

Solitons and autowaves in biopolymers

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History

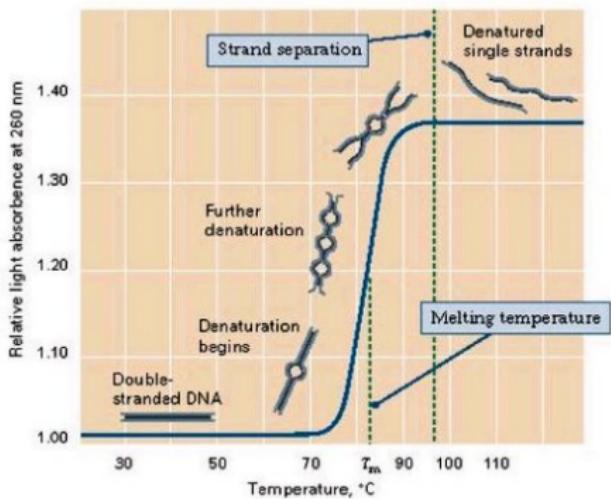
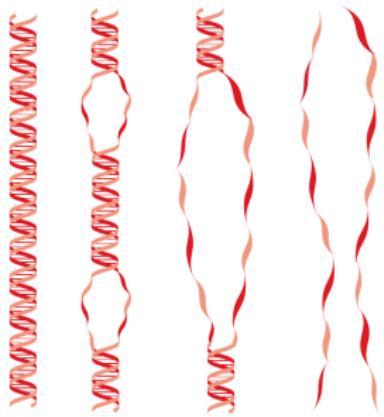
45 years of solitons in polymer chains

A.S. Davydov, N.I. Kislukha, Phys. Stat. Sol. B **59**, 465 (1973)

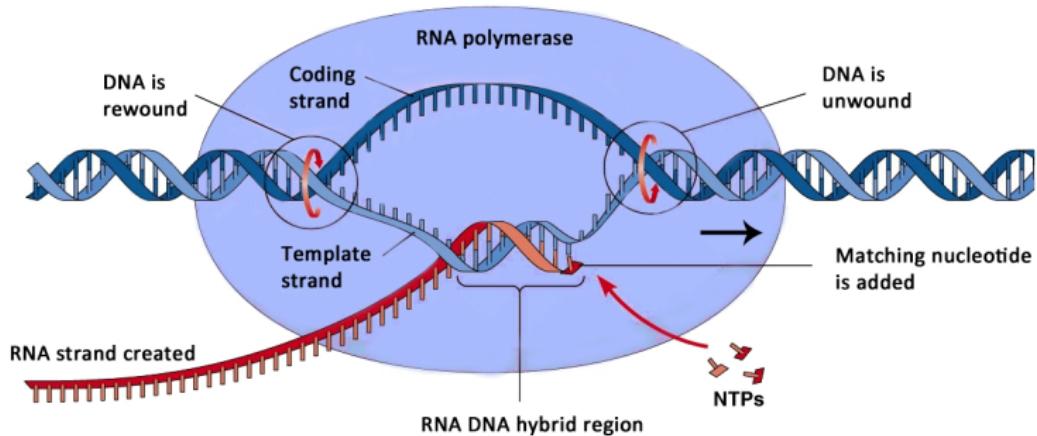
25 years of solitons in microtubules

M.V. Sataric, J. A. Tuszynski, R. B. Zakula, Phys. Rev. E **48**, 589 (1993).

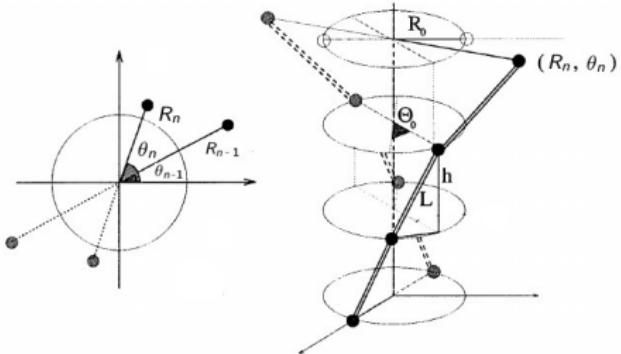
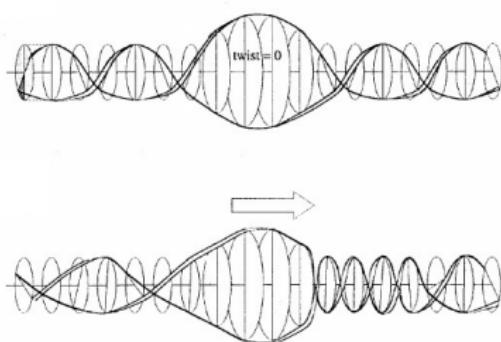
Thermal denaturation



Transcription



Helicoidal model of DNA



$$H = \frac{1}{2} \sum_n \left[m(\dot{R}_n^2 + R_n^2 \dot{\theta}_n^2) + 2V(R_n - R_0) + C(R_{n+1} - R_n)^2 e^{-b(R_{n+1} + R_n - 2R_0)} + K(L_{n,n+1} - L_0)^2 + G(\theta_{n+1} + \theta_{n-1} - 2\theta_n)^2 \right], \quad (1)$$

