

Soliton propagation in homogeneous and inhomogeneous models for DNA torsion dynamics.

M. Cadoni¹, **R. De Leo**^{1,2}, S. Demelio¹, G. Gaeta³

¹INFN, sez. di Cagliari, Italy

²Department of Mathematics
University of Cagliari, Italy

³Department of Mathematics
University of Milano, Italy

Brighton - December 7th

A rough sketch of DNA's structure

DNA is a double chain of nucleotides
there are ~ 30 atoms / nucleotide
a DNA chain has 10^5 – 10^{10} nodes.

A rough sketch of DNA's structure

DNA is a double chain of nucleotides
there are ~ 30 atoms / nucleotide
a DNA chain has 10^5 – 10^{10} nodes.

Nucleotides have two components:
a *Sugar-Phosphate group* (backbone)
and a *Nitrogen Base*.

The SP group is the same for all nodes,
the sequence of NB is the genetic info.

A rough sketch of DNA's structure

DNA is a double chain of nucleotides
there are ~ 30 atoms / nucleotide
a DNA chain has 10^5 – 10^{10} nodes.

Nucleotides have two components:
a *Sugar-Phosphate group* (backbone)
and a *Nitrogen Base*.

The SP group is the same for all nodes,
the sequence of NB is the genetic info.

There are four types of NB:
Adenine, Guanine, Cytosine, Thymine.
Covalent bonds link NB with SP,
H-bonds bet. facing NB link the two chains.

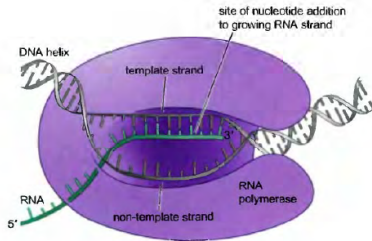
What solitons have to do with DNA

It is an old conjecture¹ that rotational kinks and breathers could play a functional role in DNA's **transcription** and **denaturation** phenomena.

¹see A. Davydov, *Solitons in Molecular Systems*, Kluwer (1981),
S. Engländer et al., PNAS USA **77** (1980)

What solitons have to do with DNA

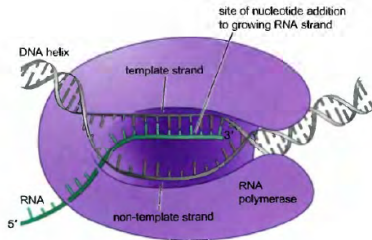
It is an old conjecture¹ that rotational kinks and breathers could play a functional role in DNA's **transcription** and **denaturation** phenomena.



¹see A. Davydov, *Solitons in Molecular Systems*, Kluwer (1981),
S. Englander et al., PNAS USA **77** (1980)

What solitons have to do with DNA

It is an old conjecture¹ that rotational kinks and breathers could play a functional role in DNA's **transcription** and **denaturation** phenomena.



These phenomena are quite complex – involving the interaction with enzymes, cell environment and so on – hence the focus has been set on formulating a reliable model describing in simple terms the dynamics of DNA as a mechanical system.

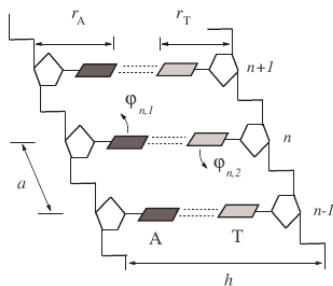
¹see A. Davydov, *Solitons in Molecular Systems*, Kluwer (1981),
S. Engländer et al., *PNAS USA* **77** (1980)

Our Main Goal

Our main goal is to understand whether the *essentially inhomogeneous* DNA molecule, seen as a mechanical system, supports the existence of narrow (of the order of 10bp) twist solitons (kinks) able to move for long enough distances (of the order of 100bp) at the natural speeds for the transcription and duplication phenomena (in the range 50–10³bp/s) under an external force and dissipation.

Starting point: the Salerno and Yakushevich models

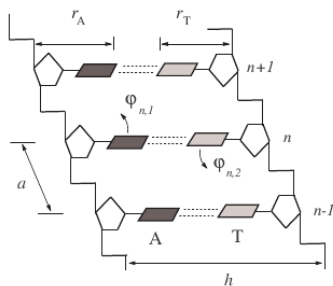
Starting point: the Salerno and Yakushevich models



$$\Delta\varphi_{n,1} = \varphi_{n,1} - \varphi_{n-1,1}$$

$$\Delta\varphi_{n,2} = \varphi_{n,2} - \varphi_{n-1,2}$$

Starting point: the Salerno and Yakushevich models

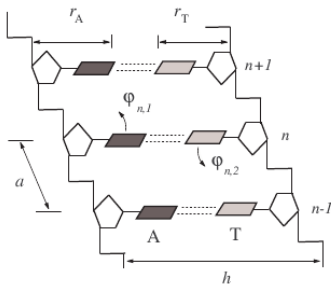


$$\Delta\varphi_{n,1} = \varphi_{n,1} - \varphi_{n-1,1}$$

$$\Delta\varphi_{n,2} = \varphi_{n,2} - \varphi_{n-1,2}$$

$$H_S = \underbrace{\sum_n \left(\frac{l_{n,1}}{2} \dot{\varphi}_{n,1}^2 + \frac{l_{n,2}}{2} \dot{\varphi}_{n,2}^2 \right)}_{\text{Kinetic Energy}} + \underbrace{K_{n,1}^{ts} (\Delta\varphi_{n,1})^2 + K_{n,2}^{ts} (\Delta\varphi_{n,2})^2}_{\text{Torsion + Stacking}} + \underbrace{K_n^P \bar{r}^2 [1 - \cos(\varphi_{n,1} - \varphi_{n,2})]}_{\text{Pairing (physical pendulum)}}$$

Starting point: the Salerno and Yakushevich models



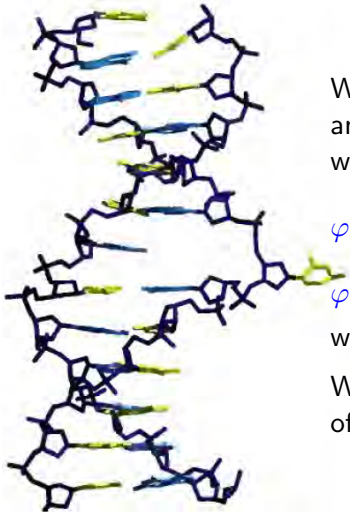
$$\Delta\varphi_{n,1} = \varphi_{n,1} - \varphi_{n-1,1}$$

$$\Delta\varphi_{n,2} = \varphi_{n,2} - \varphi_{n-1,2}$$

$$H_S = \underbrace{\sum_n \left[\frac{I_{n,1}}{2} \dot{\varphi}_{n,1}^2 + \frac{I_{n,2}}{2} \dot{\varphi}_{n,2}^2 \right]}_{\text{Kinetic Energy}} + \underbrace{K_{n,1}^{ts} (\Delta\varphi_{n,1})^2 + K_{n,2}^{ts} (\Delta\varphi_{n,2})^2}_{\text{Torsion + Stacking}} + \underbrace{K_n^P \bar{r}^2 [1 - \cos(\varphi_{n,1} - \varphi_{n,2})]}_{\text{Pairing (physical pendulum)}}$$

$$H_Y = \underbrace{\sum_n \left[\frac{I_{n,1}}{2} \dot{\varphi}_{n,1}^2 + \frac{I_{n,2}}{2} \dot{\varphi}_{n,2}^2 \right]}_{\text{Kinetic Energy}} + \underbrace{K_{n,1}^{ts} (1 - \cos \Delta\varphi_{n,1}) + K_{n,2}^{ts} (1 - \cos \Delta\varphi_{n,2})}_{\text{Torsion + Stacking}} + \underbrace{K_n^P [r_{n,1}(r_{n,1} + r_{n,2})(1 - \cos \varphi_{n,1}) + r_{n,2}(r_{n,1} + r_{n,2})(1 - \cos \varphi_{n,2}) - r_{n,1}r_{n,2}(1 - \cos(\varphi_{n,1} - \varphi_{n,2}))]}_{\text{Pairing (harmonic potential in the distance between facing bases)}}$$

