Solitons in DNA and neutron scattering. Possibilities and perspectives.

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Abstract

Recent achievements of scientists in obtaining samples of oriented fibers of DNA makes it possible to investigate nonlinear dynamical properties of DNA by the method of neutron scattering [1]. Preliminary calculations of the dynamical factor of inelastic scattering by DNA were presented in this paper. Calculations were made on the basis of nonlinear mathematical model of DNA proposed in [2], and approximate model of statistics of assemble of DNA solitons proposed in [3].

Introduction

Thermal (or slow) neutrons with de Broglie wavelengths between 2 and 20 Å are a versatile probe of the dynamics of DNA [4]. The direction of propagation of the scattered neutron with respect to the incident neutron is defined by the polar angle θ and azimuthal angle Φ . If the flux of incident neutrons, defined as the number of per unit area per unit time, is N, then the number scattered per unit time into the element of solid angle $\Omega = \sin\theta \, d\theta \, d\Phi$ is

$$N(d\sigma/d\Omega) \, d\Omega \quad ; \tag{1}$$

where $(d\sigma/d\Omega)$ is the differential cross-section.

The basic conservation equations governing the interaction between a quantum of incident radiation and a scattering center are given by

$$\hbar\mathbf{x} = \hbar(\mathbf{k}' - \mathbf{k}''); \quad \text{(momentum)} \tag{2}$$

$$\hbar w = E' - E''; \quad \text{(energy)} \tag{3}$$

where $\hbar\mathbf{x}$ and $\hbar w$ are the momentum and energy transfers, respectively ($\hbar$= Planck's constant/2π). The initial and final wavevectors and energies are denoted by $\mathbf{k}'$, $\mathbf{k}''$ and E', E''.

Some fraction of radiation is usually scattered elastically. It is the so-called elastic scattering which is characterized by the relation $k' = k''$ ($k' = |\mathbf{k}'|$, $k'' = |\mathbf{k}''|$) and produces $\mathbf{x}$-dependent diffraction patterns related by Fourier transformation to the real-space structure. The other fraction of the radiation, however, will be scattered inelastically, i.e. it will exchange energy with thermal vibrations and other excitations in the sample. Thus just this inelastic scattering is of most interest because it carries information about internal motions in the system investigated.

With the exception of spin-echo instruments, all neutron spectrometers provide data in the form of a double differential cross-section, $\partial^2\sigma/d\Omega \, dE'$. For the simplest case of a monoatomic assembly of target nuclei this is given by

$$\partial^2\sigma/\partial\Omega\,\partial E' \sim N(k''/k')[\sigma_{inc} S_{inc}(\boldsymbol{x},w) + \sigma_{coh} S_{coh}(\boldsymbol{x},w)]; \quad (4)$$

where σ_{inc} and σ_{coh} are incoherent and coherent scattering cross-sections, respectively; and $S_{coh}(\boldsymbol{x},w)$, $S_{incoh}(\boldsymbol{x},w)$ are the dynamical factors of coherent and incoherent scattering. In the case of DNA, the role of target nuclei will play the DNA bases.

In the thermal neutron experiment oriented DNA fibers are usually used [5]. Methodically, this probe offers the advantage of a dominant incoherent cross section for hydrogens and the simultaneous exploration of a wide range of frequency (w) and momentum ($\boldsymbol{x}$) space [1].

A major problem is the availability of large enough oriented samples of DNA in order to exploit the discrimination of atomic displacements by means of the projection on $\boldsymbol{x}$. Existing thermal neutron sources require about 1 cm^3 DNA in order to reach the level of statistical significance for signals due to collective excitations within the practical limits of days measuring time. This problem has been partly overcome by the development and perfection of the wet-spinning method [6]. This method allows the controlled production highly oriented (within a few degrees) thin films (1 to 100 μm) by winding up DNA fibers which are continuously stretched during precipitation into an aqueous alcohol solution. Films up to 45×275 mm^2 have been obtained in this way.

Just this result stimulated us to continue our calculations of the dynamical factor of neutron scattering by DNA solitons. The first preliminary calculations were made by us several years ago [3] and we stopped the studies because there was not a possibility for experimenters to organize neutron scattering experiment and to check the results of calculations. Recent achievements in obtaining samples of oriented fibers gave us a new hope and stimulated to continue the calculations by using a more accurate model of DNA nonlinear dynamics.