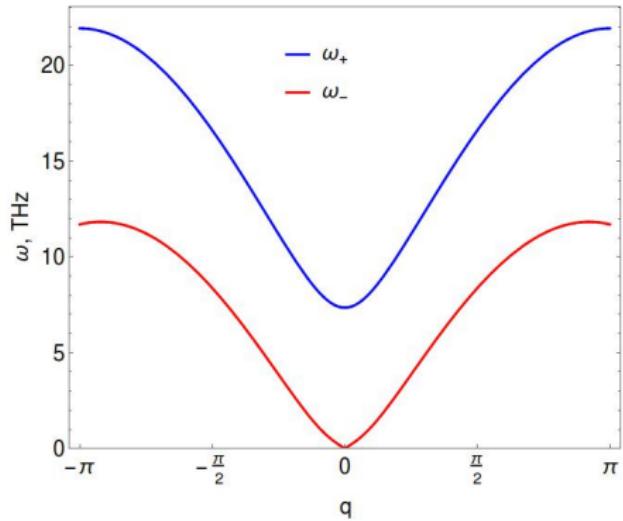
$$L_{n,n+1} = \sqrt{h^2 + R_n^2 + R_{n+1}^2 - 2R_n R_{n+1} \cos(\theta_{n+1} - \theta_n)},$$

$$L_0 = \sqrt{h^2 + 4R_0^2 \sin^2(\theta_0/2)}.$$

M. Barbi, S. Cocco, M. Peyrard, S. Ruffo J.Biol.Phys. 1999 **24**, 97.

M. Barbi, S. Lepri, M. Peyrard, N. Theodorakopoulos Phys. Rev. E. 2003 **68**, 061909.

Dispersion curves



$$R_n, \theta_n \sim e^{i(\omega t - qn)}$$

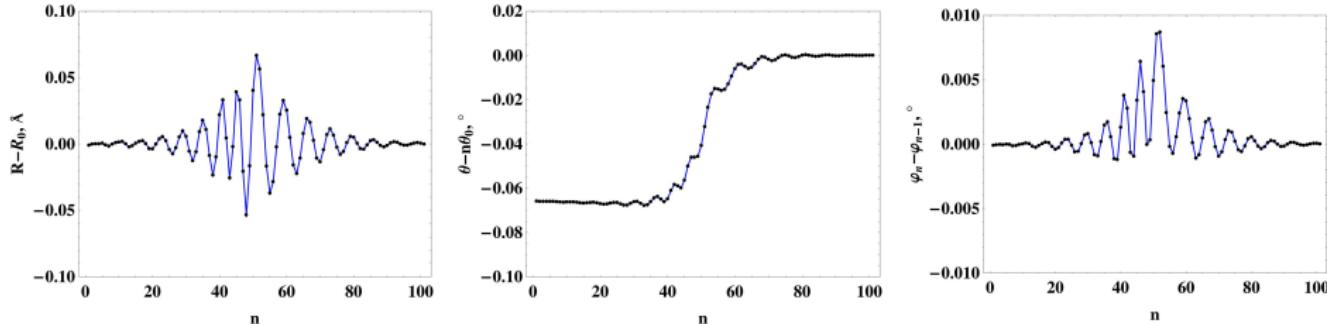
$$\omega_+ \approx \omega_+^{(0)} + \omega_+^{(2)} q^2,$$

$$\omega_- \approx \omega_-^{(1)} q - \omega_-^{(3)} q^3.$$

Known solutions: breather

M. Barbi, S. Cocco and M. Peyrard, Physics Letters A 253 (1999), 358

C.B. Tabi, A. Mohamadou, T.C. Kofane, Physics Letters A 373 (2009) 2476.



$$u_n = R_n / R_0 - 1, \quad \varphi_n = \theta_n - n\theta_0.$$

$$i \frac{\partial \psi}{\partial \tau} + P \frac{\partial^2 \psi}{\partial \zeta^2} + Q |\psi|^2 \psi = 0. \quad (2)$$