Twist Solitons in DNA



We consider a double chain with N nodes and look for solutions $\varphi_{n,i}(t)$ with boundary conditions

$$\varphi_{1,1}(t) = 0, \varphi_{1,2}(t) = 0$$

$$\varphi_{N,1}(t) = 2\pi p, \varphi_{N,2}(t) = 2\pi q$$

with $p, q \in \mathbb{Z}$.

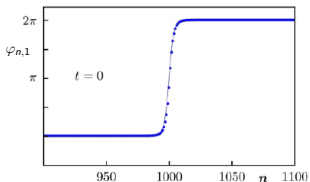
We call (p, q) the *topological type* of the solution.

REMARK: in the continuous homogeneous limit the (1, 1) solutions of H_Y are symmetric and each one is exactly a sine-Gordon kink, i.e. a kink solution of

$$\mu \partial_{tt} \varphi(x, t) = K \partial_{xx} \varphi(x, t) - \kappa \sin \varphi(x, t)$$

Twist Solitons in DNA

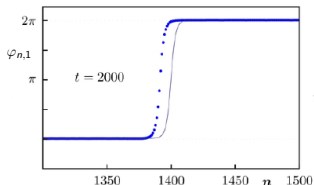
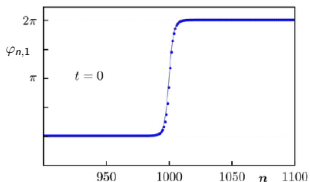
REMARK: in the continuous homogeneous limit the $(1, 1)$ solutions of H_Y are symmetric and each one is exactly a sine-Gordon kink, i.e. a kink solution of

$$\mu \partial_{tt} \varphi(x, t) = K \partial_{xx} \varphi(x, t) - \kappa \sin \varphi(x, t)$$


Twist Solitons in DNA

REMARK: in the continuous homogeneous limit the $(1, 1)$ solutions of H_Y are symmetric and each one is exactly

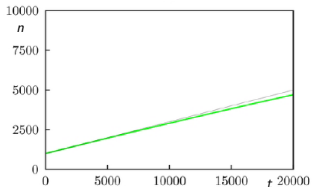
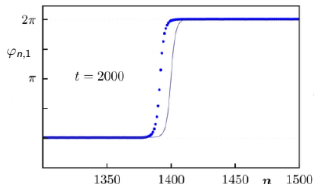
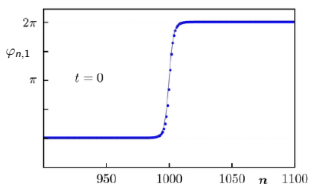
a sine-Gordon kink, i.e. a kink solution of

$$\mu \partial_{tt} \varphi(x, t) = K \partial_{xx} \varphi(x, t) - \kappa \sin \varphi(x, t)$$


Twist Solitons in DNA

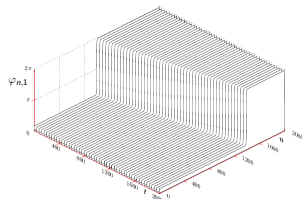
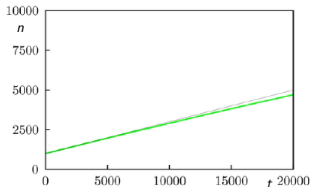
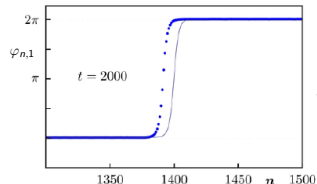
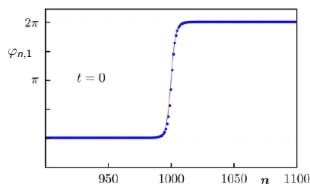
REMARK: in the continuous homogeneous limit the $(1, 1)$ solutions of H_Y are symmetric and each one is exactly

a sine-Gordon kink, i.e. a kink solution of

$$\mu \partial_{tt} \varphi(x, t) = K \partial_{xx} \varphi(x, t) - \kappa \sin \varphi(x, t)$$


Twist Solitons in DNA

REMARK: in the continuous homogeneous limit the $(1, 1)$ solutions of H_Y are symmetric and each one is exactly a sine-Gordon kink, i.e. a kink solution of

$$\mu \partial_{tt} \varphi(x, t) = K \partial_{xx} \varphi(x, t) - \kappa \sin \varphi(x, t)$$


Motion of kinks in the inhomogeneous Salerno model

$$H = \sum_i \frac{I_i^\psi}{2} (\dot{\psi}_i)^2 + \frac{I_i^\theta}{2} (\dot{\theta}_i)^2 + \frac{k_i^\psi}{2} (\psi_i - \psi_{i-1})^2 + \frac{k_i^\theta}{2} (\theta_i - \theta_{i-1})^2 + \eta_i [1 - \cos(\psi_i - \theta_i)].$$

238

E. Lennholm, M. Hörnquist / Physica D 177 (2003) 233–241

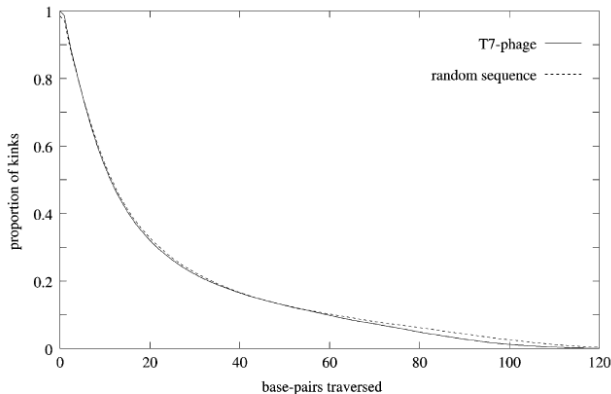


Fig. 3. Fraction of kinks that moves at least the number of base-pairs given by the x -axis. The solid line corresponds to the real genome of the T7-phage, while the dashed line corresponds to a random sequence.

