\tfrac{1}{2}I[(\psi_t^+)^2+(\psi_t^-)^2]$$
$$+\tfrac{1}{2}K_S\delta^2[(\psi_z^+)^2+(\psi_z^-)^2]+W(\psi^+,\psi^-;\lambda)\}\,dz\,, \tag{9}$$

where the factor $1/\delta$ keeps the energy scale equal to the one of the discrete model.

4. Solitons

As we have anticipated, we are particularly interested in soliton solutions, i.e. in the case

$$\psi^\pm(z,t)=\psi^\pm(z-vt)\equiv\psi^\pm(x)\,. \tag{10}$$

Substituting this into (7) we get the *equation for Yakushevich solitons*

$$(Iv^2-K_S\delta^2)\psi^\pm_{xx}=-\frac{\partial W}{\partial\psi^\pm}\,. \tag{11}$$

On physical grounds, we want that for $x\to\pm\infty$ the solution goes to one of the minima of W; noticing that W is 2π-periodic in ψ^+ and ψ^-, this means that we ask

$$\psi_x^+(\pm\infty)=\psi_x^-(\pm\infty)=0\,,$$
$$\psi^+(\pm\infty)=2\pi n_\pm\,,\quad \psi^-(\pm\infty)=2\pi m_\pm\,. \tag{12'}$$

Without any loss in generality we can take $n_-=m_-=0$, so that the second equation above is

$$\psi^+(-\infty)=\psi^-(-\infty)=0\,,$$
$$\psi^+(\infty)=2\pi n\,,\quad \psi^-(\infty)=2\pi m \tag{12''}$$

and a solution of (11) satisfying (12) will be called an (n,m) soliton.

Equation (11) can be seen, if we look at x as a "time", as describing the motion of a particle of "effective mass" $Iv^2-K_S\delta^2$ under the effect of the potential W.

By remarking that $W=0$ at the minima, and that (12) fix the energy of this motion to be $E=0$, we conclude that the desired solutions can exist only if the "effective mass" is negative; this poses a bound on the speed v of the solitons:

$$|v|<\sqrt{K_S\delta^2/I}=v_M\,. \tag{13}$$

We also write

$$\mu=K_S\delta^2-Iv^2\leqslant K_S\delta^2=\mu_M\,, \tag{14}$$

so that (11) become simply

$$\mu\psi^\pm_{xx}=\frac{\partial W}{\partial\psi^\pm}\,. \tag{15}$$

Multiplying these by, respectively, ψ_x^+ and ψ_x^-, and summing, we get a relation among complete differentials; this can be integrated once to give

$$\tfrac{1}{2}\mu[(\psi_x^+)^2+(\psi_x^-)^2]=W(\psi^+,\psi^-;\lambda)\,, \tag{16}$$

where the constant of integration is set to zero by the boundary conditions (12).

If we substitute (10) into (8), (9), we get the Lagrangian and Hamiltonian for Yakushevich solitons:

$$L=-\frac{1}{\delta}\int_{-\infty}^{\infty}\{\tfrac{1}{2}\mu[(\psi_x^+)^2+(\psi_x^-)^2]$$
$$+W(\psi^+,\psi^-;\lambda)\}\,dx\,, \tag{17}$$

$$H=\frac{1}{\delta}\int_{-\infty}^{\infty}\{\tfrac{1}{2}\nu[(\psi_x^+)^2+(\psi_x^-)^2]$$
$$+W(\psi^+,\psi^-;\lambda\}\,dx\,, \tag{18}$$

where

$$\nu=Iv^2+K_S\delta^2\,. \tag{19}$$

The energy of a solution $\bar\psi^+,\bar\psi^-$ of (16) is therefore

$$E(\bar\psi^+,\bar\psi^-;\lambda)=\frac{K_S\delta^2}{\delta}\int_{-\infty}^{\infty}[(\bar\psi_x^+)^2+(\bar\psi_x^-)^2]\,dx\,. \tag{20}$$

5. The nonhelicoidal case

It is instructive to discuss the "non-helicoidal" case

$K_H=0$; now W reduces actually to $V_T(\psi^+, \psi^-)$, and the parameter λ does simply disappear.