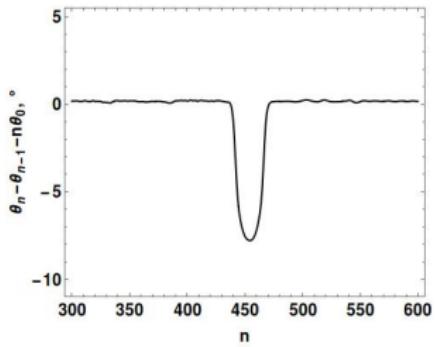
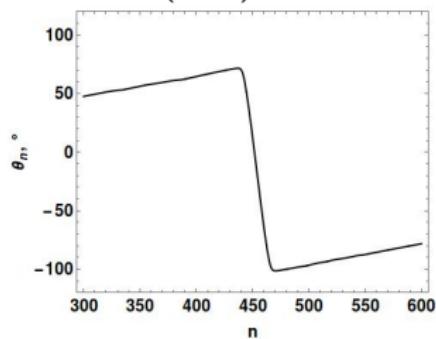
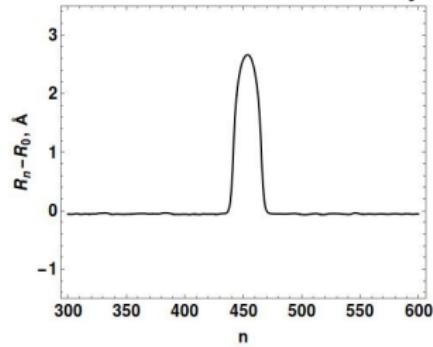
$$u = (\nu_{11} - i\nu_{12} \frac{\partial}{\partial \zeta}) \psi e^{i(\omega t - qn)} + c.c. + \nu_1 |\psi|^2 + \nu_3 \psi^2 e^{2i(\omega t - qn)} + c.c. \quad (3)$$

$$\varphi = (\nu_0 + \nu_2) \int |\psi|^2 d\zeta + (\nu_0 - i\nu_{22} \frac{\partial}{\partial \zeta}) \psi e^{i(\omega t - qn)} + \nu_4 \psi^2 e^{2i(\omega t - qn)} + c.c. \quad (4)$$

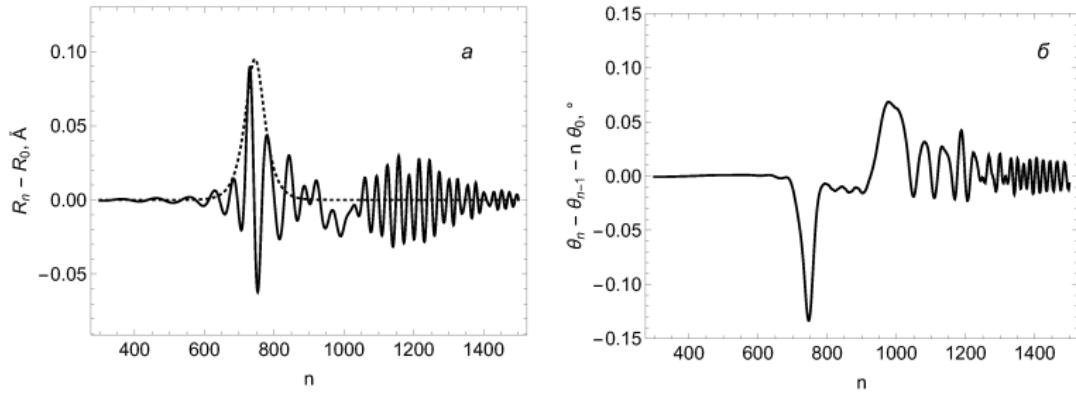
Known solutions: denaturation bubble

A. Campa, Phys. Rev. E, 63 (2001) 021901.

G. Gaeta, L. Venier, Phys. Rev. E, 78 (2008), 011901.



New solution: breather-twist solitons



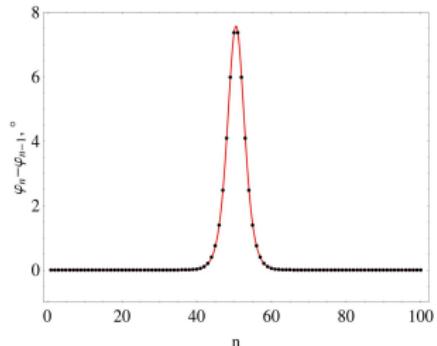
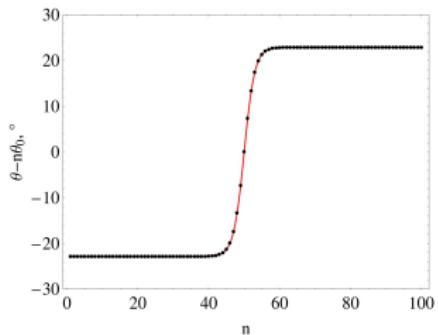
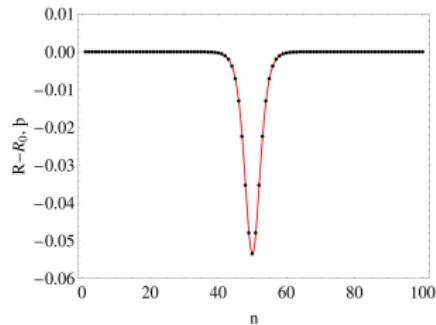
$$i \frac{\partial \psi}{\partial \tau} + P \frac{\partial^2 \psi}{\partial \zeta^2} + G_1 \chi \psi = 0. \quad (5)$$

$$i \frac{\partial \chi}{\partial \tau} + G_2 \frac{\partial}{\partial \zeta} |\psi|^2 = 0. \quad (6)$$

$$\psi = \frac{A_0 \sqrt{W}}{\lambda} \operatorname{sech} \left(\frac{\zeta - W\tau}{\lambda} \right) e^{iW\zeta - \Phi} \quad (7)$$

$$\chi = -\frac{B_0}{\lambda^2} \operatorname{sech}^2 \left(\frac{\zeta - W\tau}{\lambda} \right) \quad (8)$$

