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САНКТ-ПЕТЕРБУРГСКИЙ ГОСУДАРСТВЕННЫЙ ПОЛИТЕХНИЧЕСКИЙ УНИВЕРСИТЕТ

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LECTURE 16

The system of nonlinear differential equations describing the behavior of DNA (II)

Lecture slides
for Bachelors of Technical Sciences

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Sine–Gordon kinks in living cellular structures

- Yomosa (1983-1984) considered the standard Watson–Crick double–helix B–form DNA model, in which conformation and stability of DNA and the polynucleotide double helices are determined by:

  – The energy of the hydrogen **H**-bonds between inter-strand complementary base pairs, given by:

$$E_B = \sum_n B[1 - \cos(\theta_n - \theta'_n - \pi)],$$

where B is a parameter associated with the H-bond energy.

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– The stacking energy between intra-strand adjacent bases, given by:

$$E_S = \sum_n S[1 - \cos(\theta_n - \theta_{n-1} - \alpha_0)] + S[1 - \cos(\theta'_n - \theta'_{n-1} - \alpha_0)],$$

where S is a parameter associated with the stacking energy of DNA chains.

- Next, by adding the rotational kinetic energy:

$$T_{\mathrm{rot}} = \frac{1}{2} \sum_n I[\dot{\theta}_n^2 + \dot{\theta}_n'^2],$$

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to the potential energies, the following SG–chain Hamiltonian for DNA and synthetic polynucleotide double–helices was formulated:

$$\begin{aligned} H &= T_{\rm rot} + E_B + E_S = \frac{1}{2}\sum_n I[\dot{\theta}_n^2 + \dot{\theta}_n'^2] + \sum_n B[1-\cos(\theta_n - \theta_n' - \pi)] \\ &+ \sum_n \left\{ S[1-\cos(\theta_n - \theta_{n-1} - \alpha_0)] + S[1-\cos(\theta_n' - \theta_{n-1}' - \alpha_0)] \right\}. \end{aligned}$$

Via canonical Hamiltonian formalism, the following two sets of coupled equations of motion were derived:

$$\begin{aligned} I\ddot{\theta}_n + B\sin(\theta_n - \theta_n' - \pi) + S[\sin(\theta_n - \theta_{n-1} - \alpha_0) - \sin(\theta_{n+1} - \theta_n - \alpha_0)] &= 0, \\ I\ddot{\theta}_n' + B\sin(\theta_n - \theta_n' - \pi) + S[\sin(\theta_n' - \theta_{n-1}' - \alpha_0) - \sin(\theta_{n+1}' - \theta_n' - \alpha_0)] &= 0. \end{aligned}$$

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- By linearizing this coupled ODE-system and performing the continuum limit:

$$\begin{aligned} I\theta_{tt} - S\theta_{xx} &= -B\sin(\theta - \theta' - \pi), \\ I\theta'_{tt} - S\theta'_{xx} &= B\sin(\theta - \theta' - \pi). \end{aligned}$$

- Zhang (1985) clarified the approach of Yomosa and proposed the following modified Hamiltonian:

$$\begin{aligned} H &= \frac{1}{2}\sum_n I[\dot{\theta}_n^2 + \dot{\theta}_n'^2] + \sum_n V(\theta_n, \theta'_n) \\ &+ \frac{1}{2}\sum_n \left[S(\theta_n - \theta_{n-1})^2 + S(\theta'_n - \theta'_{n-1})^2\right] \end{aligned}$$

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- From the Hamiltonian, the following equations of motion can be derived:

$$
\begin{aligned}
&I\ddot{\theta}_n + B\sin(\theta_n - \theta'_n) + \beta[3\sin\theta_n\cos\theta'_n - \sin(\theta_n - \theta'_n)] + \lambda\sin\theta_n \\
&\qquad = S(\theta_{n+1} - 2\theta_n + \theta_{n-1}), \\
&I\ddot{\theta}'_n - B\sin(\theta_n - \theta'_n) + \beta[3\cos\theta_n\sin\theta'_n + \sin(\theta_n - \theta'_n)] + \lambda\sin\theta'_n \\
&\qquad = S(\theta'_{n+1} - 2\theta'_n + \theta'_{n-1}).
\end{aligned}
$$

- The continuum analog takes the form:

$$
\begin{aligned}
\phi_{xx} - (1/c_0^2)\phi_{tt} &= (1/l^2)\sin\phi + (2/d^2)\sin(\phi/2)\cos(\psi/2) \\
\psi_{xx} - (1/c_0^2)\psi_{tt} &= (1/l^2)\sin\psi + (2/d^2)\sin(\psi/2)\cos(\phi/2)
\end{aligned}
$$

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- Salerno (1991) introduced the following refined discreet Hamiltonian (the most commonly used):

$$H = \frac{1}{2}\sum_{n=1}^{N} I[\dot{\psi}_n^2 + \dot{\theta}_n^2] + \sum_{n=1}^{N} K\left[(\psi_{n+1} - \psi_n)^2 + (\theta_{n+1} - \theta_n)^2\right] + \sum_{n=1}^{N} \eta_n[1 - \cos(\psi_n - \theta_n)],$$

- From the Hamiltonian the following equations of motion were derived:

$$I\ddot{\psi}_n = K(\psi_{n+1} - 2\psi_n + \psi_{n-1}) - \frac{\beta}{2}\lambda_n \sin(\psi_n - \theta_n),$$

$$I\ddot{\theta}_n = K(\theta_{n+1} - 2\theta_n + \theta_{n-1}) - \frac{\beta}{2}\lambda_n \sin(\theta_n - \psi_n).$$

Conclusion

- All the studied PDE systems cannot be solved by analytical means, therefore one needs to apply numerical methods such as the explicit finite difference scheme or to use available mathematical software to evaluate the results.
- Discreet systems can be more conveniently solved by the means of numerical methods, because of its simplicity. For example it can be Verlet integration, leap-frog or another suitable method of Molecular Dynamics.