

# Soliton chaos models for mechanical and biological elastic chains

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The possibility of purely spatial chaos of loop and envelope soliton localization in long elastic strings is considered. Possible connections to some problems in molecular biology are discussed.

## 1. Introduction and preliminary remarks

There has been an increased interest in complexity and spatial chaos in recent years [1–5]. In particular, since the discovery of loop solitons and their interaction [6,7] as well as the possibility of a purely spatial chaos [8], there is a renewed interest in the Euler elastica and its applications [9].

El Naschie established the connection between the loop soliton and the Milke–Holmes chaotic elastica using a dynamical version of the Euler elastica [5,9]. He also drew attention to the possibility of interpreting the instability waves in curved compressed thin material surfaces (i.e. shells) as envelope soliton turbulence [9,10]. Thompson and Virgin were the first to publish a numerical confirmation of the theoretical results of Milke and Holmes using an elementary but neat model [11].

There is some intriguing likeness, at least a purely visual one, between the elastica configurations and protein transformations. The primary structure of protein [12], which is made up of long linear chains of covalently linked amino acids, for instance, re-

sembles the periodic instability waves of compressed elastica. Depending on certain geometrical parameters, a long elastica inside a long circular pipe would lose stability when compressed and form a helical structure [13]. The secondary structure also looks very close to the soliton loops of the chaotic elastica. Finally, the tertiary structure looks very much like the strongly coiled elastica anticipated theoretically in ref. [5] and confirmed numerically in refs. [9,13].

Protein chains are not rigid. Similar to the elastica, they are flexible. This elasticity is essential in understanding protein deformation [12,14]. Not unlike DNA, soliton chaos of the elastica also conveys a definite code when translated into symbolic dynamics.

In the present work we study numerically what we may term spatial strange attractors in the elastica. This might be of interest, since strange attractors are regarded occasionally as generators of information.

Due to the analogy between the Hamiltonian of the elastica and the Hamiltonian of a circular elastic ring under external pressure [15], the similarity may be extended to circular DNA. In fact in some elementary demonstration using a long twirled and stretched elastic band, we observe not only the spatial complexity and pseudo-random loops shown in refs. [5,9], but we can more frequently and very

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clearly observe supercoiling in the elastic band very similar to that of DNA. It seems also that spatial chaos generated by periodic fluctuation in the elastica may fit well into a known analogy between polymer chains and Brownian motion and this in turn is another connection to fractals.

We may recall as explained in detail in refs. [5,9] that for a soliton loop to form in the planar elastica, very large deformation is needed first, then we must assume that the ends can pass without obstruction through each other, which is of course physically impossible. If the planar two-dimensional constraint is removed however, the loop soliton forms in three dimensions without the need for a large deflection. This might be related to another observation in protein. There the primary structures can be considered planar, however, the secondary structures must be taken as three-dimensional [14]. Nevertheless, if the lateral movement of the elastica is restrained in some way, for instance through electromagnetic forces as in electric conductors [16] or by elastic forces as in axisymmetrical deformation of beams attached laterally to the elastic medium [9], then there can be a possibility for another type of soliton in two dimensions and without very large deflection. This is the envelope soliton well known from the solution of the nonlinear Schrödinger equation [17]. In the present work we give numerical confirmation for the conjecture made in refs. [5,10] that elastic material surfaces, such as shells, exhibit under certain conditions purely spatial and statical soliton chaos.

In all the problems considered here we study the influence of band-limited white noise on the randomness of the soliton [18,19], and we show that this spatial chaos may be eliminated or reduced by adding noise. Needless to say a phenomenon indistinguishable from spatial chaos can only be observed in the unforced system by adding band-limited white noise.

The idea of using soliton to model DNA is of course not new at all. It has been considered in some pioneering work by Davydov and Kislukla [20]. Highly interesting results were reported in numerous excellent papers by Scott [21].

These researchers go of course far deeper into the real and far more difficult problems of molecular biology. We on the other hand are familiar only with the global logic of molecular biology and are not in

a position to comment in depth on the exact nature of the analogy suggested here.