Model

Let us model DNA by two parallel chains of pendula interacting with each other by longitudinal and transverse springs (*Fig. 1*).Here pendula imitates DNA bases, two chains of longitudinal springs imitate sugar-phosphate chains and transverse springs imitate hydrogen bonds between bases. This model can be considered as a modification of the well known

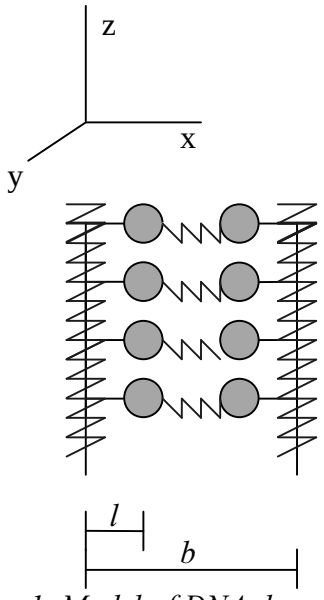

Fig. 1. Model of DNA dynamics.

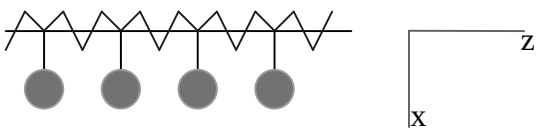

Fig. 2. Chain of pendula.

mechanical model proposed by Scott [7] and applied to DNA by Englander and co-authors [8] (*Fig. 2*).The model consists of one horizontal chain of pendula placed in the gravitational field of the Earth, each pendulum being able rotate in the *xy* plane. To receive the modified model it is enough to "remove" gravitational field and to add one more chain of pendula interacting weakly with the pendula of the first chain by transverse springs. The model shown in *Fig. 1* looks like a one dimensional lattice with two pendula per unit cell. So, to describe the model system, we can introduce the basic vector **a** = {0; 0; a}, and the lattice vector $\boldsymbol{R}^0_n$ defined as $\boldsymbol{R}^0_n = n\boldsymbol{a}$, where *a* is the distance between the neighboring pendula and *n* is the integer (*n* = 1, 2, ... *N*).

The equilibrium positions of the masses of pendula within a unit cell can be denoted by vectors $\boldsymbol{d}_1 = \{l; 0; 0\}$ and $\boldsymbol{d}_2 = \{b-l; 0; 0\}$, where *b* is the distance between the chains and *l* is
the length of pendula. Then the position vector $\boldsymbol{R}^0_{n,j}$ of the *j*-th pendulum mass (*j* = 1,2) in the *n*-th cell is given by

$$\boldsymbol{R}^0_{n,\,j} = \boldsymbol{R}^0_{\,n} + \boldsymbol{d}_j. \tag{5}$$

Taking into account that every pendulum rotates only in the *xy* plane, we can write possible displacements of masses as

$$\begin{aligned} \boldsymbol{u}_{n,1} &= \boldsymbol{R}_{n,1}(t) - \boldsymbol{R}^0_{n,1} = \{-l(1-\cos\varphi_{n,1});\ l\sin\varphi_{n,1};\ 0\};\\ \boldsymbol{u}_{n,2} &= \boldsymbol{R}_{n,2}(t) - \boldsymbol{R}^0_{n,2} = \{\ l(1-\cos\varphi_{n,2});\ l\sin\varphi_{n,2};\ 0\}; \end{aligned} \tag{6}$$

where $\varphi_{n,j}$ is the angular displacement of the *n*-th pendulum of the *j*-th chain.

The model hamiltonian will have then the form

$$H = \sum_n \{M\dot{\boldsymbol{u}}^2_{n,1}/2 + M\dot{\boldsymbol{u}}^2_{n,2}/2\} + \sum_n \{K|\boldsymbol{u}_{n,1} - \boldsymbol{u}_{n-1,1}|^2/2 + K|\boldsymbol{u}_{n,2} - \boldsymbol{u}_{n-1,2}|^2/2 + k|\boldsymbol{u}_{n,1} - \boldsymbol{u}_{n,2}|^2/2\}; \tag{7}$$

where K and k are the rigidities of longitudinal and transverse springs, correspondingly. If we insert now (6) into (7) and use linear approximation according to φ in the terms describing interactions along the chains (rigid springs) and nonlinear approximation in the terms describing interactions between chains (soft springs), the final model hamiltonian will have then the form

$$\begin{aligned} H = &\sum_n \{M\dot{\varphi}^2_{n,1}/2 + M\dot{\varphi}^2_{n,2}/2\} + \sum_n \sum_j Ka^2\{|\varphi_{n,j} - \varphi_{n-1,j}|^2\}/2 +\\ &+ \sum_n ka^2\{2(1-\cos\varphi_{n,1}) + 2(1-\cos\varphi_{n,2}) - [1-\cos(\varphi_{n,1} + \varphi_{n,2})]\}. \end{aligned} \tag{8}$$

