3rd CONFERENCE ON NONLINEARITY

Stability analysis of solutions in the helicoidal Peyrard - Bishop model of DNA molecule

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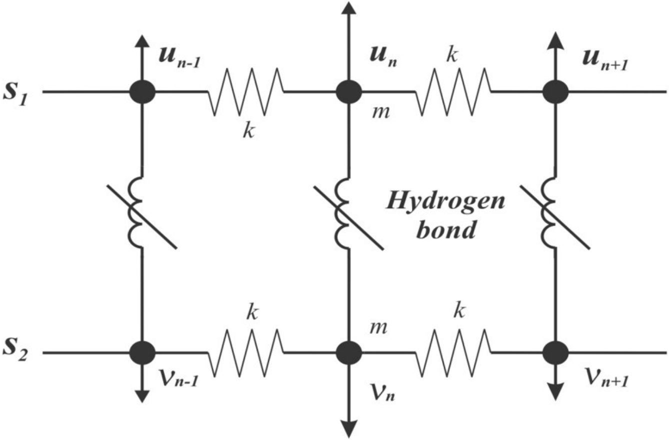
Simple model for DNA strands



$$H = \sum \left\{ \frac{m}{2}(\dot{u}_n^2 + \dot{v}_n^2) + \frac{k}{2}\left[(u_n - u_{n-1})^2 + (v_n - v_{n-1})^2\right] + V_M(u_n - v_n) \right\}$$

Helicoidal Peyrard-Bishop model of DNA

The Hamiltonian describing the HPB model is [1]

$$H = \sum \frac{m}{2}(\dot{u}_n^2 + \dot{v}_n^2) + \frac{k}{2}\left[(u_n - u_{n-1})^2 + (v_n - v_{n-1})^2\right]$$
$$+ \frac{K}{2}\left[(u_n - v_{n+h})^2 + (u_n - v_{n-h})^2\right] + D\left[e^{-a(u_n - v_n)} - 1\right]^2,$$

where u_n and v_n are displacements of the nucleotides at the position n from their equilibrium positions. The parameters k and K are coupling contants, m is the average nucleotide mass, and D and a are the depth and inverse width of the Morse potential well, respectively.

Second order ODE

After continuum approximation, and introducing unified variable $\xi = \kappa x - \omega t$, we get [2]

$$\alpha\psi'' - \rho\psi' + \psi - \psi^2 = 0, \tag{1}$$

where $\rho > 0$ is parameter proportional to the viscosity coefficient. The parameter α has the form

$$\alpha = C(V^2 - c^2), \quad C > 0,$$

where V and c are the solitonic and linear sound velocities, respectively. So, if

- $\alpha > 0$ solitary wave is supersonic,
- $\alpha < 0$ solitary wave is subsonic.

Solutions

Using the modified extended tanh-function (METHF) method, the following two solutions were obtained [2]

$$\psi_1(\xi) = \frac{1}{4}\left(1 + 2\tanh(w) + \tanh^2(w)\right), \quad (2)$$

$$\psi_2(\xi) = \frac{1}{4}\left(3 + 2\tanh(w) - \tanh^2(w)\right), \quad w = \frac{5\xi}{12\rho}. \quad (3)$$

ψ_1 corresponds to a positive $\alpha = \alpha^{(1)}$, and ψ_2 to a negative $\alpha = \alpha^{(2)}$, [2]

$$\alpha^{(1)} = \frac{6\rho^2}{25}, \quad \alpha^{(2)} = -\frac{6\rho^2}{25}.$$

Neglected viscosity - solutions

In the case $\rho = 0$, or viscosity is neglected, from (1) we get

$$\alpha\psi'' + \psi - \psi^2 = 0,$$

and solutions are expressed through the parameters $a_2^{(1)}$ and $a_2^{(2)}$

$$\begin{aligned}
\psi_{10}(\xi) &= \frac{1}{2}\left[-1 + 3\tanh^2\left(\sqrt{\frac{3}{2a_2^{(1)}}}\xi\right)\right], \quad a_2^{(1)} > 0, \\
\psi_{20}(\xi) &= \frac{3}{2}\left[1 - \tanh^2\left(\sqrt{-\frac{3}{2a_2^{(2)}}}\xi\right)\right], \quad a_2^{(2)} < 0.
\end{aligned}$$