Nevertheless we hope that our detailed knowledge of the elastica and statical chaos may be of some value, however limited, to the specialist who may be able to draw a clearer picture. In addition we hope that this work clearly shows that soliton and chaos are not contradictory and even essential as noted in a different context by Ueda and Noguchi [22].

## 2. The dynamical elastica – loop soliton

Consider the following nonlinear differential equation which describes the dynamical behaviour of the elastica,

$$W_{tt} + W_{xx} + 2\varepsilon [W_{xx}(1 + W_x^2)^{-3/2}]_{xx} = 0, \quad (1)$$

where  $( )_x = d/dx$  and  $( )_t = d/dt$ . Here  $W$  is the nondimensional displacement,  $\varepsilon = \alpha/2PA$ ,  $\alpha$  is the bending stiffness.  $A$  is the cross-sectional area of the elastica,  $P$  is the axial force,  $x$  is the axial coordinate and  $t$  is the time.

Introducing the stretched coordinates

$$x_1 = x + t \quad \text{and} \quad t_1 = \varepsilon t,$$

noting that when a loop forms in the elastica, then compression is reversed into tension [13] and using  $\phi$  and  $s$  as coordinate system where  $\phi$  is the slope of the central line and  $s$  is the arch length, our PDE reduces to

$$\dot{\phi} + \cos \phi (\sec \phi \phi_{ss})_s = 0, \quad (2)$$

where a dot denotes  $d/dt$  and  $( )_s = d/ds$ . Using the inverse scattering transformation, this equation can be shown to possess a loop soliton solution [6,7,26–28]. Some elementary experimental demonstrations of these loops were reported in ref. [13]. The time independent version of the last equation is nothing but the familiar nonlinear ODE of the Euler elastica,

$$\phi_{ss} + \sin \phi = 0. \quad (3)$$

Now we perturb this equation by first adding periodic spatial forcing (imperfection),

$$\phi_{ss} + \sin \phi = a \sin \omega s, \quad (4)$$

and then adding band-limited white noise perturbation to it:

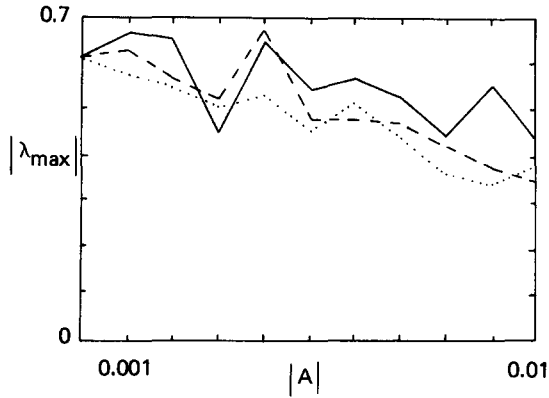


Fig. 1. The most probable value of the distribution of maximum Lyapunov exponents  $|\lambda_{\max}|$  for eq. (5) versus noise intensity  $A$ :  $a=0.01$ ,  $\omega=1$ ,  $\phi(0)=2$ ,  $\phi'(0)=0$ ; (---)  $\nu_{\min}=0.5$ ,  $\nu_{\max}=3.5$ ; (····)  $\nu_{\min}=0.5$ ,  $\nu_{\max}=1.5$ ; (---)  $\nu_{\min}=2.5$ ,  $\nu_{\max}=3.5$ .

$$\phi_{ss} + \sin \phi = a \sin \omega s + A \sum_{i=1}^N \sin(\nu_i s + \gamma_i), \quad (5)$$

where  $\nu_i$  and  $\gamma_i$  are random variables.

The second component of eq. (5) is an approximation of a band-limited white noise with a spectral density

$$S(\nu) = \sigma / (\nu_{\max} - \nu_{\min}), \quad \nu \in [\nu_{\min}, \nu_{\max}], \\ = 0 \quad \nu \notin [\nu_{\min}, \nu_{\max}], \quad (6)$$

$\sigma$  is constant,  $\nu_{\min}$  and  $\nu_{\max}$  are the band frequencies of the noise.  $\gamma_i$  are independent random variables with uniform distribution on the interval  $[0, 2\pi]$ ,  $A$  and  $\nu_i$  are given by

$$A = \sqrt{2\sigma/N}, \quad \nu_i = (i-0.5)\Delta\nu + \nu_{\min}, \\ \Delta\nu = (\nu_{\max} - \nu_{\min})/N. \quad (7)$$