Corresponding dynamical equations take the form

$$I\ddot{\varphi}_{n,1} = Kl^2(\varphi_{n+1,1} - 2\varphi_{n,1} + \varphi_{n-1,1}) - kl^2[2\sin\varphi_{n,1} - \sin(\varphi_{n,1} + \varphi_{n,2})];$$

(9)

$$I\ddot{\varphi}_{n,2} = Kl^2(\varphi_{n+1,2} - 2\varphi_{n,2} + \varphi_{n-1,2}) - kl^2[2\sin\varphi_{n,2} - \sin(\varphi_{n,2} + \varphi_{n,1})].$$

In the continuum limit when

$$a \to 0;\ N \to \infty;\ na \to z;\ \varphi_{n,j}(t) \to \varphi_j(z,t);\ \Sigma \to \int dz.$$

equations (9) can be rewritten in the form

$$I\ddot{\varphi}_{1t} = Kl^2a^2\varphi_{1zz} - kl^2[2\sin\varphi_1 - \sin(\varphi_1 + \varphi_2)];$$
$$I\ddot{\varphi}_{2t} = Kl^2a^2\varphi_{2zz} - kl^2[2\sin\varphi_2 - \sin(\varphi_2 + \varphi_1)]. \qquad (10)$$

It is convenient to rewrite equations (10) in the form

$$\ddot{\varphi}_{1t} - C_0^2\varphi_{1zz} + w_0^2\{2\sin\varphi_1 - \sin(\varphi_1 + \varphi_2)\} = 0;$$
$$\ddot{\varphi}_{2t} - C_0^2\varphi_{2zz} + w_0^2\{2\sin\varphi_2 - \sin(\varphi_2 + \varphi_1)\} = 0; \qquad (11)$$

where $C_0 = Kl^2a^2/I;\ w_0^2 = kl^2/I.$

One of the most interesting solutions of equations (11) has the form [9]

$$\varphi_1(z,t) = -\varphi_2(z,t) = 4\arctan\{\exp[\gamma(z-vt)/d]\}; \qquad (12)$$

shown schematically in *Fig.* 3. It has a simple interpretation of a local conformational deformation of size $d = C_0/(2^{1/2} w_0)$ moving along the DNA molecule with velocity v. Here $\gamma = (1-v^2/C_0^2)^{-1/2}$. In *Fig.* 4 a qualitative picture corresponding to the solution (12) is shown. Sugar-phosphate chains of DNA are shown here as long lines and the bases are shown with the help of short transverse rods.

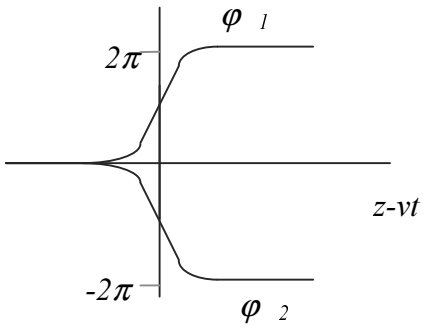

Fig. 3. Two coupled kinks.

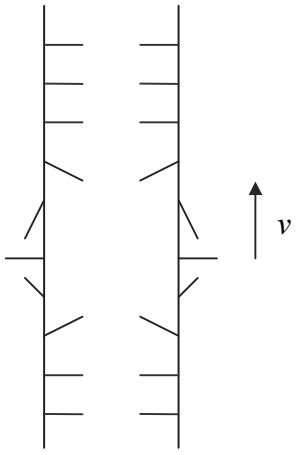

Fig. 4. Moving local deformation.

Dynamical factor of inelastic coherent scattering

Now let us apply the results described above to calculate the dynamical factor of inelastic coherent scattering.