Equation (16) is now

$$\tfrac{1}{2}\mu[(\psi_x^+)^2+(\psi_x^-)^2]=V_T(\psi^+, \psi^-) \tag{21}$$

and this is invariant under the rescaling

$$\mu\to\alpha^2\mu\,, \quad x\to\alpha x\,. \tag{22}$$

In other words, if $\psi^+=f(x;\mu)$, $\psi^-=g(x;\mu)$ solve (21), then for $\mu\to\alpha^2\mu=M$ we have the solution

$$\psi^{+\prime}=f(x;M)\equiv f(x/\alpha;\mu)\,,$$
$$\psi^{-\prime}=g(x;M)\equiv g(x/\alpha;\mu)\,. \tag{23}$$

Obviously, this does just correspond to the fact that particles of different masses moving in a potential, with the same initial position, same energy, and collinear initial velocities, move along the same trajectories with different speed.

If now we use (20) and denote $E_0(\mu)$ the energy of the soliton for $K_H=0$ and velocity corresponding to μ by (14), we get

$$E_0(\alpha^2\mu)$$
$$=K_S\delta\int_{-\infty}^{\infty}\left(\frac{d}{dx}[f(x/\alpha;\mu)+g(x/\alpha;\mu)]\right)^2 dx$$
$$=\frac{1}{\alpha^2}E_0(\mu)\,,$$

which can be rewritten as

$$E_0(\mu_1)=\frac{\mu_0}{\mu_1}E_0(\mu_0)\,. \tag{24}$$

This shows that, once (n, m) are chosen, see (12), the solitons with lower energy are those with lower speed, as is indeed entirely natural.

In particular, if $v_0=0$, $\mu_0=\mu_M$ and $v_1=\gamma v_M$, by (14), (13) we have

$$\mu_1=(1-\gamma^2)\mu_M \tag{25}$$

and we can revert (24) into a scaling relation for energy versus speed of solitons

$$E_0(\gamma)=\frac{1}{1-\gamma^2}E_0(0)\,. \tag{26}$$

6. Scaling laws for the helicoidal case

Let us now go back to the general case $K_H\neq0$; now the nonlocal potential W is not invariant under (22), (23). We can anyway restore invariance by allowing for a rescaling of the parameter λ as well. Indeed, the non-invariance of W is due to terms like $\psi^+(x+\lambda)-\psi^+(x)$; if we set, say,

$$A_0(\mu,\lambda)=f(x+\lambda;\mu)-f(x;\mu)\,,$$

we see that this is invariant under (22), (23) provided that $\lambda\to\lambda'=\alpha\lambda$, i.e.

$$A_0(\alpha^2\mu,\lambda')=f\left(\frac{x+\lambda'}{\alpha};\mu\right)-f\left(\frac{x}{\alpha};\mu\right)$$

and $A_0(\alpha^2\mu, \alpha\lambda)=A_0(\mu,\lambda)$. This reasoning applies to the ψ^- as well to the ψ^+ terms.

We write now a solution to (16) as

$$\psi^\pm=f^\pm(x;\mu,\lambda)\,.$$

The above discussion shows that

$$f^\pm(x;\alpha^2\mu,\lambda)=f^\pm(x/\alpha;\mu,\lambda)\,. \tag{27}$$

By substituting this into (20), we get

$$E(\lambda,\mu_1)=\frac{\mu_0}{\mu_1}E(\sqrt{\mu_1/\mu_0}\,\lambda,\mu_0)\,, \tag{28}$$

or, passing again to v dependence and choosing $v_0=0$, see (25), (26),

$$E(\lambda,\gamma)=\frac{1}{1-\gamma^2}E(\sqrt{1-\gamma^2}\lambda,0) \tag{29}$$

Therefore now, in order to evaluate the dependence of soliton energy (with fixed soliton number) on the speed of solitons – with fixed $\lambda=\lambda_0$ – we could proceed by considering λ as a variable parameter and studying the dependence of energy of stationary solutions (i.e. solitons with zero speed) on this parameter λ. (It can be worth remarking that the physical case of $v<10^3$ base/s corresponds to $\gamma\simeq10^{-8}$.)