Some of the obtained numerical results for  $a=0.01$ ,

$0.00 \leq A \leq 0.01$  and three different perturbation frequency bands  $0.5 \leq \nu_i \leq 3.5$ ,  $0.5 \leq \nu_i \leq 1.5$  and  $2.5 \leq \nu_i \leq 3.5$ ,  $N=300$  are shown in figs. 1 and 2. Two different representations are used: A spatial plot which shows the actual form which the infinite elastica should take and also the plot of the most probable value of the maximum Lyapunov exponent distribution over a number of noise realizations  $|\lambda_{\max}|$  (100 realizations of noise for different  $\gamma_i$  have been considered) [18,19] versus noise intensity  $A$ . As has been shown in refs. [18,19] a positive value of  $|\lambda_{\max}|$  indicates a chaotic stochastic process while a non-positive one is characteristic for a regular stochastic process. The results agree qualitatively with some experimental demonstration reported in refs. [5,9].

To conclude this part we consider the influence of positive damping as well as what might appear as somewhat artificial spatial forcing. This forcing arises however in a natural way in the parametric forcing of the corresponding damped pendulum problem. Thus we study the following equation of the elastica,

$$\phi_{ss} + \delta\phi_s + b \sin \phi \\ = a \sin \omega s \sin \phi + A \sum_{i=1}^N \cos(\nu_i s + \gamma_i) \quad (8)$$

for different parametric values as well as initial conditions.

For the deterministic and noise perturbed nonlinear dynamics we plot the corresponding spatial strange attractor in the region of the strange attractor [23]. Fig. 3 shows clearly the immense richness of information which these looping patterns can produce for infinitely long  $s$ . This may be relevant to some problems in molecular biology.

From the plot of the most probable value of the Lyapunov exponent distribution  $|\lambda_{\max}|$  shown in fig. 4 we can observe that for some value of noise inten-

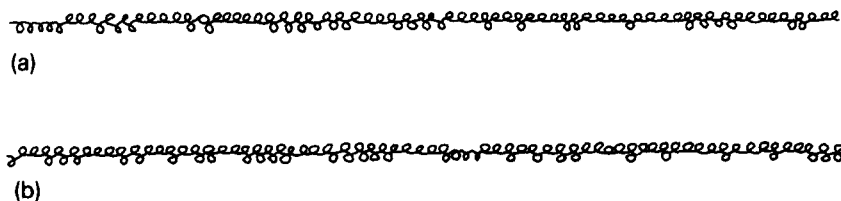


Fig. 2. Examples of spatial plot for eq. (5) : (a)  $A=0.0015$ ; (b)  $A=0.0080$ .