New solution: twist solitons



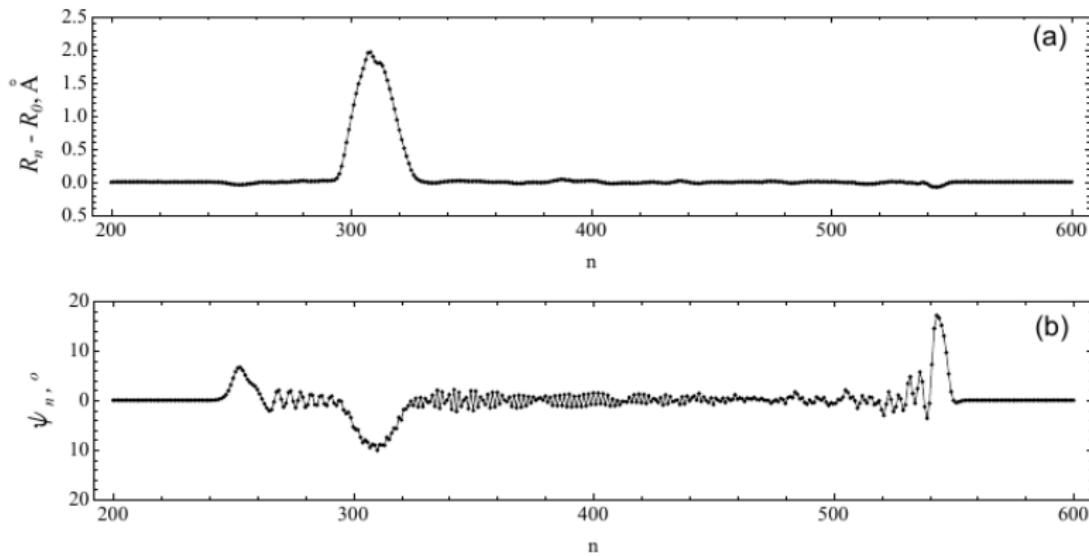
$$\frac{\partial f}{\partial \tau} + \gamma_1 f \frac{\partial f}{\partial \xi} + \gamma_2 \frac{\partial^3 f}{\partial \xi^3} = 0. \quad (9)$$

$$f = \frac{3\gamma_2}{\gamma_1 \lambda^2} \operatorname{sech}^2 \left(\frac{\xi - \gamma_2 \tau / \lambda^2}{2\lambda} \right) \quad (10)$$

$$u = f(\xi, \tau), \quad (11)$$

$$\varphi = -\mu_1 \int f(\xi, \tau) d\xi - \int \left(\mu_2 f^2(\xi, \tau) - \mu_3 \frac{\partial^2 f}{\partial \xi^2} \right) d\xi \quad (12)$$

Modeling of transcription



New solution: dissipative soliton

$$i\frac{\partial\psi}{\partial t} + P\frac{\partial^2\psi}{\partial\eta^2} + Q|\psi|^2\psi = -\frac{i\gamma}{2}\psi - \frac{i\alpha\varepsilon_0}{2}\psi^*\mathrm{e}^{i\delta t}, \quad (13)$$

$$\delta = 2\omega - \Omega$$

$$\psi_s = i\sqrt{\frac{2P}{Q}}\rho \operatorname{sech}[\rho(nl_0)] \mathrm{e}^{i\Phi_{ph}}, \quad (14)$$

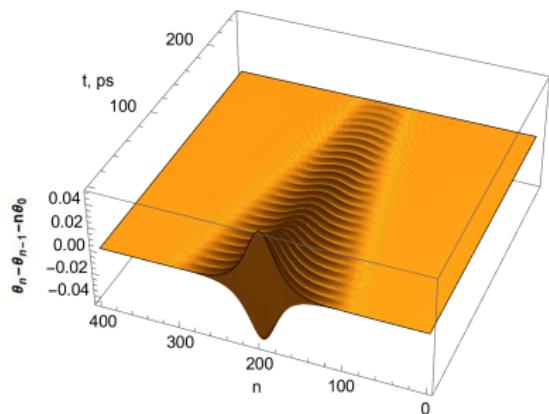
$$\Phi_{ph\pm}(t) = \frac{1}{2} \left(\delta t \mp \arccos \frac{\gamma}{\alpha\varepsilon_0} \right), \quad (15)$$

$$\rho_{\pm} = \sqrt{\frac{\delta}{2P} \pm \frac{\alpha\varepsilon_0}{P} \sqrt{1 - \left(\frac{\gamma}{\alpha\varepsilon_0}\right)^2}} \quad (16)$$

