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MICROWAVE AND THERMAL GENERATION OF SOLITONS IN DNA

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Abstract - Models for soliton generation in DNA strands are presented. First, soliton generation from interaction with an electromagnetic field is discussed, modelling DNA as a homogeneous, cylindrical rod with nonlinear elasticity using the Ostrovskii-Sutin equation. Then the problem of thermally generated solitons is considered. The thermal equilibrium number of solitons as a function of absolute temperature and the number of base pairs in the DNA molecule is computed. The calculation is effected by modelling DNA as a Toda lattice with parameters chosen to match experimentally measured properties of DNA.

1 - INTRODUCTION

In the controversial problem of solitons playing a role in the dynamics of DNA /1-5/, there is a particular aspect related to the question if solitons will be generated at physiological temperature. Sobell /1/ has suggested, on the basis of biochemical evidence, that a localized nonlinear state (which he calls the "premelton") should be observed in DNA at 310 K. Van Zandt /2/, on the other hand, claims that nonlinearity plays no role in DNA dynamics at that temperature. Our aim here is to present an overview of two models introduced by the authors in /4/ and /5/, showing that solitons are expected at physiological temperature. The first soliton theory uses a continuous model for the DNA molecule, and considers nonlinear effects in a microwave experiment /4/. The second one uses a discrete model for the DNA strand, and by using well-developed analytical techniques allows to compute the number of solitons as a function of temperature /5/. The continuous model is presented in Section 2, while the discrete one is given in Section 3.

2 - THE CONTINUOUS MODEL

One of the simplest models for DNA dynamics is a uniform cylindrical rod /3/. Since Ostrovskii and Sutin /6/ have studied longitudinal wave motion on a uniform rod with nonlinear elasticity in considerable detail, in /4/ their equation has been considered as model for DNA dynamics when dispersive and nonlinear effects are taken into account. In terms of the longitudinal displacement U, the Ostrovskii-Sutin equation (OSE) reads /4/:

\[
\frac{\partial^2 U}{\partial T^2} = c^2 \frac{\partial^2 U}{\partial X^2} + \frac{c^2}{3} \frac{\partial^2 U}{\partial X^2 \partial T^2} + \delta U + \frac{1}{c^2} \frac{\partial U}{\partial T} + \frac{1}{c^2} \frac{\partial U}{\partial T}.
\]

Here X and T are laboratory space and time, and the subscripts indicate partial derivative; c is the wave velocity, c/c² is the dispersive parameter and δ is the nonlinear parameter.

In order to model a microwave experiment /4/, the OSE, seen as Newton's second law, must be augmented by a damping term to represent the viscosity of water /2/ and a driving term to represent the microwave field. The considered equation is then
Introducing the following normalizing transformations

\[ U = - \frac{c^2}{\delta} u , \quad X = \frac{\sqrt{\epsilon}}{c} x , \quad T = \frac{\sqrt{\epsilon}}{c^2} t \]

\[ A = \frac{c^2}{\delta} \alpha , \quad \Omega = \frac{c^2}{\sqrt{\epsilon}} \omega , \quad F(X) = - \frac{c^2}{\delta \sqrt{\epsilon}} \Gamma f(x) , \]

Eq. (2.2) takes the form

\[ u_{tt} = u_{xx} + u_{xxtt} - (\frac{u_x^2}{X})_x - \alpha u_x + \Gamma f(x) \cos(\omega t) . \]

Considering periodic boundary conditions which correspond to DNA closed in a loop of normalized length \( L_c = \sqrt{\epsilon} \) (L is the physical length of the molecule), an exact cnoidal wave solution of the unperturbed OSE (Eq. (2.4) with \( \alpha = 0 \) and \( \Gamma = 0 \)) can be easily obtained /4/. Moreover, the following quantities are constants of motion

\[ I_1 = \int u_x \, dx = 0 , \]  

the momentum

\[ I_2 = \int u_t \, dx , \]  

and the energy

\[ H = \int \left[ \frac{1}{2} u_x^2 + \frac{1}{2} u_t^2 + \frac{1}{2} u_{xt}^2 - \frac{1}{3} u_x^3 \right] \, dx . \]

