FREQUENCY DEPENDENCE OF AMPLITUDE OF NONLINEAR TRANSVERSE WAVES IN DNA MOLECULE

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We use the nonlinear Peyrard-Bishop model for describing the transversal oscillations of nucleotides. The potential for hydrogen bonds connecting AT or CG base pairs is modeled by a Morse potential. The Hamiltonian for DNA is [1, 2]

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

It is convenient to introduce the new coordinates

$$x_n = (u_n + v_n)/\sqrt{2}\,,\ y_n = (u_n - v_n)/\sqrt{2}\,. \quad (2)$$

The equations for the transversal oscillation of nucleotides are

$$m\ddot{x}_n = c\left(x_{n+1} + x_{n-1} - 2x_n\right),\ m\ddot{y}_n = c\left(y_{n+1} + y_{n-1} - 2y_n\right) + 2\sqrt{2}aD\left(\mathrm{e}^{-a\sqrt{2}y_n} - 1\right)\left(\mathrm{e}^{-a\sqrt{2}y_n}\right). \quad (3)$$

The first equation describes the usual linear waves (photons). The second one describes the nonlinear waves (breathers). For the equation (3) we shall be used the solution in form of traveling wave

$$y_n = A\cos(\omega t - knh) = A\cos x\,. \quad (4)$$

Here ω is frequency, which dependent from the amplitude *A*; k is the wave number; *h* is distance between neighboring nucleotides of same strand.

After substitution (4) in (3) we find relation

$$m\omega^2 A\cos x = 2cA(1 - \cos kh)\cos x - 2\sqrt{2}aD\left[\mathrm{e}^{-2a\sqrt{2}A\cos x} - \mathrm{e}^{-a\sqrt{2}A\cos x}\right]. \quad (5)$$

According to Galerkin method we multiply (6) on cos*x* and then integrate over the *x* from -π to π. In result we obtain the equation for frequency ω as function the amplitude *A* and the wave number *k*

$$\frac{\omega}{\omega_0} = \sqrt{2(1 - \cos kh) + \frac{4\sqrt{2}aD}{cA}\left(I_1(2\sqrt{2}aA) - I_1(\sqrt{2}aA)\right)}\,. \quad (6)$$

Here $\omega_0 = \sqrt{c/m}$, $I_1(x)$ is Bessel function of imaginary argument. The equation (6) given the sharp increase the amplitude at variation the frequency in bounded limits. The relation (6) describes the optical modes due to the nonlinear dependence of frequency from amplitudes. We may to support the assumption that local DNA denaturation is due to local strand separation.

References

1. *Yakushevich L.V.* Nonlinear physics of DNA. – Willey, 1998. 204 p.
2. *Zdravkovic S., Sataric M.* Single-molecule unzippering experiments on DNA and Peyard-Bishop-Dauxois model // Phys. Rev. E **Vol. 73**, 2006. Pp. 021905-1-11.