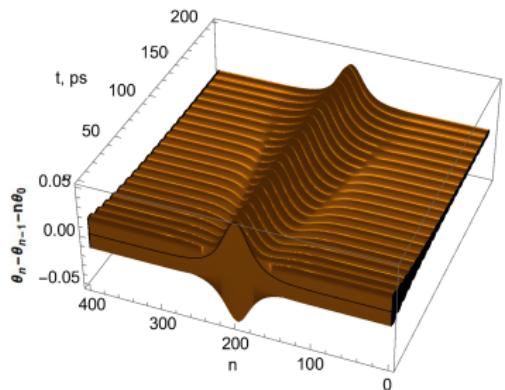
$$\frac{\gamma}{s_1\omega_0} < \varepsilon_0 \ll 1 \quad (17)$$

Excitation of dissipative soliton

$$\varepsilon = 0$$

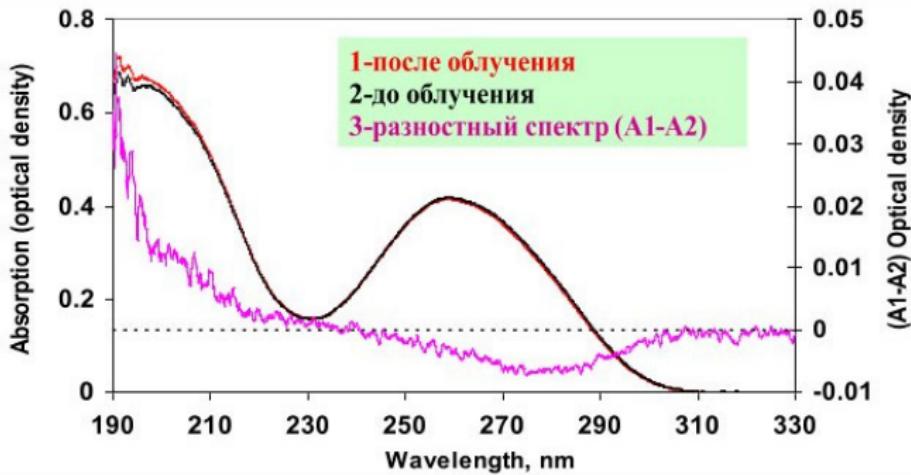


$$\varepsilon \neq 0$$



Experiment: THz radiation induces changes in DNA UV absorption spectra

3.6THz, 15mW/cm²

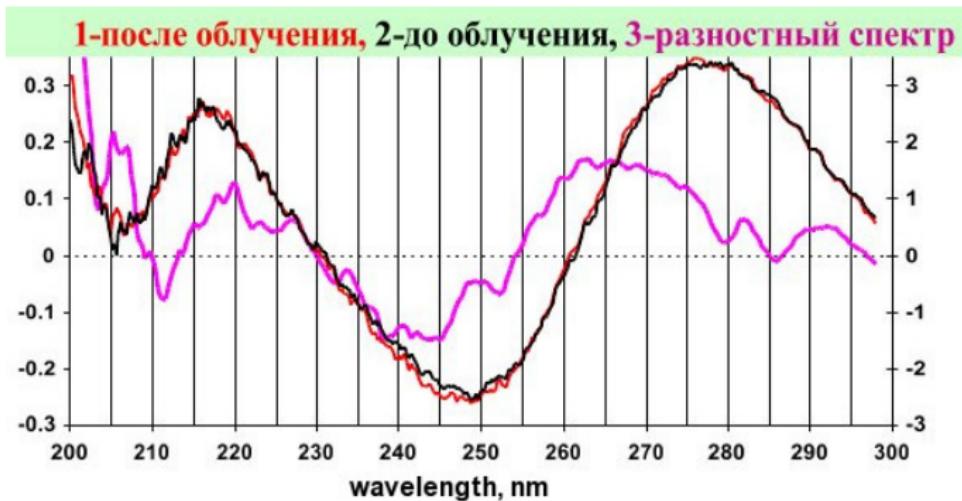


O.P.Cherkasova et al, V International Symposium on Modern Problems of Laser Physics, Novosibirsk, Russia, August 24-30, 2008.

V.I. Fedorov, Biomedical Radioelectronics, 2011, No.2, P.17-27.

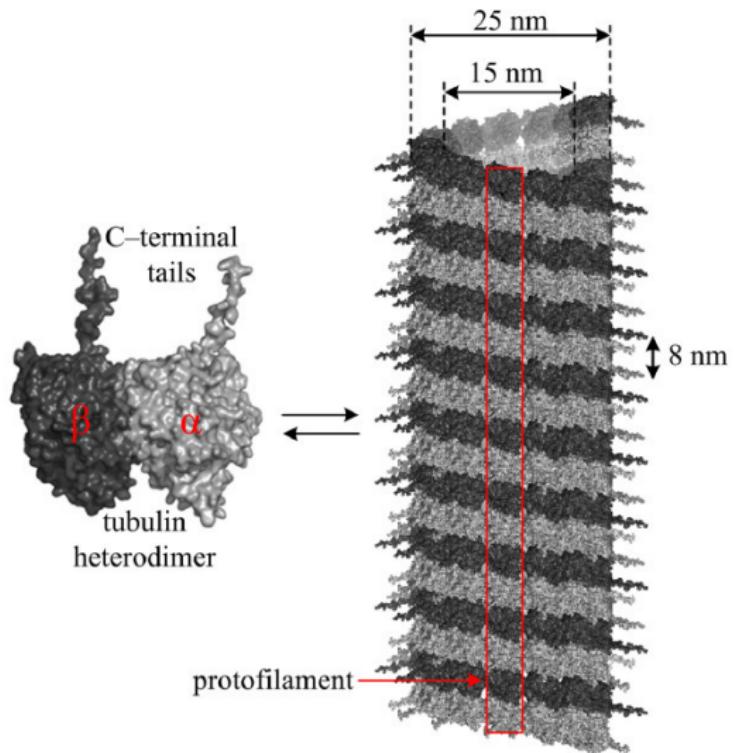
Experiment: THz radiation induces changes in DNA circular dichroism spectra