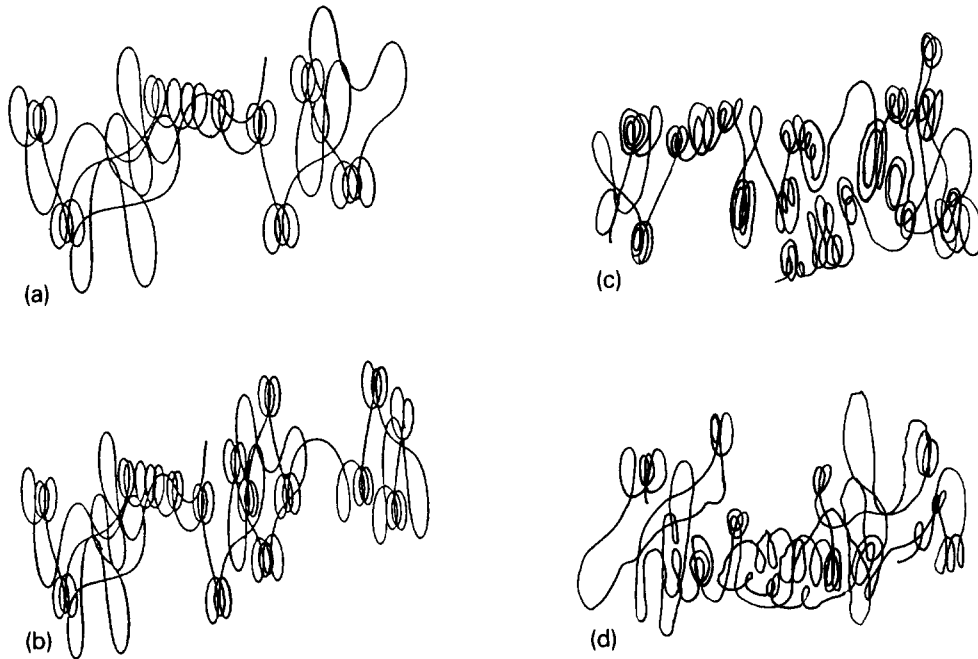


Fig. 3. Spatial strange attractors for eq. (8),  $\delta=0.15$ ,  $b=1$ ,  $a=0.94$ ; (a)  $\omega=1.56$ ,  $A=0$ ; (b)  $\omega=1.58$ ,  $A=0$ ; (c)  $\omega=1.56$ ,  $A=0.1$ ; (d)  $\omega=1.58$ ,  $A=0.15$ .

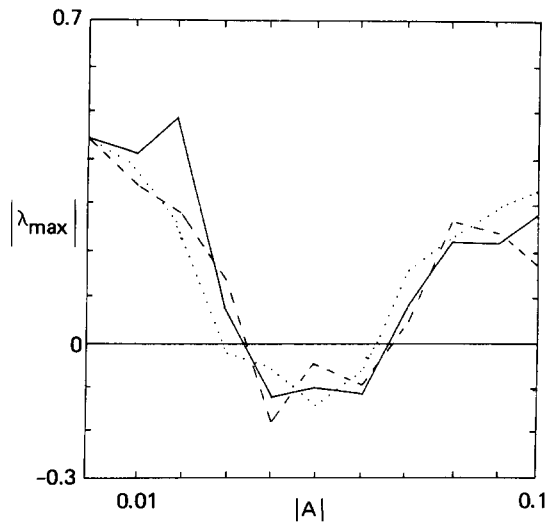


Fig. 4. The most probable value of the distribution of maximum Lyapunov exponents  $-|\lambda_{\max}|$  for eq. (8) versus noise intensity  $A$ ,  $a=0.15$ ,  $\delta=0.01$ ,  $\omega=1$ ,  $b=0.0272222$ ,  $\phi(0)=6$ ,  $\phi(0)=0$ ; (----)  $\nu_{\min}=0.5$ ,  $\nu_{\max}=3.5$ ; (.....)  $\nu_{\min}=0.5$ ,  $\nu_{\max}=1.5$ ; (-.-)  $\nu_{\min}=2.5$ ,  $\nu_{\max}=3.5$ .

sity  $A$ ,  $|\lambda_{\max}|$  is negative, which implies elimination of chaos (transition from chaotic to regular stochastic process) in the sense of symbolic dynamics as shown in the spatial plot of fig. 5b. The shape of

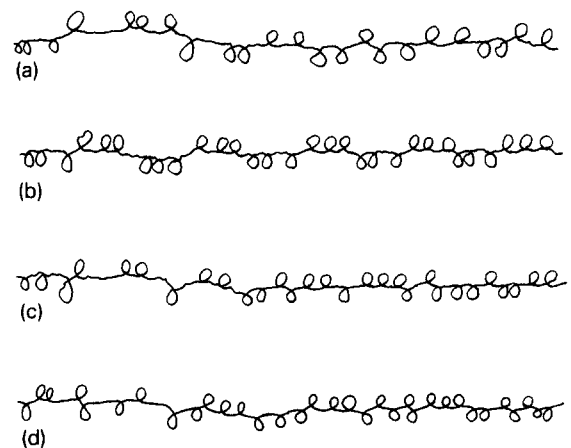


Fig. 5. Examples of spatial plot for eq. (8): (a)  $A=0.02$ ; (b)  $A=0.05$ ; (c)  $A=0.08$ ; (d)  $a=0$ ,  $N=2$ ,  $\nu_1=1$ ,  $\nu_2=\sqrt{2}/10$ ,  $A=0.1$ .

loops in the spatial plot is not the same because of random forcing, but if we indicate the upper loop as 1 and the lower one as 0 we obtain a periodic sequence of symbols:

000111000111000111000111... ,

while for the chaotic spatial plots of figs. 5a and 5c we have aperiodic sequences:

000111100001001000110001...

and

000111011100111010011100... .