The effects of the damping and driving terms present in the perturbed equation (2.4) on the conserved quantities \( I_1, I_2, \) and \( H \) are the following:

\[ \dot{I}_1 = 0 , \]  

\[ \dot{I}_2 = - \alpha I_1 + \Gamma \cos(\omega t) \int f(x) \, dx , \]  

\[ \dot{H} = - \alpha \int u_t^2 \, dx + \Gamma \cos(\omega t) \int f(x) u_t \, dx . \]

Eq. (2.6a) implies that \( I_1 \) is a constant of motion for the perturbed equation (2.4). Eq. (2.6b) implies that the time average of \( I_2 \) will relax to zero as \( \exp(-\alpha t) \). Eq. (2.6c) is an expression of conservation of energy for the equation. The first term on the right-hand side gives the power dissipated in viscous drag, the second one gives the power input from the microwave field. For steady state oscillations the time average over a period of these two terms must be equal.

In /4/ a detailed analysis of the damped-driven OSE, Eq. (2.4), has been performed for different choices of the driver, and comparison with a linear study has been done. Here we only report one of the calculations, shown in Fig. 2.1, for computing the energy \( H \) as a function of the driving frequency \( \omega \), with \( \alpha = 0.02 \), the normalized length \( L_c = 51.2 \), and driving function \( f(x) = 0.4 \delta(x) \). An absorption spectrum similar to the one calculated by van Zandt /2/ is evident. In /4/ it has been shown that the linewidth of a resonance peak is not simply related to the damping constant as in the linear cases. This is an anharmonic effect. Moreover, resonance peaks of the damped-driven OSE exhibit a multicomponent character that is related to "bunched" multisoliton solutions. The energy in laboratory units, \( E \), is given by the relation

\[ E = \frac{\rho_c c^2 \sqrt{\epsilon}}{\delta^2} \equiv E_0 \]

where \( \rho_c = 2.0 \times 10^{-3} \) kg/meter is the linear mass density, and \( H \) the normalized energy shown in Fig. 2.1. If realistic parameter values for the dispersive and nonlinear coefficients are considered /4/, values for the energy \( E \) can be computed. These are shown in Table 1. At physiological temperature (310 K), the thermal energy in an oscillatory mode is
Here $k_B T = 4.28 \times 10^{-21}$ joules. \hfill (2.8)

Here $k_B$ is Boltzmann constant, and $T$ is absolute temperature.

Fig. 2.1 - Total energy $H$ versus frequency $\omega$ computed for Eq. (2.4) with $\alpha = 0.02$, $\Gamma = 0.4$, and $f(x) = \delta(x)$; normalized length $l = 51.2$.

Since in Fig. 2.1 for the first peak the normalized energy is about $H = 1$, then the actual energy is the one given in Table 1. For those entries for which

$$k_B T > E$$

we would expect thermal excitation of the mode to at least the level indicated in Fig. 2.1. These entries are indicated by a "bullet" in the upper right-hand corner of Table 1.

Table 1 - Values of the normalizing energy, $E_0$, for various values of the dispersion parameter, $\varepsilon$, and the anharmonicity parameter, $\delta$.