3.6THz, 15mW/cm²



O.P.Cherkasova et al, V International Symposium on Modern Problems of Laser Physics, Novosibirsk, Russia, August 24-30, 2008.
V.I. Fedorov, Biomedical Radioelectronics, 2011, No.2, P.17-27.

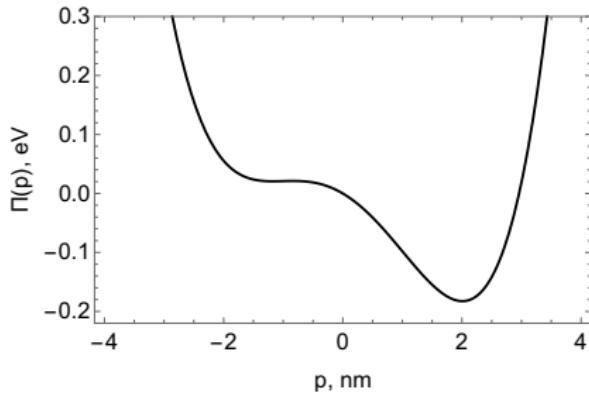
Structure of microtubules



Effective Hamiltonian and equations of motion

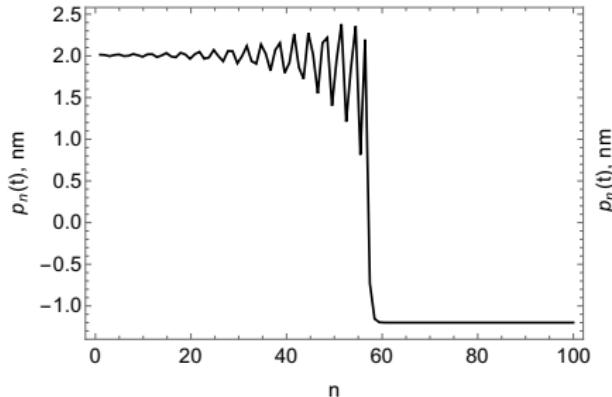
$$H = \sum_n \left[\frac{m}{2} \dot{p}_n^2 + \frac{K}{2} (p_{n+1} - p_n)^2 - \frac{1}{2} A p_n^2 + \frac{1}{4} B p_n^4 - q E_0 p_n \right]. \quad (18)$$

$$m \ddot{p}_n = K(p_{n+1} + p_{n-1} - 2p_n) + Ap_n - Bp_n^3 + qE_0(1 + \varepsilon(t)) - m\gamma \dot{p}_n. \quad (19)$$

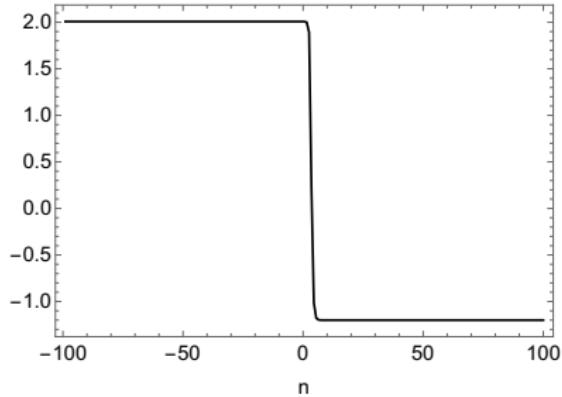


Kinks

Underdamped case $\frac{\gamma}{\omega} \ll 1$



Overdamped case $\frac{\gamma}{\omega} \gg 1$

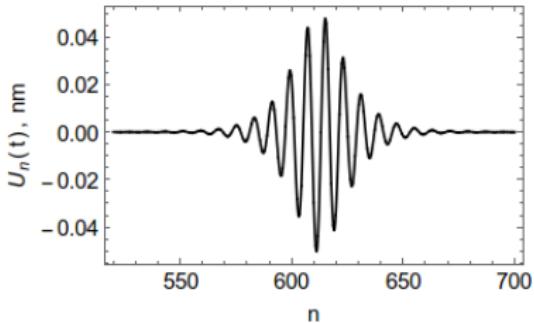
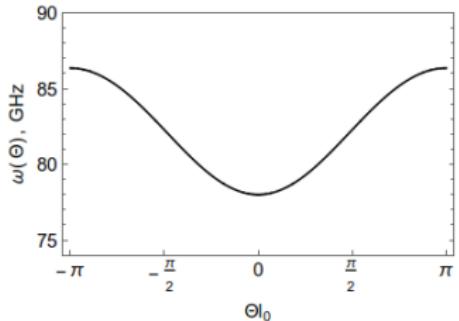


$$p(n, t) = \sqrt{\frac{A}{B}} \left(a_0 - \sqrt{1 - 3a_0^2} \tanh[b(nl_0 - vt)] \right), \quad (20)$$