Using (28), we can scale up to reduce the length scale of helicoidal interaction to the lattice size, i.e.

$$\lambda_0=\sqrt{\mu_1/\mu_0}\,\lambda=\delta\,, \tag{30}$$

which gives

$$E(\lambda, \mu_1) = (\lambda/\lambda_0)^2 E(\lambda_0, \mu_0) ,$$

$$\mu_0 = (\lambda/\lambda_0)^2 \mu_1 . \tag{31}$$

Since $\lambda_0 = \delta$, we can now use the approximation (6′) for V_H as well; this gives

$$V_H = K_H \int_{-\infty}^{\infty} [1 - \cos(2\psi^- + \nabla\psi^-) \cos(\nabla\psi^+)] \, dx \tag{32}$$

and we have transformed V_H into a local potential.

The cosine nonlinearity prevents one from applying scaling arguments; we can go back to the original form of V_H proposed by Yakushevich – corresponding to slowly varying fields over the λ length scale – to write the integrand in the above as

$$1 - [\cos 2\psi^- - 2(\sin 2\psi^-)\nabla\psi^- - 4(\cos 2\psi^-)(\nabla\psi^-)^2][1 - \tfrac{1}{2}(\nabla\psi^+)^2]. \tag{33}$$

Even in this form, we still have two differences with respect to the nonhelicoidal case: (i) the transversal and stacking parts of the potential are now interacting, precisely due to terms originated by V_H; (ii) the dependence of V_H on gradients is not of homogeneous degree, and scaling does not hold even in the approximation (33). Both of these problems are solved if $\psi^-(x) \equiv 0$; this is the case for the (1, 0) soliton of minimal energy, and we will now concentrate on this case.

7. Energy scaling for the (1, 0) helicoidal soliton

It is quite clear from the expression of V that for the (1, 0) soliton we have a solution with $\psi^- \equiv 0$, and that this has minimal energy among the (1, 0) soliton solutions; we will study this. For the (1, 0) soliton in the slowly varying field approximation, we have

$$V_H = \tfrac{1}{2} K_H \delta^2 \int_{-\infty}^{\infty} (\nabla\psi^+)^2 \, dx \tag{34}$$

and the equivalent of (21) is now

$$\tfrac{1}{2}(\mu + K_H\delta^2)(\psi_x^+)^2 = V_T(\psi^+, 0) . \tag{35}$$

Redefining the "helicoidal effective mass" μ_H as

$$\mu_H = \mu + K_H\delta^2 \equiv (K_S + K_H)\delta^2 - Iv^2 \leqslant (K_S + K_H)\delta^2 = \mu_{HM} , \tag{36}$$

we have

$$\tfrac{1}{2}\mu_H(\psi_x^+)^2 = V_T(\psi^+, 0) , \tag{37}$$

which is formally analogous to (21); if $\psi^+ = f(x; \mu_H)$ solves this, we have as solution for $\mu'_H = \alpha^2 \mu_H$,

$$\psi^{+\prime} = f(x; \alpha^2\mu_H) = f(x/\alpha; \mu_H) . \tag{38}$$

If now we write $E_0(\mu_H)$ for the energy of the soliton in this approximation, i.e. $E(\delta, \mu) = E_0(\mu_H)$, we have a scaling relation analogous to (24), i.e.

$$E_0(\mu_H) = \frac{\mu_H^*}{\mu_H} E_0(\mu_H^*) . \tag{39}$$

Combining (31), (36) and (39), we get

$$E(\lambda, \mu) = (\lambda/\delta)^2 E(\delta, (\lambda/\delta)^2\mu)$$
$$= (\lambda/\delta)^2 E_0((\lambda/\delta)^2\mu + K_H\delta^2)$$
$$= \left(\frac{\lambda}{\delta}\right)^2 \frac{\mu_H^*}{(\lambda/\delta)^2\mu + K_H\delta^2} E_0(\mu_H^*) ,$$

or, with constants A, B defined by comparison with the above,

$$E(\lambda, \mu) = \frac{A}{B + \mu} E_0(\mu_H^*) . \tag{40}$$

If we want to pass to γ dependence – in which case it is entirely natural to choose $\mu_H^* = \mu_{HM}$, corresponding to zero speed – we will get

$$E(\lambda, \gamma) = \frac{A'}{B' - \gamma^2} E_0(\mu_H^*) . \tag{41}$$

The determination of A, B, A', B' is a matter of straightforward algebra, which gives (with the choice $\mu_H^* = \mu_{HM}$)

$$A = (K_S + K_H)\delta^2 , \quad B = K_H\delta^4/\lambda^2 ,$$

$$A' = 1 + K_H/K_S , \quad B' = 1 + (K_H/K_S)\delta^2/\lambda^2 . \tag{42}$$

Notice that for $K_H = 0$ we find again (26), as it should be; we also recall that $(\delta/\lambda)^2 = \frac{1}{25}$, so that the main correction is due to the K_H/K_S term in A'.