Motion of kinks in the inhomogeneous Yakushevich model

$$H = \sum_n \left\{ \frac{1}{2} I_{n,1} \dot{\varphi}_{n,1}^2 + \frac{1}{2} I_{n,2} \dot{\varphi}_{n,2}^2 + \epsilon_{n,1} \sin^2 \frac{\varphi_{n+1,1} - \varphi_{n,1}}{2} + \epsilon_{n,2} \sin^2 \frac{\varphi_{n+1,2} - \varphi_{n,2}}{2} + V_{\alpha\beta}(\varphi_{n,1}, \varphi_{n,2}) \right\} \quad 12$$

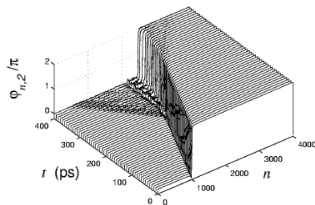
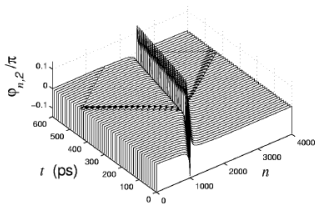
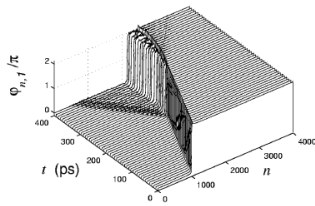
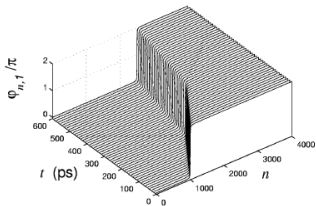
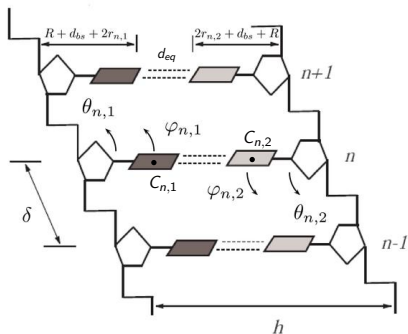


FIG. 11: Movement of soliton with $\mathbf{q}=(1,0)$, $s=0.5$ through the boundary between homogeneous AT and GC regions.

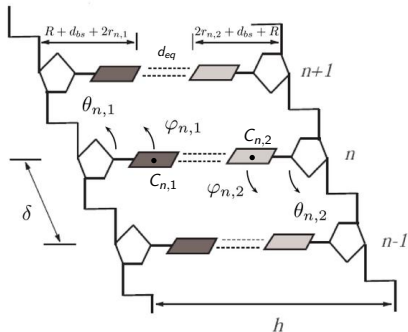
FIG. 12: Entering two component soliton (charge $\mathbf{q}=(1,1)$), velocity $s=0.5$) the random inhomogeneous region of the chain, and further disintegration of the soliton.

Our composite model for DNA



	A	T	G	C	mean	Sugar
m	134	125	150	110	130	85
I	3.6×10^3	3.0×10^3	4.4×10^3	2.3×10^3	3.3×10^3	2.9×10^3
l	3.9	2.9	4.1	2.7	3.4	3.1
d_{bs}	1.0	1.0	1.0	1.0	1.0	-
d_{eq}	3.0	3.0	3.0	3.0	3.0	-

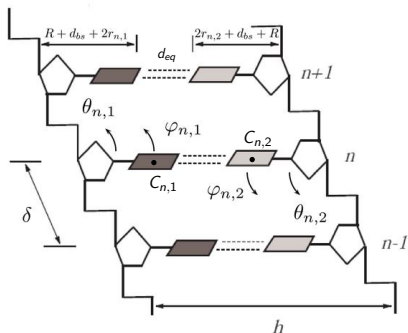
Our composite model for DNA



	A	T	G	C	mean	Sugar
m	134	125	150	110	130	85
I	3.6×10^3	3.0×10^3	4.4×10^3	2.3×10^3	3.3×10^3	2.9×10^3
l	3.9	2.9	4.1	2.7	3.4	3.1
d_{bs}	1.0	1.0	1.0	1.0	1.0	-
d_{eq}	3.0	3.0	3.0	3.0	3.0	-

$$H = T + V_t + V_s + V_p + V_h + V_w$$

Our composite model for DNA

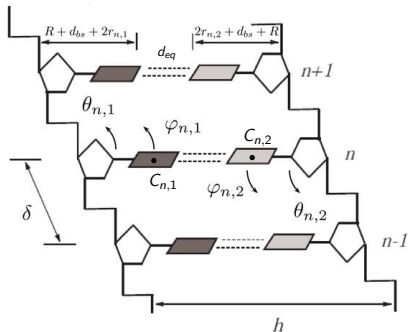


	A	T	G	C	mean	Sugar
m	134	125	150	110	130	85
I	3.6×10^3	3.0×10^3	4.4×10^3	2.3×10^3	3.3×10^3	2.9×10^3
l	3.9	2.9	4.1	2.7	3.4	3.1
d_{bs}	1.0	1.0	1.0	1.0	1.0	-
d_{eq}	3.0	3.0	3.0	3.0	3.0	-

$$H = T + V_t + V_s + V_p + V_h + V_w$$

$$T = \frac{1}{2} \sum_{n=1}^N \sum_{i=1}^2 \left[I_t \dot{\theta}_{n,i}^2 + m_{n,i} \dot{C}_{n,i}^2 \right]$$

Our composite model for DNA



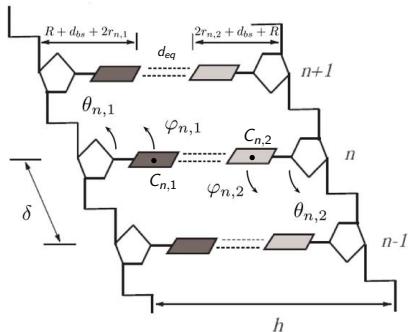
	A	T	G	C	mean	Sugar
m	134	125	150	110	130	85
I	3.6×10^3	3.0×10^3	4.4×10^3	2.3×10^3	3.3×10^3	2.9×10^3
l	3.9	2.9	4.1	2.7	3.4	3.1
d_{bs}	1.0	1.0	1.0	1.0	1.0	-
d_{eq}	3.0	3.0	3.0	3.0	3.0	-

$$H = T + V_t + V_s + V_p + V_h + V_w$$

$$T = \frac{1}{2} \sum_{n=1}^N \sum_{i=1}^2 \left[I_t \dot{\theta}_{n,i}^2 + m_{n,i} \dot{C}_{n,i}^2 \right]$$

$$V_t = \sum_{n=1}^N \sum_{i=1}^2 K_t [1 - \cos(\Delta\theta_{n,i})]$$

Our composite model for DNA



	A	T	G	C	mean	Sugar
m	134	125	150	110	130	85
I	3.6×10^3	3.0×10^3	4.4×10^3	2.3×10^3	3.3×10^3	2.9×10^3
l	3.9	2.9	4.1	2.7	3.4	3.1
d_{bs}	1.0	1.0	1.0	1.0	1.0	-
d_{eq}	3.0	3.0	3.0	3.0	3.0	-

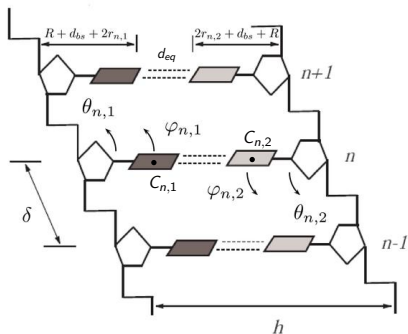
$$H = T + V_t + V_s + V_p + V_h + V_w$$

$$T = \frac{1}{2} \sum_{n=1}^N \sum_{i=1}^2 \left[I_t \dot{\theta}_{n,i}^2 + m_{n,i} \dot{C}_{n,i}^2 \right]$$

$$V_t = \sum_{n=1}^N \sum_{i=1}^2 K_t [1 - \cos(\Delta\theta_{n,i})]$$

$$V_s = \frac{1}{2} \sum_{n=1}^N \sum_{i=1}^2 K_s \frac{d_{xy}^2(C_{n+1,i}; C_{n,i})}{(d_{bs} + \bar{r})^2}$$