Stability analyses

In order to examine stability of the solutions (2) and (3) we will apply substitution in equation (1)

$$\tilde{\psi} = \psi - \psi_0, \tag{4}$$

where ψ_0 stands for ψ_1 or ψ_2. Then we get

$$\alpha\tilde{\psi}'' - \rho\tilde{\psi}' + \tilde{\psi} - \tilde{\psi}^2 - 2\psi_0\tilde{\psi} = 0. \tag{5}$$

Now, if we denote $\tilde{\psi}' = \tilde{\theta}$, we can get this system of the first order differential equations

$$\begin{aligned} \frac{d\tilde{\psi}}{d\xi} &= \tilde{\theta}, \\ \frac{d\tilde{\theta}}{d\xi} &= \frac{\rho}{\alpha}\tilde{\theta} - \frac{1}{\alpha}\tilde{\psi} + \frac{1}{\alpha}\tilde{\psi}^2 + \frac{2}{\alpha}\psi_0\tilde{\psi}, \end{aligned} \tag{6}$$

with stationary solution at $(0, 0)$.

Supersonic solution

Substitution ψ_1 instead of ψ_0, and linearization give the system

$$\frac{d\tilde{\psi}}{d\xi} = \tilde{\theta}, \qquad \frac{d\tilde{\theta}}{d\xi} = -\frac{1}{2\alpha}\tilde{\psi} + \frac{\rho}{\alpha}\tilde{\theta}. \tag{7}$$

Corresponding eigenvalues are

$$\lambda_{1,2} = \frac{\rho \pm \sqrt{\rho^2 - 2\alpha}}{2\alpha}. \tag{8}$$

Since we know that $\rho > 0$, and $\alpha > 0$ real parts of these eigenvalues ($Re\lambda_{1,2}$) are positive, so our solution ψ_1 is **unstable**.

Subsonic solution

Similarly, if we put ψ_2 instead of ψ_0, we get the linearized system

$$\begin{aligned} \frac{d\tilde{\psi}}{d\xi} &= \tilde{\theta}, \\ \frac{d\tilde{\theta}}{d\xi} &= \frac{1}{2\alpha}\tilde{\psi} + \frac{\rho}{\alpha}\tilde{\theta}, \end{aligned} \tag{9}$$

with stationary solution at $(0,0)$.
Corresponding eigenvalues are

$$\lambda_{1,2} = \frac{\rho \pm \sqrt{\rho^2 + 2\alpha}}{2\alpha}. \tag{10}$$

In the case of ψ_2, ρ is positive and α is negative, which means that the solution ψ_2 is **stable**.

Our equation is

$$\alpha\psi'' + \psi - \psi^2 = 0, \tag{11}$$

and solutions we found are

$$\psi_{10}(\xi) = \frac{1}{2}\left[-1 + 3\tanh^2\left(\sqrt{\frac{3}{2a_2^{(1)}}}\xi\right)\right], \quad a_2^{(1)} > 0, \tag{12}$$

$$\psi_{20}(\xi) = \frac{3}{2}\left[1 - \tanh^2\left(\sqrt{-\frac{3}{2a_2^{(2)}}}\xi\right)\right], \quad a_2^{(2)} < 0. \tag{13}$$

If we try to examine stability of these solutions, and apply substitution

$$\tilde{\psi} = \psi - \psi_{00}, \tag{14}$$

where ψ_{00} stands for ψ_{10} or ψ_{20}, we'll get

$$\alpha\tilde{\psi}'' + \tilde{\psi} - \tilde{\psi}^2 - 2\psi_{00}\tilde{\psi} = 0. \tag{15}$$

Linearized system

Second order differential equation (15) can be written as the system

$$\frac{d\tilde{\psi}}{d\xi} = \tilde{\theta},$$
$$\frac{d\tilde{\theta}}{d\xi} = -\frac{1}{\alpha}\tilde{\psi} + \frac{1}{\alpha}\tilde{\psi}^2 + \frac{2}{\alpha}\psi_{00}\tilde{\psi}, \tag{16}$$

where $\tilde{\psi}' = \tilde{\theta}$.
Using (12) for ψ_{00} we can obtain linearized system

$$\frac{d\tilde{\psi}}{d\xi} = \tilde{\theta},$$
$$\frac{d\tilde{\theta}}{d\xi} = -\frac{2}{\alpha}\tilde{\psi}. \tag{17}$$