8. Explicit solution for the (1, 0) soliton

In the case of the (1, 0) soliton of minimal energy it is actually possible, thanks to $\psi^-=0$, to give the explicit solution, which we derive here.

The equation is now (see (21), (35))

$$\tfrac{1}{2}\mu(\psi_x^+)^2=2\alpha(1-\cos\psi^+)$$

which, writing $a=\sqrt{2\alpha/\mu}$, reduces to

$$\int\frac{\mathrm{d}\psi^+}{\sqrt{1-\cos\psi^+}}=\sqrt{2}\,a\int\mathrm{d}x\,. \tag{43}$$

The integral on the left hand side gives

$$\int\frac{\mathrm{d}\psi^+}{\sqrt{1-\cos\psi^+}}=-\sqrt{2}\,\operatorname{arcsinh}\left(\frac{1+\cos\psi^+}{|\sin\psi^+|}\right)$$
$$=-\sqrt{2}\,\operatorname{arcsinh}\left(\sqrt{\frac{1+\cos\psi^+}{1-\cos\psi^+}}\right)$$
$$\equiv-\sqrt{2}\,\operatorname{arcsinh}[F(\psi^+)]\,.$$

Equation (43) reduces therefore to

$$F(\psi^+)=\sinh(c-ax)\equiv\sqrt{f(x)}\,,$$

or, using the explicit form of $F(\psi^+)$ and with some straightforward algebra,

$$\psi^+(x)=\arccos\left(\frac{f(x)-1}{f(x)+1}\right).$$

Here c is the integration constant from (43); it is immediate to check that the behaviour of $\psi^+(x)$ at infinity does not depend on it: indeed, as it had to be by (12),

$$\lim_{x\to\pm\infty}\frac{f(x)-1}{f(x)+1}=1\,,\quad\lim_{x\to\pm\infty}\psi^+(x)=\arccos(1)\,.$$

The constant c determines the position of the soliton at time $t=0$; it is immediate to check that requiring $\psi^+(0)=\pi$ yields $c=0$.

With this, the explicit solution reads

$$\psi^+(x)=\arccos\left(\frac{\sinh^2(ax)-1}{\sinh^2(ax)+1}\right), \tag{44}$$

which satisfies the scaling relations obtained above; in fig. 1 we plot $\psi^-(x)$ for $a=1$.

It would also be possible, along the same lines,to derive the (0, 1) soliton of minimal energy: now by (21) and $\psi^+=0$ we have