<table>
<thead>
<tr>
<th>$\varepsilon/c^2$</th>
<th>$4.8 \times 10^{-21}$</th>
<th>$3.6 \times 10^{-20}$</th>
<th>$4.8 \times 10^{-19}$</th>
<th>meter$^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\delta/c^2$ = 1</td>
<td>$4.0 \times 10^{-19}$</td>
<td>$1.1 \times 10^{-18}$</td>
<td>$4.0 \times 10^{-18}$</td>
<td>joules</td>
</tr>
<tr>
<td>9.2</td>
<td>$4.7 \times 10^{-21}$</td>
<td>$1.3 \times 10^{-20}$</td>
<td>$4.7 \times 10^{-20}$</td>
<td>joules</td>
</tr>
<tr>
<td>20</td>
<td>$9.9 \times 10^{-22}$</td>
<td>$2.7 \times 10^{-21}$</td>
<td>$9.9 \times 10^{-21}$</td>
<td>joules</td>
</tr>
</tbody>
</table>

We emphasize that this point of view assumes that anharmonic modes (solitons) share $k_B T$ of thermal energy in thermal equilibrium, just as do harmonic modes. From Table 1 it is evident that the calculations involve mode energy of the order $k_B T$, under reasonable assumptions for the anharmonicity and the dispersive parameter.

3 - THE DISCRETE MODEL

Another of the simplest models for DNA dynamics is a simple nonlinear spring and mass system, where each mass of the model represents a single base pair, and the nonlinear spring represents the van der Waals potential between adjacent base pairs. Since the Toda lattice /7,8/ is exactly integrable, and well-developed analytical techniques can be used to efficiently count the number of solitons, it is considered as model for DNA dynamics, when the problem of thermally generated solitons at physiological temperature is analysed /5/. Newton's second law for the longitudinal motion of the masses is the set of ordinary differential equations (N denotes the number of masses)

$$M \ddot{y}_j = V'(y_{j+1} - y_j) - V'(y_j - y_{j-1})$$ \hfill (3.1)

where dots indicate time derivative and prime denotes derivative with respect to the argument. For the Toda lattice the nonlinear spring potential is /7/
\[ V(y_{j+1} - y_j) = \frac{a}{b} \exp\left[-\frac{b(y_{j+1} - y_j)}{a}\right] + a(y_{j+1} - y_j) \] (3.2)

where \(a\) and \(b\) are arbitrary parameters, and \(j = 1, 2, \ldots, N\).

An important physical point is the determination of the parameters \(a\) and \(b\) in (3.2) to match experimentally measured properties of DNA. This is easily done /5/. From the known structure and density of DNA, the mass is

\[ M = 1.26 \times 10^{-24} \text{ kg m} \] (3.3)

By fitting the exponential function (3.2) with a more realistic potential function between base pairs, that is the generalized van der Waals function

\[ V(y_{j+1} - y_j) = \frac{A}{(y_{j+1} - y_j)^n} - \frac{B}{(y_{j+1} - y_j)^m} \] (3.4)

and considering a 6-12 potential \((n = 12, \ m = 6)\) then

\[ b = 6.18 \times 10^{-10} \text{ meters}^{-1} \] (3.5)

Near the minimum \((y_{j+1} - y_j = 0)\), the potential (3.2) reduces to a harmonic one, with a spring force constant \(k = ab\). From the experimentally measured sound speed \((c = \sqrt{k/M} = 1.69 \times 10^3 \text{ meters/sec})\), the value for the parameter \(a\) is readily obtained

\[ a = 5.13 \times 10^{-10} \text{ newtons} \] (3.6)

Since our interest is in the knowledge of the amount of solitons thermally generated at physiological temperature, we have used well-known techniques to efficiently count the number of solitons as a function of temperature /8/.