According to the general theory of neutron scattering [10], let us assume that interaction of the incident neutron having mass m and coordinate $\boldsymbol{r}$ with a pendulum having mass M and coordinate $\boldsymbol{R}_{n,j}(t)$ can be described by Fermi pseudo-potential

$$V_{n,j} = (2\pi \hbar^2 B_{nj}/m)\delta (\boldsymbol{r} - \boldsymbol{R}^0_{n,j}); \qquad (13)$$

where $B_{n,j}$ is the scattering length. Then the interaction of the incident neutron with a rigid array of $2N$ pandula is described by the potential

$$V = (2\pi \hbar /m)\sum_n \sum_j B_{n,j}\delta (\boldsymbol{r} - \boldsymbol{R}^0_{n,j}(t)). \qquad (14)$$

and the master formula for differential cross section will have then the form similar to (4)

$$\partial^2\sigma /\partial \Omega \partial E' = 2N(\bar{k}''/\bar{k}')\{(\bar{B}^2 - B^2) S_{inc}(\boldsymbol{x},w) + B^2 S_{coh}(\boldsymbol{x},w);. \qquad (15)$$

where

$$S_{coh}(\boldsymbol{x},w) = (4\pi \hbar N)^{-1}\int dt\, exp(-iwt)\sum_n \sum_{n'} \sum_j \sum_{j'} <exp(-i\boldsymbol{x}\boldsymbol{R}_{n,j}(0)), exp(i\boldsymbol{x}\boldsymbol{R}_{n',j'}(t))>; \qquad (16)$$

$$S_{inc}(\boldsymbol{x},w) = (4\pi \hbar N)^{-1}\int dt\, exp(-iwt)\sum_n \sum_j <exp(-i\boldsymbol{x}\boldsymbol{R}_{n,j}(0)), exp(i\boldsymbol{x}\boldsymbol{R}_{n,j}(t))>; \qquad (17)$$

and <...> is the averaging over states of assemble of pendula.

The term describing the contribution of coherent inelastic scattering is of most interest. And the formula for corresponding dynamical factor can be simplified and take the form

$$S_{coh.,inel.}(\boldsymbol{x},w) = [exp(-2W_x)/(4\pi \hbar N)]\sum_n \sum_{n'} \sum_j \sum_{j'} exp[-i\boldsymbol{x}(\boldsymbol{R}^0_{n,j} - \boldsymbol{R}^0_{n',j'})]$$

$$\int dt\, exp(-iwt) <exp(-i\boldsymbol{x}\boldsymbol{u}_{n,j}(0)), exp(i\boldsymbol{x}\boldsymbol{u}_{n',j'}(t))>; \qquad (18)$$

where vectors $\boldsymbol{u}_{n,j}$ (n = 1,2) are determined by formulas (6).

Algorithm of further calculations is the following:

1. Insert (6) and (12) into (18).
2. Pass to the continuum approximation

$a \to 0;\ N \to \infty\ ;\ na \to z;\ \varphi_{n,j}(t) \to \varphi_j(z,t);\ \sum \to \int dz.$

3. Apply approximation of the ideal gas as it was done in [3]

$$<...> \rightarrow N<...>_1; \quad (19)$$

where $<...>_1$ is the averaging over the states of a pendulum, and $\bar{N}$ is the average number of local conformational deformations in the model system.

The result of the calculations is

$$S_{coh.,inel.}(\boldsymbol{x},w) = \{[4l^2\gamma_0 d \exp(-2W_x)\,(E_0/2\pi k_BT)^{1/2}]/[\hbar C_0 a x_z K_1(E_0/k_BT)]\}$$

$$\exp(-E_0/k_BT)\exp(-E_0\gamma/k_BT)\{X^2(1+\cos x_y h) - 2XY\sin x_y h +$$

$$+ Y^2(1-\cos x_y h)\}; \quad (20)$$

where $X = x_x(\pi dx_z/\gamma_0)/sh(\pi dx_z/2\gamma_0)$; $Y = x_y(\pi dx_z/\gamma_0)/ch(\pi dx_z/2\gamma_0)$; $\gamma_0 = (1-v_0^2/C_0^2)^{-1/2}$; $v_0 = w/x_z$; $\boldsymbol{x} = \{x_x; x_y; x_z\}$; $E_0 = 8al^2(2Kk)^{1/2}$; $K_1(x)$ is the Macdonald function; $h = b-2l$.

So, the result obtained shows that in the spectrum of scattering we can expect an existence of a central peak with characteristics depending on the wave vector $\boldsymbol{x}$ and on temperature T according to formula (20).

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