$$\tfrac{1}{2}\mu(\psi_x^-)^2=2\alpha(1-\cos\psi^-)^2 \tag{45}$$

and, with $a=2\sqrt{\alpha/\mu}$ we have

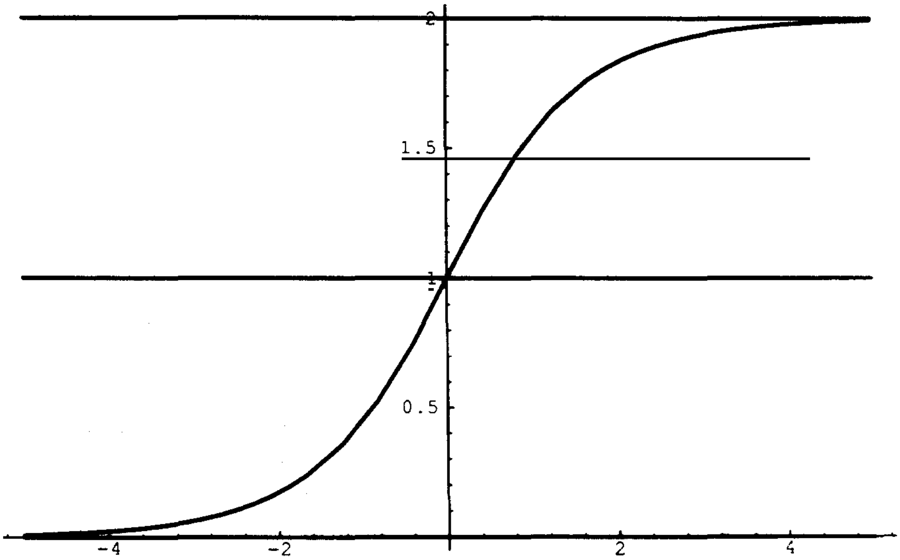

Fig. 1. The (1, 0) soliton (in units of π), as given by formula (44) with $a=1$.

$$\int \frac{d\psi^-}{1-\cos\psi^-} = a \int dx\,. \tag{46}$$

Performing the integration, imposing $\psi^-(0)=\pi$ (which puts again the integration constant to zero) and with some simple algebra, we arrive at

$$\psi^-(x) = \arccos\left(\frac{a^2x^2-1}{a^2x^2+1}\right). \tag{47}$$

It should not be forgotten anyway that this is a solution to the *planar* Yakushevich model. While in the (1, 0) case the helicoidal term could be taken care of, by a careful use of rescalings, by a μ scaling, eq. (33) shows that such a correspondence between solutions to the planar and helicoidal Yakushevich models does not hold in this (0, 1) case.

We would also like to stress that the explicit formulas (44), (47) imply, as it can be seen by straightforward algebra, that the size of the soliton (defined as the length of the interval over which $\phi^\pm$ differs from its asymptotic value by more than an arbitrary but fixed small quantity) satisfies

$$s_\pm(\mu) = c_\pm\sqrt{\mu/\alpha}\,, \quad s_\pm(\gamma) = k_\pm\sqrt{1-\gamma^2}\,,$$

with $c_\pm$, $k_\pm$ numerical constants that can be explicitly and easily computed. This scaling is coherent with (22), (23) and (27).

9. Numerical results for the helicoidal case

In the previous section we were able to determine an explicit solution for the (1, 0) soliton, thanks to $\psi^-=0$. In the general case, as already remarked, we are not only unable to give exact solutions or scaling properties, but we are also in general unable to have qualitative information on the behaviour of the energy as a function of soliton speed.

We revert therefore to a numerical approach: we fix the constants α, K_S, K_H of the model, as well as the soliton number, and let μ vary between 0 and μ_M; for each value of μ we determine numerically (on a linear lattice of 100 points) te configuration $\bar\psi^+$, $\bar\psi^-$ which makes extremal, with boundary values as above, the soliton Lagrangian (17). We can then compute the soliton energy $E(\mu)$ or $E(v)$ by plugging $\bar\psi^+$, $\bar\psi^-$ into (18) or, more simply, by (20).

The numerical minimization is performed by a Monte Carlo algorithm. Let us call $S(\mu)$ the extremal value of L, i.e.

$$S(\mu) = \frac{1}{\delta}\int_{-\infty}^{\infty} \{\tfrac{1}{2}\mu[(\bar\psi_x^+)^2 + (\bar\psi_x^-)^2] + W(\bar\psi^+, \bar\psi^-)\}\,dx\,.$$

Using (16) and (20), and recalling (14), we get for the energy of the soliton

$$H(\mu) = \frac{\mu_M}{\mu} S(\mu)\,.$$

With the notation used in (25) we have for the energy as a function of γ

$$H(\gamma) = \frac{1}{1-\gamma^2} S(\mu(\gamma)) \equiv \frac{1}{1-\gamma^2} S((1-\gamma^2)\mu_M)\,.$$

We have performed our numerical computations with the following values of the parameters: $\alpha=0.13$ eV, $K_H=0.009$ eV, $K_S=0.025$ eV, $\delta=3.4$ Å; with this μ varies between 0 and $\mu_M=0.025\delta^2$; in the numerical results we choose units in which $\delta=1$.