Another interesting type of behaviour can be observed if we consider a particular form of eq. (5) by taking  $a=0$ ,  $N=2$  and  $\nu_1$  and  $\nu_2$  to be incommensurable. In this case we can observe the behaviour presented in fig. 5d which seems to be chaotic. It is chaotic in the sense that it has an aperiodic sequence in the symbolic representation:

0111001001110001110101110010100... ,

but we have no sensitive dependence on the initial conditions as the Lyapunov exponents are negative. This type of spatial strange behaviour is related to the so-called strange nonchaotic attractors [23–25].

### 3. Instability waves in an elastic structure – envelope soliton

Consider the following nonlinear partial differential equation which may be used to describe the propagation of buckling waves in an elastic medium such as the axisymmetrical deformation of an axially compressed cylindrical shell,

$$\alpha W'''' + \sigma W'' + c_1 W - c_2 W^2 + \rho \dot{W} = 0. \quad (9)$$

For a radial strain obeying a logarithmic law, this equation was used in refs. [9,13] to study the instability waves due to buckling.

Now depending on the number of slow spaces and slow time, different reduced differential equations for the complex amplitude of deflection  $A$  may be obtained. For instance, using

$$x = x_0, \quad x_1 = \varepsilon x_0, \quad x_2 = \varepsilon^2 x, \\ t = t_0, \quad t_1 = \varepsilon t_0, \quad t_2 = \varepsilon^2 t_1,$$

one finds the following Ginzburg–Landau type equation [17]:

$$\alpha_1 A'' - \alpha_2 A + i\alpha_3 A' + i\alpha_4 \dot{A} + \alpha_5 A |A|^2 = 0, \quad (10)$$

where  $i = \sqrt{-1}$ , an accent denotes  $d/dx$  and a dot denotes  $d/dt$ .

On the other hand the PDE may be drastically reduced to an ODE by reducing stretching to only  $x_1 = \varepsilon x$ . This leads to the following stationary nonlinear Schrödinger equation [17],

$$\alpha_1 A'' - \alpha_2 A + \alpha_5 A |A|^2 = 0. \quad (11)$$

This equation is easily integrated by elementary methods and gives the soliton solution

$$A = \frac{6}{\sqrt{19}} \operatorname{sech}\left(\frac{19}{12}x_1\right), \quad (12)$$

for  $\alpha = c_1 = c_2 = c_3 = r = 1$ . The homoclinicity of this solution may be established easily as shown in ref. [9].

An optimum choice of the number of slow spaces and slow times which restores the dynamical character of the problem we have, however, when we take

$$x_1 = \varepsilon x_0, \quad t_1 = \varepsilon t_0, \quad t_2 = \varepsilon^2 t_1.$$

This leads to the nonlinear Schrödinger equation

$$\alpha_1 A'' - \alpha_2 A + i\alpha_4 \dot{A} + \alpha_5 A |A|^2 = 0, \quad (13)$$

with the well-known solution [17]

$$A(x, t) |_{t=t_0} = a \operatorname{sech} bx \cos cx, \quad (14)$$

where  $a$ ,  $b$  and  $c$  are constant.

Either way we expect spatial forcing to yield spatial envelope soliton chaos. Thus we consider first the periodically forced equation

$$A'' + k_1 A' - k_2 A + k_3 A^3 = k_4 \cos k_5 s. \quad (15)$$

The results of the numerical integrations for different parameter values which are:  $k_1 = 0.01$ ,  $k_2 = 0.25$ ,  $k_3 = 19/(4 \times 18)$ ,  $k_5 = 1$  and different values of  $k_4$  are shown in fig. 6. They fully confirm the expectations expressed earlier in refs. [5,9,13].