Our composite model for DNA



	A	T	G	C	mean	Sugar
m	134	125	150	110	130	85
I	3.6×10^3	3.0×10^3	4.4×10^3	2.3×10^3	3.3×10^3	2.9×10^3
l	3.9	2.9	4.1	2.7	3.4	3.1
d_{bs}	1.0	1.0	1.0	1.0	1.0	-
d_{eq}	3.0	3.0	3.0	3.0	3.0	-

$$H = T + V_t + V_s + V_p + V_h + V_w$$

$$T = \frac{1}{2} \sum_{n=1}^N \sum_{i=1}^2 \left[I_t \dot{\theta}_{n,i}^2 + m_{n,i} \dot{C}_{n,i}^2 \right]$$

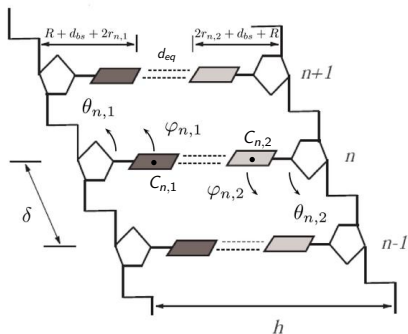
$$V_t = \sum_{n=1}^N \sum_{i=1}^2 K_t [1 - \cos(\Delta\theta_{n,i})]$$

$$V_s = \frac{1}{2} \sum_{n=1}^N \sum_{i=1}^2 K_s \frac{d_{xy}^2(C_{n+1,i}; C_{n,i})}{(d_{bs} + \bar{r})^2}$$

$$V_p = \sum_{n=1}^N D_n \left[1 - e^{-\mu(d(C_{n+1,i}; C_{n,i}) - d_{eq})} \right]^2$$

(Morse potential)

Our composite model for DNA



	K_t	K_s	K_p	D_{AT}	D_{GC}	a	K_h
lo bd	130kJ/mol	-	3.5 N/m	30 meV	45 meV	2\AA^{-1}	$K_t/100$
up bd	720kJ/mol	16.6N/m	30 N/m	50 meV	75 meV	4\AA^{-1}	$K_t/25$
	g_t	g_s	g_p	d_{AT}	d_{GC}	μ	g_h
lo bd	0.58	-	0.91	0.013	0.02	8.8	$g_t/100$
up bd	3.2	1.6	7.8	0.02	0.03	17.6	$g_t/25$

	A	T	G	C	mean	Sugar
m	134	125	150	110	130	85
I	3.6×10^3	3.0×10^3	4.4×10^3	2.3×10^3	3.3×10^3	2.9×10^3
l	3.9	2.9	4.1	2.7	3.4	3.1
d_{bs}	1.0	1.0	1.0	1.0	1.0	-
d_{eq}	3.0	3.0	3.0	3.0	3.0	-

$$H = T + V_t + V_s + V_p + V_h + V_w$$

$$T = \frac{1}{2} \sum_{n=1}^N \sum_{i=1}^2 \left[I_t \dot{\theta}_{n,i}^2 + m_{n,i} \dot{C}_{n,i}^2 \right]$$

$$V_t = \sum_{n=1}^N \sum_{i=1}^2 K_t [1 - \cos(\Delta\theta_{n,i})]$$

$$V_s = \frac{1}{2} \sum_{n=1}^N \sum_{i=1}^2 K_s \frac{d_{xy}^2(C_{n+1,i}; C_{n,i})}{(d_{bs} + \bar{r})^2}$$

$$V_p = \sum_{n=1}^N D_n \left[1 - e^{-\mu(d(C_{n+1,i}; C_{n,i}) - d_{eq})} \right]^2$$

(Morse potential)

The initial profiles of the kinks were determined by looking for extremals of the action after the “constant speed” discrete ansatz

$$\dot{q}_n = v(q_n - q_{n+1})/\delta, \text{ where } q_n = (\theta_{n,1}, \theta_{n,2}, \phi_{n,1}, \phi_{n,2}).$$

For the evolution, since all systems we deal with are conservative, we decided to use geometric integrators in order to minimize the error sources.

We started by using a *Lagrangian* approach to study kinks evolution in the Yakushevich model, mainly because several geometric integrators for Lagrangian systems were available on the net, in particular those developed by Ernst Hairer (GNI_IRK2).

The initial profiles of the kinks were determined by looking for extremals of the action after the “constant speed” discrete ansatz

$$\dot{q}_n = v(q_n - q_{n+1})/\delta, \text{ where } q_n = (\theta_{n,1}, \theta_{n,2}, \phi_{n,1}, \phi_{n,2}).$$

For the evolution, since all systems we deal with are conservative, we decided to use geometric integrators in order to minimize the error sources.

We started by using a *Lagrangian* approach to study kinks evolution in the Yakushevich model, mainly because several geometric integrators for Lagrangian systems were available on the net, in particular those developed by Ernst Hairer (GNI_IRK2).

The initial profiles of the kinks were determined by looking for extremals of the action after the “constant speed” discrete ansatz

$$\dot{q}_n = v(q_n - q_{n+1})/\delta, \text{ where } q_n = (\theta_{n,1}, \theta_{n,2}, \phi_{n,1}, \phi_{n,2}).$$

For the evolution, since all systems we deal with are conservative, we decided to use geometric integrators in order to minimize the error sources.

We started by using a *Lagrangian* approach to study kinks evolution in the Yakushevich model, mainly because several geometric integrators for Lagrangian systems were available on the net, in particular those developed by Ernst Hairer (GNI_IRK2).

When we switched to our composite model we found out that no geometric integrators were available instead for Lagrangians whose kinetic energy depends on the spatial coordinates (e.g. double pendulum). We contacted Hairer and were suggested to switch to the *Hamiltonian* approach, for which he kindly provided to us several geometric integrators (GRKAAD).

Finally, we repeated some of the numerical results using non-symplectic ODEs algorithms from the GSL and found an excellent agreement.

REMARK: there is a time scale inerent in our numerical analysis.

Consider the simplest case of the Yakushevich model (SG):

$$\mu \partial_{tt} \varphi(x, t) = K \partial_{xx} \varphi(x, t) - \kappa \sin \varphi(x, t)$$

We have $\mu \simeq 1.3 \cdot 10^{-25} \text{ kKs}^2 / \text{mol}$ while $K \simeq \kappa \simeq 1 \text{ kJ/mol}$. In order to have constants of the same order of magnitude we must change time unit to $TU = 3.4 \cdot 10^{-13} \text{ s!}$.

When we switched to our composite model we found out that no geometric integrators were available instead for Lagrangians whose kinetic energy depends on the spatial coordinates (e.g. double pendulum). We contacted Hairer and were suggested to switch to the *Hamiltonian* approach, for which he kindly provided to us several geometric integrators (GRKAAD).