The simplest case in which none of ψ^+, ψ^- is identically zero is provided by the (1, 1) soliton; our numerical results for this case are reported in fig. 2 (with logarithmic scale for γ), and turn out to be in very good agreement with the exact results obtained above for the (1, 0) soliton, as it is shown by fitting

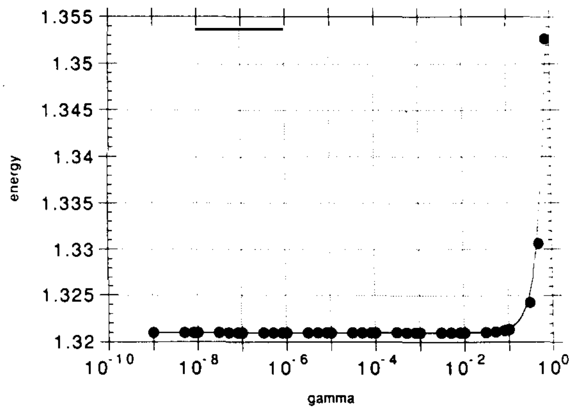

Fig. 2. Energy versus speed of the (1, 1) soliton: solid dots represent the result of Monte Carlo computations, the continuous line is the best fit of numerical data by a function of the form (41).

the numerical data with a function of the form (41).

Indeed, we have computed the energy $H(\gamma)$ for 35 different values of γ, with uniform logarithmic distribution over the range $[10^{-9}, 0.8]$: the best fitting with curves of the form $H(\gamma)=a/(b-\gamma^2)$ is obtained for $a=17.67$, $b=1.74$, with a χ^2 of 0.227; this correspond to a confidence level of over 99%.

10. Conclusions

We have considered solitons for both the planar [1] and the helicoidal [4] Yakushevich model of DNA torsion dynamics; after providing general formulas and framework, we have obtained the scaling relations obeyed by soliton solutions in terms of the physical parameters characterizing them and the model.

In the planar case, we were also able to prove that the dependence of soliton energy on its speed is given by (26); in the helicoidal case scaling involves unphysical changes in the parameter λ – fixed by the geometry of the double helix – but permits one nevertheless to predict the behaviour of energy as a function of speed for the simpler solitons, see (41).

We concentrated on the (1, 0) soliton, corresponding qualitatively to the solutions conjectured by Englander et al. [6], and were able to give the explicit solution in this case; it satisfies the above mentioned scaling properties.

Finally, we have performed numerical computations – making use of an approach based on the general formulation presented in the first part of this note – for more complicated solitons; these show a behaviour of the energy as a function of soliton speed in good agreement with the one displayed by the completely solved case.

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References

[1] L.V. Yakushevich, Phys. Lett. A 136 (1989) 413.
[2] W. Saenger, Principles of nucleic acid structure, 2nd Ed. (Springer, Berlin, 1988).
[3] G. Gaeta, An amended version of "helicoidal" models of DNA dynamics, Preprint C.P.Th. 1992, submitted to Phys. Lett. A.
[4] G. Gaeta, Phys. Lett. A 143 (1990) 227.
[5] T. Dauxois, Phys. Lett. A 159 (1991) 390.
[6] S.W. Englander et al., Proc. Natl. Acad. Sci. USA 77 (1980) 7222.
[7] M. Peyrard and A.R. Bishop, Phys. Rev. Lett. 62 (1989) 2755.
[8] S. Yomosa, Phys. Rev. A 27 (1983) 2120; 30 (1984) 474;
S. Takeno and S. Homma, Prog. Theor. Phys. 77 (1987) 548;
C.T. Zhang, Phys. Rev. A 35 (1987) 886;
L.L. Van Zandt, Phys. Rev. A 40 (1989) 6134; 42 (1990) 5036.
[9] E.W. Prohofsky, Phys. Rev. A 38 (1988) 1538;
M. Techera, L.L. Daemen and E.W. Prohofsky, Phys. Rev. A 40 (1989) 6636; 41 (1990) 4543; 42 (1990) 5033.
[10] V. Muto, A.C. Scott and P.L. Christiansen, Phys. Lett. A 136 (1989) 33; Physica D 44 (1990) 75;
V. Muto, P.S. Lomdahl and P.L. Christiansen, Phys. Rev. A 42 (1990) 7452;
V. Muto, Nonlinear models for DNA dynamics, Ph.D. Thesis (1988).