Subsequently the forcing by band-limited white noise,

$$A'' + k_1 A' - k_2 A + k_3 A^3 = A \sum_{i=1}^N \cos(\nu_i s + \gamma_i), \quad (16)$$

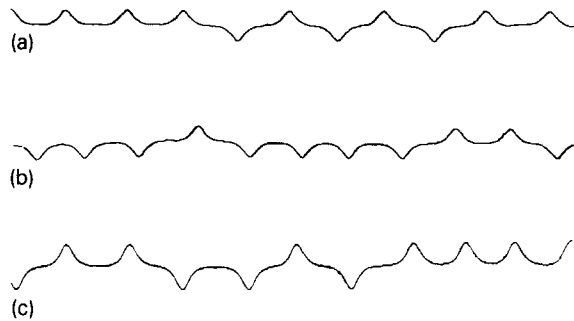


Fig. 6. Examples of spatial plot for eq. (15):  $k_1=0.01$ ,  $k_2=0.25$ ,  $k_3=19/(4 \times 18)$ ,  $k_5=1$ ,  $A(0)=1.37649$ ,  $A(0)=0$ ; (a)  $k_4=0.001$ ; (b)  $k_4=0.002$ ; (c)  $k_4=0.003$ .

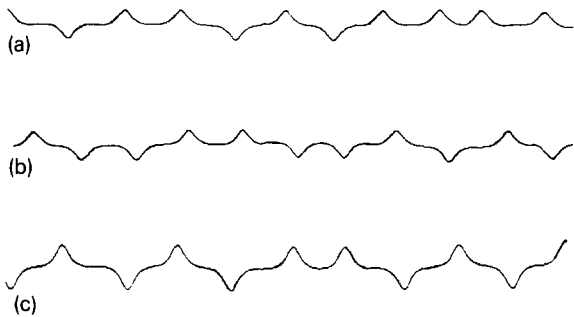


Fig. 7. Examples of spatial plot for eq. (16):  $k_1-k_3$  as in fig. 6: (a)  $A=0.001$ ,  $|\lambda_{\max}|=0.06$ ; (b)  $A=0.002$ ,  $|\lambda_{\max}|=0.07$ ; (c)  $A=0.003$ ,  $|\lambda_{\max}|=-0.03$ .

is considered. In fig. 7 we show a spatial plot of the same system as in fig. 6 this time, however, with band-limited white noise forcing.

In all the above examples the soliton strange behaviour would thus have a similar symbolic dynamic representation. However, in many cases we have no sensitive dependence on initial conditions – fig. 7c.

#### 4. Conclusions

Based on the symbolic dynamics of a single spatial plot, it is not easy if at all possible to distinguish between chaos, strange nonchaotic behaviour and random behaviour. However, based on the distribution of the maximum Lyapunov exponents, a distinction can be made between chaotic and nonchaotic “strange” behaviour.

There seems to be some likeness between the deformation of the elastica and DNA chains. The deformation in an elastic band however is in principle reversible while the transformation from DNA to RNA was never observed to be reversible.

In terms of the mechanics of deformable bodies DNA chains act as if they had in-locked internal compression inside them, a kind of pre-stressing with a very weak elastic bond, which is checked by the bending and axial stiffness of the silhouette of the chain. When through chemical reactions this stiffness and the bond are eroded, collapse follows. This is not very much unlike the coiling of a long twirled and stretched rubber band when the stretching forces are gradually released. If this outrageously elementary mechanical picture is anywhere near correct, then it is of course extremely unlikely that an increase in the stiffness could ever restore the original situation and if the analogy holds, then there can be no RNA to DNA transformation.

Of course there is still the possibility known from materials with memory which may regain the original form by an influx of energy.

We hope to have shown clearly through the numerical results that spatial chaos may help in understanding complexity. The role of random perturbation in eliminating spatial chaos sheds light on the therapeutic effect of vibration in the medical treatment of bone disorder. Based upon previous dynamical observations [18,19] this effect is fully expected although it should be regarded as counter-intuitive that a type of spatial forcing which on its own produces stochasticity should eliminate another type of chaos where intuition may suggest that more complicated behaviour is expected. The work also stresses the view expressed probably for the first time by Ueda that soliton and chaos should not be regarded as contradictory.

Finally we may note that spatial damping may be thought of as a kind of nonconservative force similar to that known in dynamical stability as follower forces [29].

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