Finally, we repeated some of the numerical results using non-symplectic ODEs algorithms from the GSL and found an excellent agreement.

REMARK: there is a time scale inerent in our numerical analysis.

Consider the simplest case of the Yakushevich model (SG):

$$\mu \partial_{tt} \varphi(x, t) = K \partial_{xx} \varphi(x, t) - \kappa \sin \varphi(x, t)$$

We have $\mu \simeq 1.3 \cdot 10^{-25} \text{ kKs}^2 / \text{mol}$ while $K \simeq \kappa \simeq 1 \text{ kJ/mol}$. In order to have constants of the same order of magnitude we must change time unit to $TU = 3.4 \cdot 10^{-13} \text{ s!}$.

When we switched to our composite model we found out that no geometric integrators were available instead for Lagrangians whose kinetic energy depends on the spatial coordinates (e.g. double pendulum). We contacted Hairer and were suggested to switch to the *Hamiltonian* approach, for which he kindly provided to us several geometric integrators (GRKAAD).

Finally, we repeated some of the numerical results using non-symplectic ODEs algorithms from the GSL and found an excellent agreement.

REMARK: there is a time scale inerent in our numerical analysis.

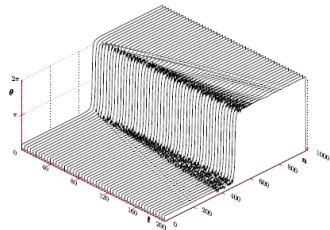
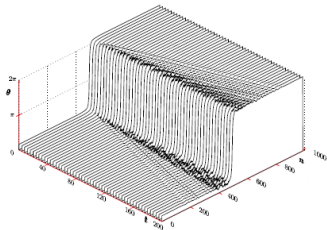
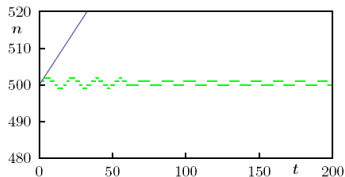
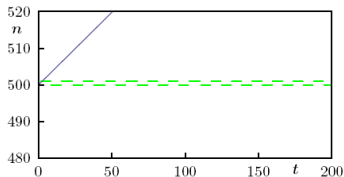
Consider the simplest case of the Yakushevich model (SG):

$$\mu \partial_{tt} \varphi(x, t) = K \partial_{xx} \varphi(x, t) - \kappa \sin \varphi(x, t)$$

We have $\mu \simeq 1.3 \cdot 10^{-25} \text{ kKs}^2 / \text{mol}$ while $K \simeq \kappa \simeq 1 \text{ kJ/mol}$. In order to have constants of the same order of magnitude we must change time unit to $TU = 3.4 \cdot 10^{-13} \text{ s!}$.

Why we do not use a harmonic pairing potential

Under the harmonic approximation, kinks in the composite model do not move *even in homogeneous chains*.



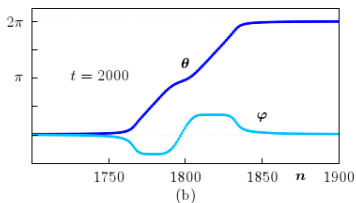
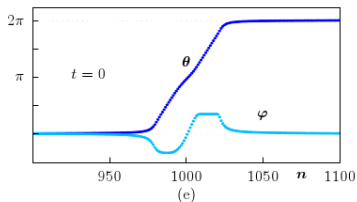
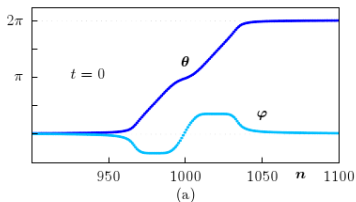
Motion of kinks in the composite homogeneous model

$$H = v^2 \sum_{n=1}^N \sum_{i=1}^2 \left[\frac{I}{2\delta^2} [\Delta\theta_{n,i}]^2 + m [\Delta C_{n,i}]^2 \right] + \sum_{n=1}^N \sum_{i=1}^2 g_\tau [1 - \cos(\Delta\theta_{n,i})] + \frac{1}{2} \sum_{n=1}^N \sum_{i=1}^2 g_s \frac{d_{xy}^2(C_{n+1,i}; C_{n,i})}{(d_{bs} + \bar{r})^2} + \sum_{n=1}^N d \left[1 - e^{-\mu(d(C_{n,1}; C_{n,2}) - d_{eq})} \right]^2 + V_h + V_w$$

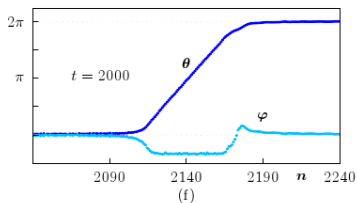
Motion of kinks in the composite homogeneous model

$$H = v^2 \sum_{n=1}^N \sum_{i=1}^2 \left[\frac{I}{2\delta^2} [\Delta\theta_{n,i}]^2 + m[\Delta C_{n,i}]^2 \right] + \sum_{n=1}^N \sum_{i=1}^2 g_t [1 - \cos(\Delta\theta_{n,i})] + \frac{1}{2} \sum_{n=1}^N \sum_{i=1}^2 g_s \frac{d_{xy}^2(C_{n+1,i}; C_{n,i})}{(d_{bs} + \bar{r})^2} + \sum_{n=1}^N d \left[1 - e^{-\mu(d(C_{n,1}; C_{n,2}) - d_{eq})} \right]^2 + V_h + V_w$$

$$\bar{i}_t = 1.1, \bar{i}_s = 1.3, g_t = 1, g_s = 0.3, g_h = 0.01, g_p = 0.02, d = 0.02, \mu = 6.3$$



$$v = 0.4$$

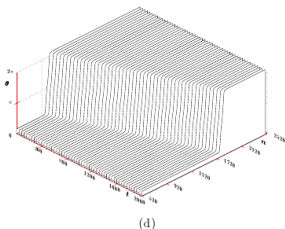
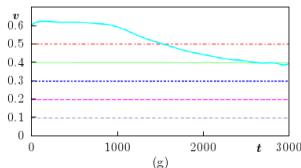
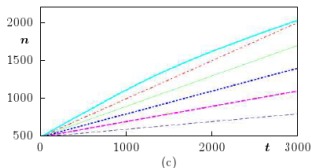


$$v = 0.62 \simeq v_{lim}$$

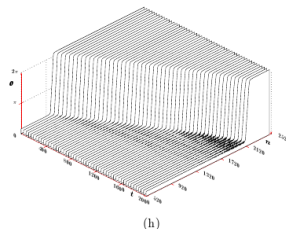
Motion of kinks in the composite homogeneous model

$$H = v^2 \sum_{n=1}^N \sum_{i=1}^2 \left[\frac{I}{2\delta^2} [\Delta\theta_{n,i}]^2 + m[\Delta C_{n,i}]^2 \right] + \sum_{n=1}^N \sum_{i=1}^2 g_t [1 - \cos(\Delta\theta_{n,i})] + \frac{1}{2} \sum_{n=1}^N \sum_{i=1}^2 g_s \frac{d_{xy}^2(C_{n+1,i}; C_{n,i})}{(d_{bs} + \bar{r})^2} + \sum_{n=1}^N d \left[1 - e^{-\mu(d(C_{n,1}; C_{n,2}) - d_{eq})} \right]^2 + V_h + V_w$$