The equations of motion (3.1) are derived from the Hamiltonian

\[ H = \sum_{j=1}^{N} \left[ \frac{1}{2} M \ddot{y}_j + V(y_j - y_{j-1}) \right] \] (3.7)

After introducing the scaling transformations

\[ \sqrt{ab} t \rightarrow t, \ \ b_y_j \rightarrow Q_j \] (3.8)

and the new dynamical variables

\[ a_j = \frac{1}{2} \exp\left[-\left(\frac{Q_j - Q_{j-1}}{2}\right)\right], \ b_j = -\frac{1}{2} \dot{Q}_j \] (3.9)

they can be written as a system of 2\(N\) coupled ordinary differential equations

\[
\begin{align*}
\dot{a}_j &= a_j (b_{j+1} - b_j) \\
\dot{b}_j &= 2(a_j^2 - a_{j-1}^2)
\end{align*}
\] (3.10)

For a cyclic system of \(N\) masses, the periodic boundary condition is expressed as

\[ a_{j+N} = a_j, \quad b_{j+N} = b_j \] (3.11)

It is easily shown that the problem (3.10) written in Lax formulism /7/ is equivalent to the eigenvalue problem

\[
\begin{align*}
L \phi &= \lambda \phi, \quad \lambda = \text{const} \\
\dot{\phi} &= B \phi
\end{align*}
\] (3.12)

where \(L\) and \(B\) are \((N \times N)\) matrices.
From the first equation of system (3.12) a discrete Hill's equation is obtained

\[ a_{j-1} \phi_{j-1}(\lambda) - b_j \phi_j(\lambda) + a_j \phi_{j+1}(\lambda) = \lambda \phi_j. \]  

(3.13)

The initial value problem (3.10) can be solved exactly for an infinite lattice /8/. In particular, solitons are specified by bounded states whose eigenvalues satisfy the condition /8/

\[ |\lambda| > 1. \]  

(3.14)

Condition (3.14) is valid with a reasonable degree of accuracy even for a periodic lattice /8/.

In order to compute the proportion of eigenvalues with absolute value greater than 1, in /5/ we have used a simple and efficient method. Defining \( x_{j+1} = \phi_{j+1}(\lambda)/\phi_j(\lambda) \), from (3.13) a recursive relation for \( x_{j+1} \) is obtained:

\[ x_{j+1} = \frac{1}{a_j} \left[ \lambda - b_j - \frac{a_{j-1}}{x_j} \right]. \]  

(3.15)

Negative values of \( x_j \) indicate zero crossings of eigenvectors of (3.13). Since the number of zero crossings of eigenvectors of (3.13) decreases as the corresponding eigenvalue increases, by choosing \( \lambda = +1 \) (\( \lambda = -1 \)) in (3.15) and counting the number of negative (positive) values of \( x_j \), we determine the number of solitons travelling to the left (right).

In order to thermalize the system, we assume that initially the masses are at their equilibrium positions, \( y_j(t=0) = 0 \), and that their initial velocity, \( v_j(t=0) = \dot{y}_j(t=0) \), is chosen from a Gaussian random distribution with variance determined by the condition

\[ \frac{1}{2} \sum_j \langle v_j^2 \rangle = k_B T. \]  

(3.16)

Here \( k_B \) is the Boltzmann constant and \( T \) is absolute temperature.

Fig. 3.1 - Logarithm to base 10 of the ratio \( N_s/N \) versus the logarithm to base 10 of the temperature measured in K, calculated for DNA parameters (Eqs. (3.3), (3.5), and (3.6)). The bullet (•) indicates a temperature of 310 K, where \( N_s/N = 0.31 \). Number of base pairs \( N = 45000 \).

With these initial conditions and the technique described above we have calculated the number of solitons \( N_s \) as a function of temperature \( T \) and the number of masses \( N \). A typical result is shown in Fig. 3.1, where \( \log(N_s/N) \) is plotted versus \( \log(T) \) for \( N = 45000 \). This result does not change as \( N \) is reduced or increased /5/. The point indicated by the bullet corresponds to physiological temperature (310 K) where the ratio is

\[ \frac{N_s}{N} = 0.31. \]  

(3.17)

Therefore, we find that at any temperature the number of thermally generated solitons \( N_s \) will be proportional to the number of base pairs \( N \). Moreover, at 310 K, the number of ther-
nally generated solitons can be calculated by multiplying the number of base pairs by the factor 0.31.

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