Eigenvalues

The characteristic equation is

$$\lambda^2 + \frac{2}{\alpha} = 0, \tag{18}$$

so we've got eigenvalues $\lambda_{1,2} = \pm\sqrt{-\frac{2}{\alpha}}$.
In the case $\alpha < 0$, solution ψ_{10} is **unstable**, but in the case $\alpha > 0$ we didn't get any answer about stability (pure imaginary eigenvalues $\lambda_{1,2} = \pm i\sqrt{\frac{2}{\alpha}}$).
Similarly, the solution ψ_{20} is **unstable** for $\alpha > 0$, and no answer in the case $\alpha < 0$.
Evan if we add the second order or the third order terms to the system (17) we will not get any different result.
At the end, we can say that analytical stability examination fails in these two cases.

If we introduce change of variables to the system (16) ($\psi_{00} = \psi_{10}$, and $\alpha > 0$)

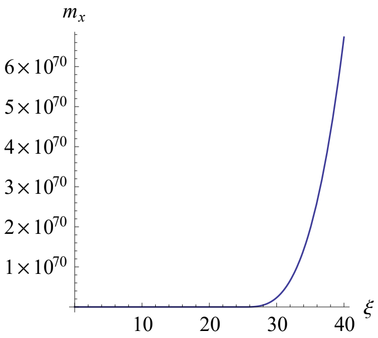
$$\tilde{\psi} = m_y, \quad \tilde{\theta} = \sqrt{\frac{2}{\alpha}} m_x \tag{19}$$

we'll get

$$\frac{dm_x}{d\xi} = -\sqrt{\frac{2}{\alpha}} m_y + \frac{1}{\alpha\sqrt{\frac{2}{\alpha}}} m_y^2 + \frac{3}{\alpha\sqrt{\frac{2}{\alpha}}} \tanh^2\left(\sqrt{\frac{3}{2a_2^{(1)}}}\xi\right) m_y,$$

$$\frac{dm_y}{d\xi} = \sqrt{\frac{2}{\alpha}} m_x. \tag{20}$$

with stationary solution at $(0, 0)$.



m_x
6×10^{70}
5×10^{70}
4×10^{70}
3×10^{70}
2×10^{70}
1×10^{70}
10
20
30
40
ξ
m_y
2.5×10^{59}
2.0×10^{59}
1.5×10^{59}
1.0×10^{59}
5.0×10^{58}
10
20
30
40
ξ

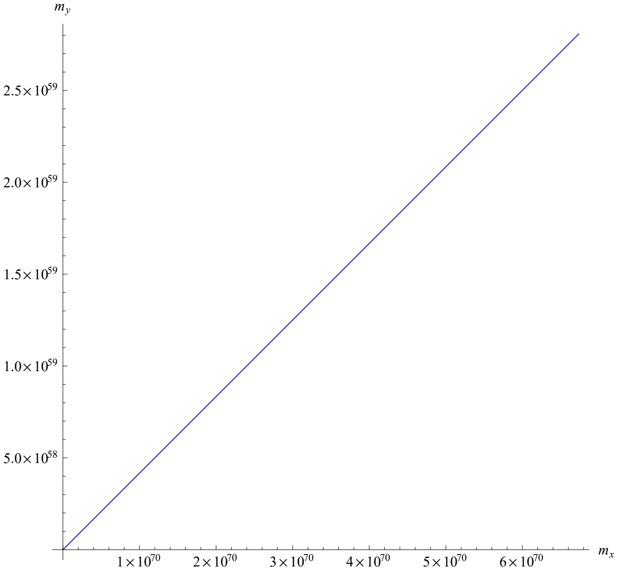
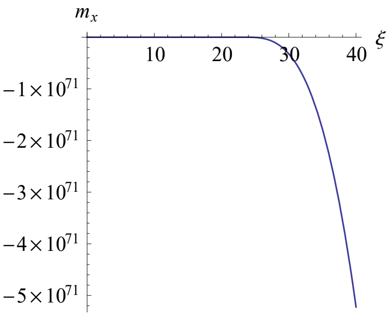
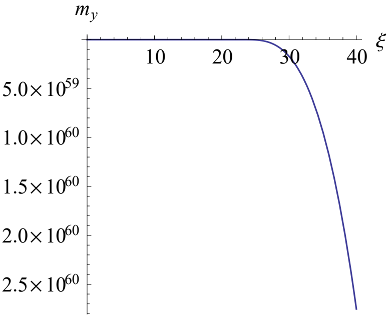