$$\bar{i}_t = 1.1, \bar{i}_s = 1.3, g_t = 1, g_s = 0.3, g_h = 0.01, g_p = 0.02, d = 0.02, \mu = 6.3$$



$$v = 0.4$$



$$v = 0.62 \simeq v_{lim}$$

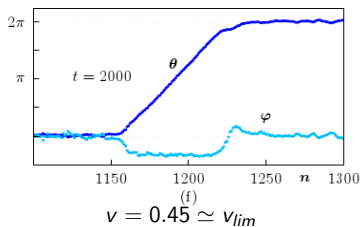
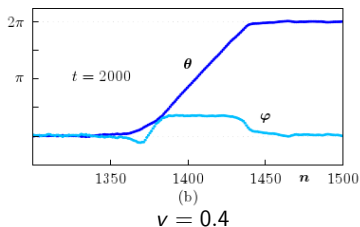
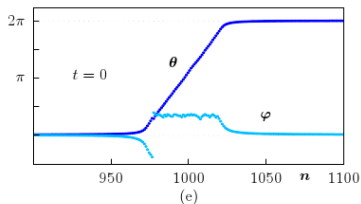
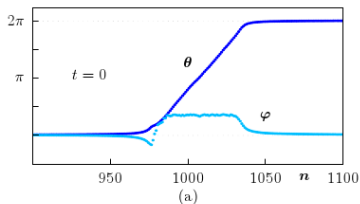
Motion of kinks in the composite inhomogeneous model

$$H = v^2 \sum_{n=1}^N \sum_{i=1}^2 \left[\frac{j_{n,i}}{2\delta^2} [\Delta\theta_{n,i}]^2 + m_{n,i} [\Delta C_{n,i}]^2 \right] + \sum_{n=1}^N \sum_{i=1}^2 g_t [1 - \cos(\Delta\theta_{n,i})] + \frac{1}{2} \sum_{n=1}^N \sum_{i=1}^2 g_s \frac{d_{xy}^2(C_{n+1,i}; C_{n,i})}{(d_{bs} + \bar{r})^2} + \sum_{n=1}^N d_n \left[1 - e^{-\mu(d(C_{n,1}; C_{n,2}) - d_{eq})} \right]^2 + V_h + V_w$$

Motion of kinks in the composite inhomogeneous model

$$H = v^2 \sum_{n=1}^N \sum_{i=1}^2 \left[\frac{i_{n,i}}{2\delta^2} [\Delta\theta_{n,i}]^2 + m_{n,i} [\Delta C_{n,i}]^2 \right] + \sum_{n=1}^N \sum_{i=1}^2 g_t [1 - \cos(\Delta\theta_{n,i})] + \frac{1}{2} \sum_{n=1}^N \sum_{i=1}^2 g_s \frac{d_{xy}^2(C_{n+1,i}; C_{n,i})}{(d_{bs} + \bar{r})^2} + \sum_{n=1}^N d_n [1 - e^{-\mu(d(C_{n,1}; C_{n,2}) - d_{eq})}]^2 + V_h + V_w$$

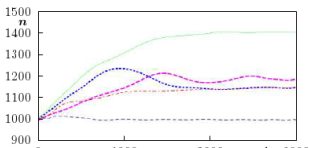
$$\bar{i}_t = 1.1, \bar{i}_s = 1.3, g_t = 1, g_s = 0.3, g_h = 0.01, g_p = 0.02, d = 0.02, \mu = 6.3$$



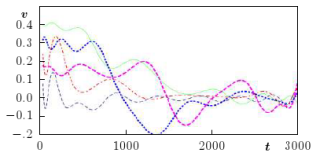
Motion of kinks in the composite inhomogeneous model

$$H = v^2 \sum_{n=1}^N \sum_{i=1}^2 \left[\frac{i_{n,i}}{2\delta^2} [\Delta\theta_{n,i}]^2 + m_{n,i} [\Delta C_{n,i}]^2 \right] + \sum_{n=1}^N \sum_{i=1}^2 g_t [1 - \cos(\Delta\theta_{n,i})] + \frac{1}{2} \sum_{n=1}^N \sum_{i=1}^2 g_s \frac{d_{xy}^2(C_{n+1,i}; C_{n,i})}{(d_{bs} + \bar{r})^2} + \sum_{n=1}^N d_n \left[1 - e^{-\mu(d(C_{n,1}; C_{n,2}) - d_{eq})} \right]^2 + V_h + V_w$$

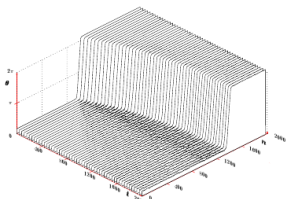
$$\bar{i}_t = 1.1, \bar{i}_s = 1.3, g_t = 1, g_s = 0.3, g_h = 0.01, g_p = 0.02, d = 0.02, \mu = 6.3$$



(c)

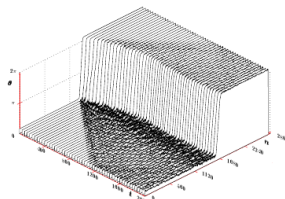


(g)



(d)

$$v = 0.4$$



(h)

$$v = 0.45 \simeq v_{lim}$$

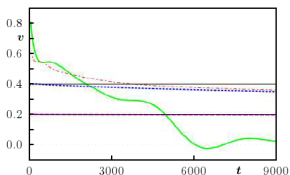
Motion of kinks in the inhomogeneous YakMorse model

$$H_Y = \sum_n \frac{I_{n,1}}{2} \dot{\varphi}_{n,1}^2 + \frac{I_{n,2}}{2} \dot{\varphi}_{n,2}^2 + g(2 - \cos \Delta\varphi_{n,1} - \cos \Delta\varphi_{n,2}) + K \left[1 - e^{-\mu(d(C_{n,1}; C_{n,2}) - d_{eq})} \right]^2$$

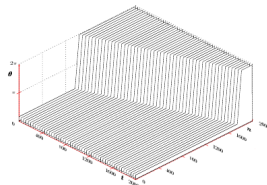
Motion of kinks in the inhomogeneous YakMorse model

$$H_Y = \sum_n \frac{I_{n,1}}{2} \dot{\varphi}_{n,1}^2 + \frac{I_{n,2}}{2} \dot{\varphi}_{n,2}^2 + g(2 - \cos \Delta\varphi_{n,1} - \cos \Delta\varphi_{n,2}) + K \left[1 - e^{-\mu(d(C_{n,1}; C_{n,2}) - d_{eq})} \right]^2$$

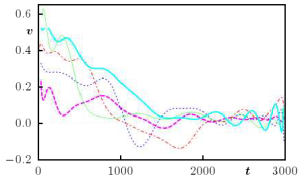
$$\bar{I} = 7, g = 7.5, K = 0.02, \mu = 11$$



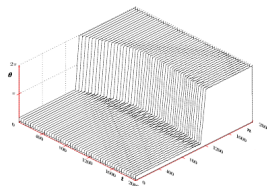
(e)



(f)