Kinks as molecular memory elements:

Sahu et al., "Multi-level memory-switching properties of a single brain microtubule"
Appl. Phys. Lett. **102**, 123701 (2013)

Breather

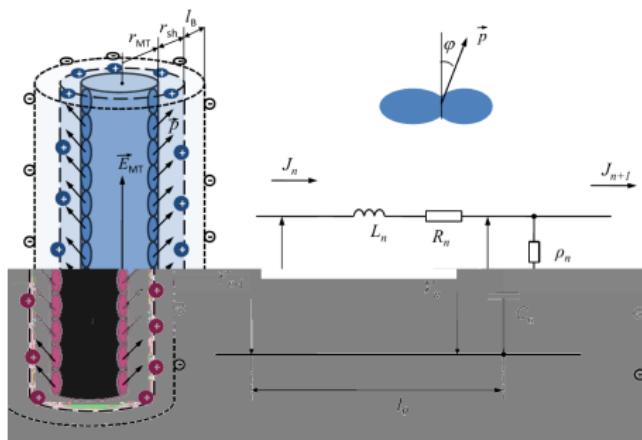


$$p_n(t) = p_R + \rho \operatorname{sech} \left(\frac{n l_0 - V_G t}{L} \right) \cos(\Theta n l_0 - \Omega_0 t) - \frac{a \rho^2}{2b} \operatorname{sech}^2 \left(\frac{n l_0 - V_G t}{L} \right) + \\ + \frac{1}{2} \delta \rho^2 \operatorname{sech}^2 \left(\frac{n l_0 - V_G t}{L} \right) \cos(2(\Theta n l_0 - \Omega_0 t)), \quad (21)$$

$$\Omega_0 = \omega(\Theta) - \frac{Q(\Theta)\rho^2}{8}, \quad (22)$$

Possible relation to collective MT vibrations, observed in
Sahu S., et al. Sci.Rep. 4, 7303 (2014)

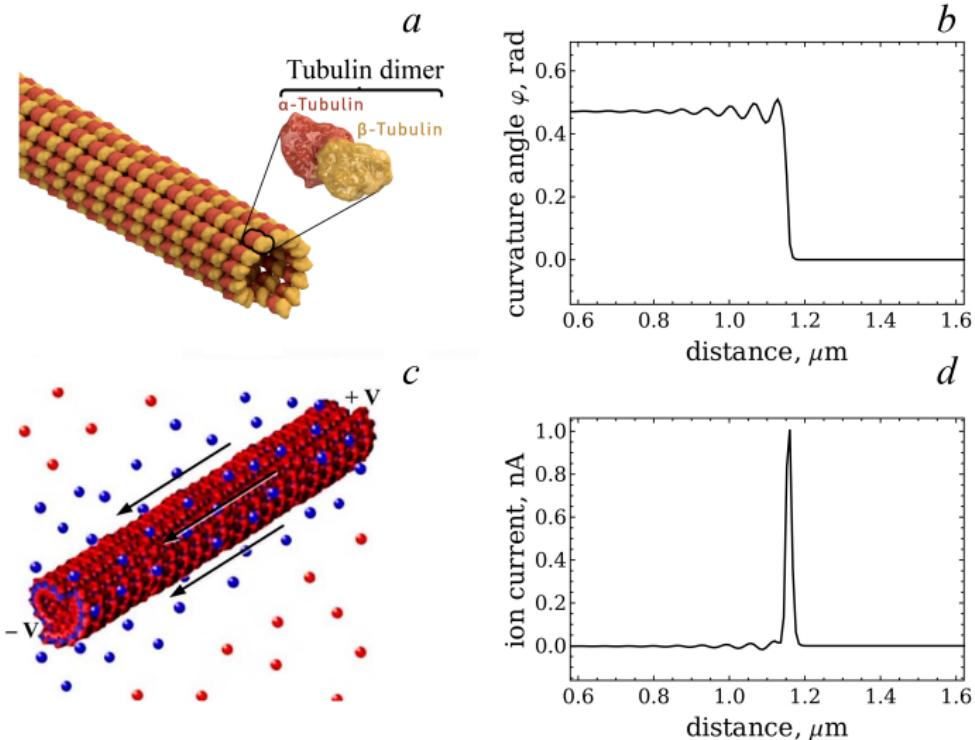
Equations for electro-mechanical excitations



$$\frac{d^2\varphi_n}{dt^2} + \gamma \frac{d\varphi_n}{dt} = \frac{K}{I}(\varphi_{n+1} + \varphi_{n-1} - 2\varphi_n) - \frac{A}{I}\varphi(\varphi_n - \varphi_u)(\varphi_n - \varphi_s) - bV_n - a\varphi_n V_n, \quad (23)$$