Fig. 1. The solution of the system, near $(0, 0)$, for $\alpha = 4$, $a_2^{(1)} = 4$, $m_{x0} = 0.0001$ and $m_{y0} = 0.0001$.


m_x
ξ
10
20
30
40
-1×10^{71}
-2×10^{71}
-3×10^{71}
-4×10^{71}
-5×10^{71}


m_y
ξ
10
20
30
40
5.0×10^{59}
1.0×10^{60}
1.5×10^{60}
2.0×10^{60}
2.5×10^{60}

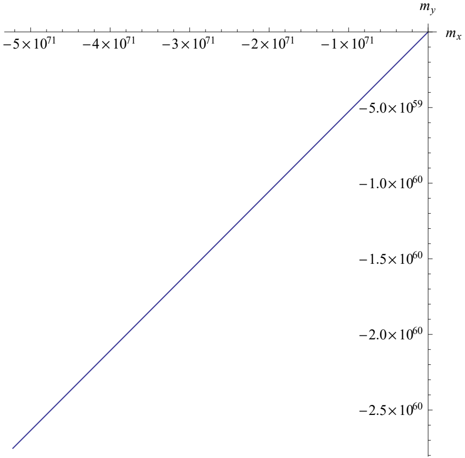


Fig. 2. The solution of the system, near $(0,0)$, for $\alpha = 4.8$, $a_2^{(1)} = 3$, $m_{x0} = 0.0001$ and $m_{y0} = 0.0001$.

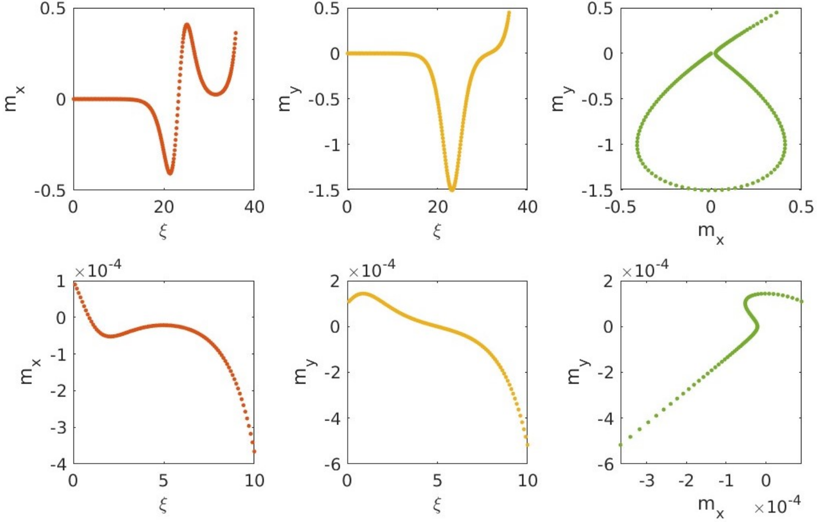


Fig. 3. The solution of the system, near $(0,0)$, for $\alpha = 4.8$, $a_2^{(1)} = 2$, $m_{x0} = 0.0001$ and $m_{y0} = 0.0001$.

According to numerical examination (using Mathematica and Matlab), we can see that solution ψ_{10} is also **unstable** for any $\alpha > 0$, and parameter $a_2^{(1)} > 0$. Analogously, the solution ψ_{20} is **unstable** for any $\alpha < 0$, and parameter $a_2^{(2)} < 0$.

Conclusion

- The functions $\psi_1(\xi)$ and $\psi_2(\xi)$ represent the supersonic and subsonic kinks, respectively.
- We show that only **subsonic** soliton is **stable**.
- We show also that the solutions $\psi_{10}(\xi)$ and $\psi_{20}(\xi)$ are **unstable**, which means that the viscosity enables the existence of the solitary waves in DNA.

References:

- **S. Zdravković**, Helicoidal Peyrard-Bishop Model of DNA Dynamics, Journal of Nonlinear Mathematical Physics **18** (2011) 463-484.
- **S. Zdravković, D. Chevizovich, A.N. Bugay, and A. Maluckov,** Chaos **29** (2019) 053118.
- **S. Zdravković**, Nonlinear Dynamics of DNA Chain, In Nonlinear Dynamics of Nanobiophysics, Edited by S. Zdravković and D. Chevizovich, Springer (2022) 29-66.