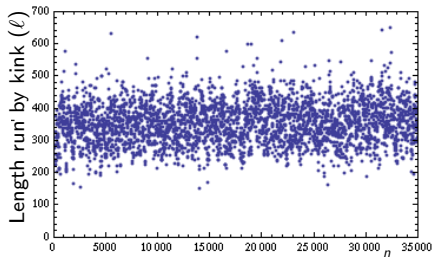
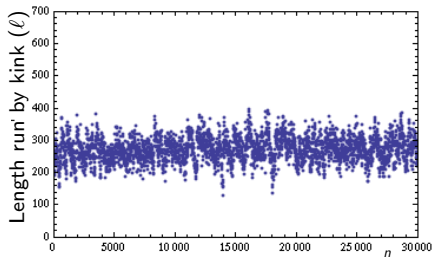
(g)



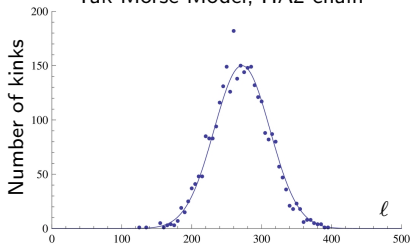
(h)

Traveled Distance vs Initial Position in the Chain

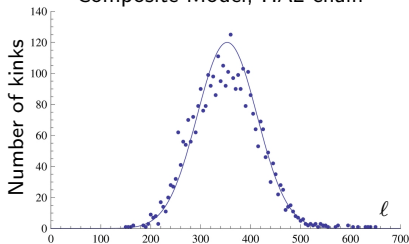
How much the traveled distance varies by the starting point at $v = 0.4$?



Yak Morse Model, HA2 chain

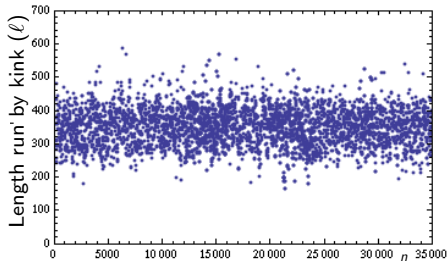


Composite Model, HA2 chain

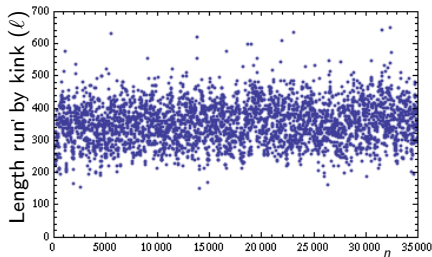


Traveled Distance vs Initial Position in the Chain

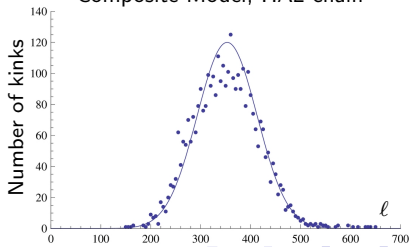
How much the traveled distance varies by the starting point at $v = 0.4$?



Composite Model, random chain

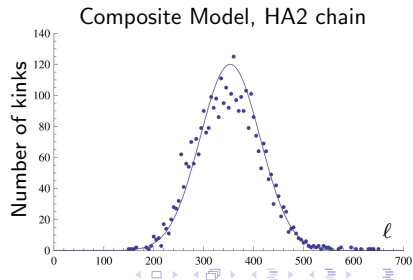
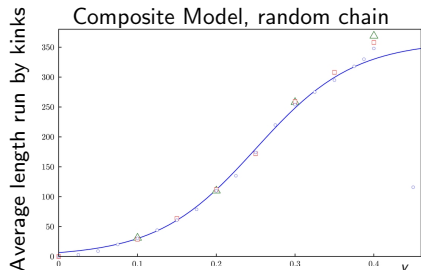
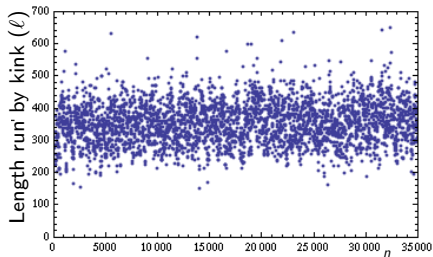
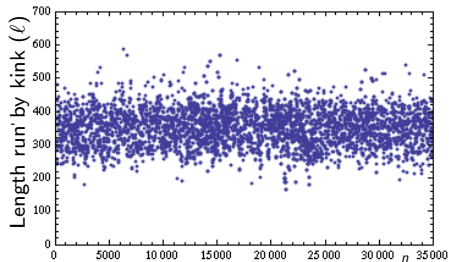


Composite Model, HA2 chain



Traveled Distance vs Initial Position in the Chain

How much the traveled distance varies by the starting point at $v = 0.4$?



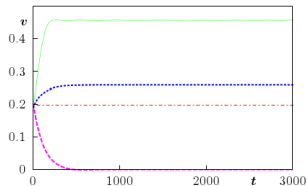
Dissipation and external forces

We introduce in the Yakushevich equations for the $\theta_{n,i}$ a new term $\nu\dot{\theta}_{n,i} + F_0$.

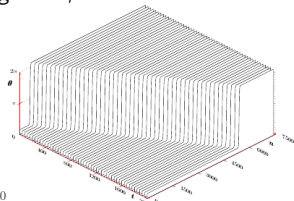
Dissipation and external forces

We introduce in the Yakushevich equations for the $\theta_{n,i}$ a new term $\nu\dot{\theta}_{n,i} + F_0$.

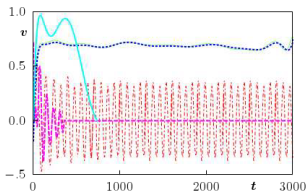
$$\nu = 0, 2, \bar{l} = 7, g = 21, K = 1$$



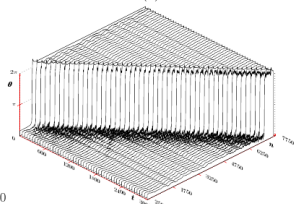
(a)



(b)



(c)



(d)

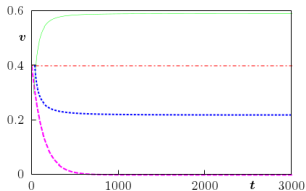
Dissipation and external forces

Now we do the same after replacing the harmonic pairing potential with a Morse one.

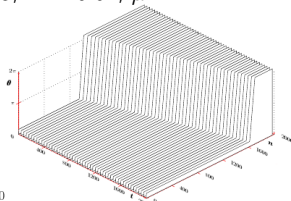
Dissipation and external forces

Now we do the same after replacing the harmonic pairing potential with a Morse one.