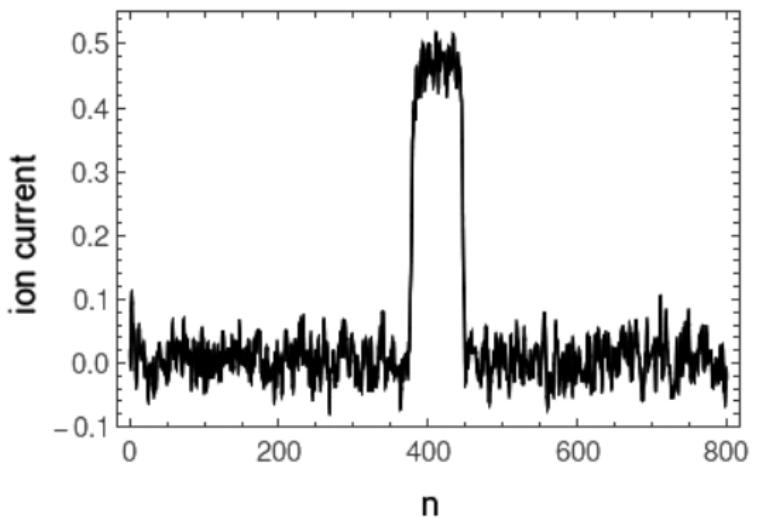
$$\frac{dV_n}{dt} = \frac{1}{RC}(V_{n+1} + V_{n-1} - 2V_n) + \alpha(\varphi_{n+1} - \varphi_n) + \beta(\varphi_{n+1}^2 - \varphi_n^2), \quad (24)$$

Electro-mechanic signal

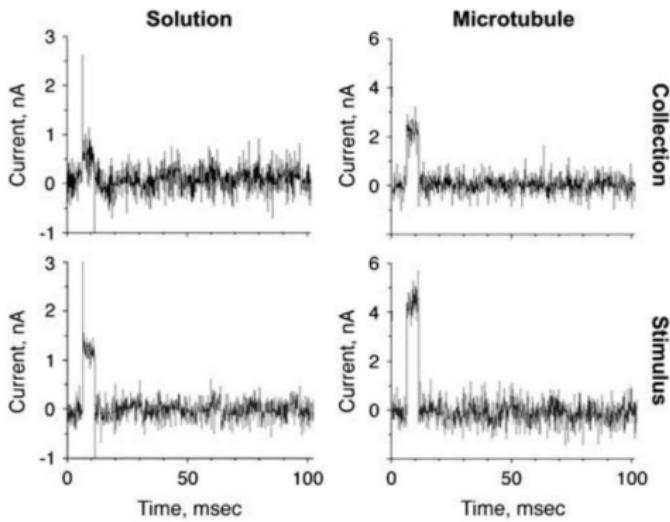
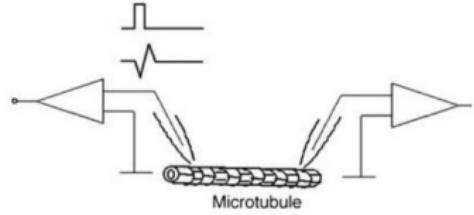


$$v_{pulse} = 6 \text{ m/s}$$

Signal stability under thermal noise ($T=310K$)



Experiment: MT amplifies injected electric current



A. Priel, A.J. Ramos, J.A. Tuszyński, and H.F. Cantiello, Biophys. J. **90**, 4639 (2006)

List of publications

- Bugay A.N. Bull. Russ. Acad. Sci. Physics. 2011. V.75. No.12. P.1579.
- Bugay A.N. Nanosystems: Physics, Chemistry, Mathematics 2012. V.3. No.1. P.51.
- Bugay A.N., Aru G.F. Nonlinear Phenomena in Complex Systems. 2014. V.17. No.1. P.1.
- Zdravkovic S., Bugay A.N., Aru G.F., Maluckov A. Chaos. 2014. V.24. No.2. P.023139.
- Bugay A.N. Nonlinear Phenomena in Complex Systems 2015. V.18. No.2. P.236.
- Sekulic D.L., Sataric B.M., Zdravkovic S., Bugay A.N., Sataric M.V. Chaos. 2016. V.26. P.073119.
- Zdravkovic S., Bugay A. N. Nonlinear Phenomena in Complex Systems. 2016. V.19, No.1. P.71.
- Zdravkovic S., Zekovic S., Bugay A.N., Sataric M.V. Applied Mathematics and Computation. 2016. V.285. P.248.
- Zdravkovic S., Bugay A.N., Parkhomenko A.Yu. Nonlinear Dynamics. 2017. V.90. P.2841.

Thank you for the attention!