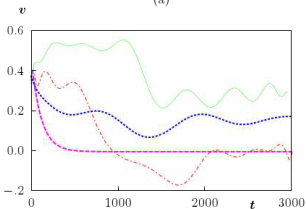
$$\nu = 0.4, \bar{T} = 7, g = 7.5, K = 0.02, \mu = 11$$



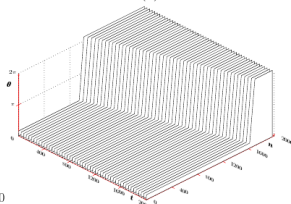
(a)



(b)



(c)



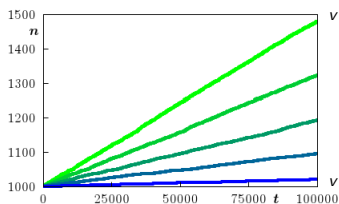
(d)

Very slow kinks

Finally we try to create very slow kinks in the Yakushevich (1st row) and YakMorse (2nd row) models

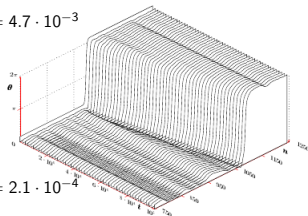
Very slow kinks

Finally we try to create very slow kinks in the Yakushevich (1st row) and YakMorse (2nd row) models



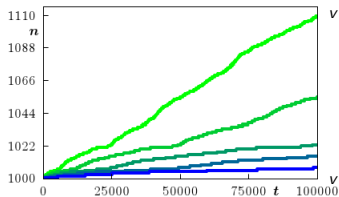
(a)

$$v = 4.7 \cdot 10^{-3}$$



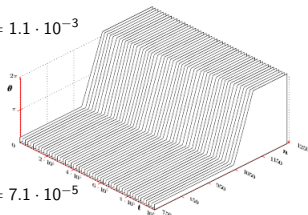
(b)

$$v = 2.1 \cdot 10^{-4}$$



(c)

$$v = 1.1 \cdot 10^{-3}$$



(d)

$$v = 7.1 \cdot 10^{-5}$$

A remark about stability

Gianne Derks (U. of Surrey) pointed out to us that $(1,1)$ solitons in the Yakushevich model are instable.
We verified numerically that this instability disappears when a Morse pairing potential is used:

A remark about stability

Gianne Derks (U. of Surrey) pointed out to us that $(1, 1)$ solitons in the Yakushevich model are unstable.
We verified numerically that this instability disappears when a Morse pairing potential is used:

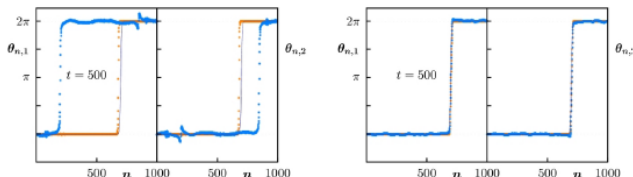


Figure 6. Motion of $(1, 1)$ kinks in the Y (left) and YM (right) models with $v = 0.4$ km/s, $I = 7$, $K_t = 21$, $K_p = 1$, $D = 0.02$, $\nu = 11$. In each picture we show three kinks starting at $n = 500$: 1. the symmetric continuous one (thin line); 2. the one with symmetric initial condition (lighter points); 3. the one with asymmetric initial conditions (darker points) – their initial profiles have been desymmetrized by modifying the position of two points on the chain 1 by 10^{-1} . In the Y model the “asymmetric” kink in the chain 1 moves backwards with speed opposite to the one on the chain 2. Moreover they are both faster than the corresponding symmetric ones, which instead behave in the expected way (including the fact that after just 500 TU it is already slightly behind the corresponding continuous one). In the YM model instead the “asymmetric” kink is virtually indistinguishable by the symmetric one and both are still keeping the pace of the corresponding continuous one.

Strong points of the model

- 1 The Salerno and Yakushevich models are so basic that, to get equations compatible with the observed dispersion relations, one must use unphysical coupling constants. Splitting the degrees of freedom of backbone and bases angles proved to be enough to allow using physical values.
- 2 In the composite model, in the Harmonic approximation for pairing, kinks do not move *even in homogeneous chains*, leading to the introduction of the Morse potential. A posteriori, Morse potential also allows motion of kinks in the Yakushevich inhom. model. Hence improving the geometry of the model also *requires* a more physical pairing potential.
- 3 In the Harmonic approx. the $(1, 1)$ solitons are unstable, with a Morse potential they are stable.

Strong points of the model

- 1 The Salerno and Yakushevich models are so basic that, to get equations compatible with the observed dispersion relations, one must use unphysical coupling constants. Splitting the degrees of freedom of backbone and bases angles proved to be enough to allow using physical values.
- 2 In the composite model, in the Harmonic approximation for pairing, kinks do not move *even in homogeneous chains*, leading to the introduction of the Morse potential. A posteriori, Morse potential also allows motion of kinks in the Yakushevich inhom. model. Hence improving the geometry of the model also *requires* a more physical pairing potential.
- 3 In the Harmonic approx. the $(1, 1)$ solitons are unstable, with a Morse potential they are stable.

Strong points of the model

- 1 The Salerno and Yakushevich models are so basic that, to get equations compatible with the observed dispersion relations, one must use unphysical coupling constants. Splitting the degrees of freedom of backbone and bases angles proved to be enough to allow using physical values.
- 2 In the composite model, in the Harmonic approximation for pairing, kinks do not move *even in homogeneous chains*, leading to the introduction of the Morse potential. A posteriori, Morse potential also allows motion of kinks in the Yakushevich inhom. model. Hence improving the geometry of the model also *requires* a more physical pairing potential.
- 3 In the Harmonic approx. the $(1, 1)$ solitons are unstable, with a Morse potential they are stable.

Future Directions

- 1 Investigate numerically about dissipation, external forces and low speed solitons for the composite model.
- 2 Analyze numerically what happens for several other real DNA sequences to prove that the “global” dynamics really does not depend on the particular sequence and look for the activation regions discussed by Salerno in his seminal paper.
- 3 Investigate numerically about the interaction DNA/RNAP studied analytically in a recent paper by G. Derks and G. Gaeta in the context of the Yakushevich model.

Future Directions

- 1 Investigate numerically about dissipation, external forces and low speed solitons for the composite model.
- 2 Analyze numerically what happens for several other real DNA sequences to prove that the “global” dynamics really does not depend on the particular sequence and look for the activation regions discussed by Salerno in his seminal paper.
- 3 Investigate numerically about the interaction DNA/RNAP studied analytically in a recent paper by G. Derks and G. Gaeta in the context of the Yakushevich model.

- 1 Investigate numerically about dissipation, external forces and low speed solitons for the composite model.
- 2 Analyze numerically what happens for several other real DNA sequences to prove that the “global” dynamics really does not depend on the particular sequence and look for the activation regions discussed by Salerno in his seminal paper.
- 3 Investigate numerically about the interaction DNA/RNAP studied analytically in a recent paper by G. Derks and G. Gaeta in the context of the Yakushevich model.

M. Salerno, "*Discrete model for DNA-promoter dynamics*", PRA **44**, 1991

L.V. Yakushevich *et al.*, "*On the nonlinear dynamics of topological solitons in DNA*", PRE **66**, 2002

M. Cadoni, R. De Leo and G. Gaeta, "*A composite model for DNA torsion dynamics*", PRE **75**, 2007

L.V. Yakushevich, "*Nonlinear dynamics of DNA: Velocity of the kinks activated in homogeneous polynucleotide chains*", IJQC **110**, 2010

M. Cadoni, R. De Leo, S. Demelio and G. Gaeta, "*Propagation of twist solitons in fully inhomogeneous DNA chains*", JNMP **17:04**, 2010

R. De Leo and S. Demelio, "*Some numerical results on motion of kinks in some model of DNA torsional dynamics*", Proceedings of SIMAI 2010

M. Cadoni, R. De Leo and S. Demelio, "*Soliton propagation in homogeneous and inhomogeneous models for DNA torsion dynamics*", JNMP **18:52**, 2011

G. Derks and G. Gaeta, "*A minimal model of DNA dynamics in interaction with RNA-Polymerase*", Physica D **240**, 2011