A Model for
Double-Stranded Excitations of DNA

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ABSTRACT

We calculate the spectrum of torsional vibrations of a double-stranded structure that models the double helix of the DNA. We come to the conclusion that within the framework of the model elementary excitations may display an asymmetry as regards their winding and direction of the propagation, depending on initial polarization. The asymmetry could have a bearing on processes that take place in molecules of the DNA.
Conformational excitations of the DNA molecule are important for understanding transformations of DNA, for example during transcription, and therefore there is an urgent need for their investigation. But, on the other hand, the latter is a difficult problem, even on the assumption that the excitations are weak enough to preserve the hydrogen bonds between base-pairs, so that the double-stranded structure is deformed but not disrupted. As to our knowledge, it was Cappelmann and Beim, [1], who were the first to attempt such a study. They gave a model of DNA that accommodates a number of modes of elastic vibrations with sophisticated spectrum, and the analysis of their bearing on the actual properties of DNA needs further studying. As usual in such cases, the most important thing is the wise choice of an initial model, which determines the final outcome; taking into account the qualitative nature of the approach, one should employ the minimal number of assumptions so as to obtain simple characteristics of the dynamics of a molecule. In our work we aim at studying elastic modes of vibrations of the double-stranded structure, which are similar to the phonon modes of crystalline lattices. We show that the asymmetry of the double helix, due to its having an orientation of the right or the left screw, may result in the propagation of pairs of waves travelling in opposite directions and producing twists of different signs in the double-stranded structure.

According to the results of [2], [3], the number of open base pairs at room temperature is very small, so that the system of H-bonds may be considered intact, within a good approximation. On the other hand the H-bonds are more fragile than the sugar-phosphate frame, and therefore it appears to be a reasonable proposition to consider excitations for either of them separately. Thus, at least for sufficiently small excitational energies, we may assume the conformation of the sugar-phosphate frame being static, while the H-bonds subject to small deformations. Hence, the minimal list of basic properties of the DNA molecule under the circumstances may be drawn as follows:

- a molecule of DNA is an elastic system at the spatial scale of the order $500 \AA$, or less;
- the discrete nature of the system is to be taken into account at the intra base-pair distances, that is $3.4 \AA$;
- the conformation of the double-stranded structure of DNA may be described, qualitatively, by the vector field $\mathbf{Y}$ defined at points of the central line of a molecule, with $\mathbf{Y} = 0$ corresponding to the unperturbed state, (cf. [4]);
- the double helix of the two strands means that the system has a twisted ground state characterized by the twist vector $\mathbf{\Omega}$.
Consequently, the dynamics of the double helix is to be determined by the twist, and therefore the vector $\vec{\Omega}$.

In accord with the requirements formulated above we may cast the energy of a molecule in the form

$$E = \sum_{i=1}^{N} \frac{1}{2M} (\partial_t \vec{P}_i)^2 + \sum_{i=1}^{N} \frac{K}{2} (\nabla \vec{Y}_i)^2 + \sum_{i=1}^{N} \frac{L}{2} \vec{Y}_i^2$$

where $\vec{Y}_i$ is the value of $\vec{Y}$ at the site corresponding to the i-th base-pair, and the covariant derivative $\nabla \vec{Y}_i$ is given by the equation

$$\nabla \vec{Y}_i = \frac{1}{a} (\vec{Y}_{i+1} - \vec{Y}_i) + \frac{1}{a} \hat{\Omega}_i \vec{Y}_i$$

in which $a$ is the distance between adjacent base-pairs and the matrix $\hat{\Omega}_i$ is determined by the formula

$$\hat{\Omega}_i = \hat{R}_i^{-1} (\hat{R}_{i+1} - \hat{R}_i)$$

Here the matrix $\hat{R}_i$ is the matrix of a rotation that transforms the local coordinates at the site $i$ towards the laboratory one. It is important that the matrix $\hat{\Omega}_i$ corresponds to the twist of the double strands of the helix, and one can describe it by the vector $\vec{\Omega}$, mentioned above. One can derive the dynamical equations for the field $\vec{Y}$ from the energy given above as usual. The set of values for the matrix $\hat{\Omega}_i$ is supposed to be fixed by the equilibrium ground state of the double helix. It is worth noting that, to a certain extent, the distribution of base-pairs of different shapes can be mimicked by the choice of $\hat{\Omega}_i$.

Assuming that the matrices $\hat{\Omega}_i$ do not depend on the site $i$, which means that some spatial homogeneity could be accepted, we are looking for eigenmodes that can be cast in the form

$$\vec{Y}_n = e^{-ina} Y_q$$

and obtain the modes having the spectrum
\[ \omega^2_{1,2} = v^2 \left[ 4A^2 \sin^2 \left( \frac{aq}{2} \right) \pm 2 \sin \phi \sin(aq) + 4 \sin^2 \phi + \Delta^2 \right] \]

\[ \omega^2_3 = 4v^2 \sin^2 \left( \frac{aq}{2} \right) \]

\[ v = \sqrt{\frac{K}{Ma^2}} \]

in which \( A^2 \) is given by the equation

\[ A^2 = 1 + 2 \sin^2 \left( \frac{\phi}{2} \right) \]

the angle \( \phi \) is that of the rotation matrix \( \hat{\Omega} \). The spectrum is illustrated in Fig.1. It is worth noting that a similar form of the spectrum is obtained for the linearized expression for matrices \( \hat{\Omega}_i \), that is the rotations

\[ \hat{R}_i^{-1} \cdot \hat{R}_{i+1} \]

being considered infinitesimal (see [5]). The agreement between the two approaches is in accord with the qualitative nature of the model we consider.

One can infer an important conclusion from the shape of the spectrum.

Let us consider the first mode \( \omega_1 \) which corresponds to the minus sign in the equation given above. The frequency \( \omega_1 \) has a pronounced minima at \( q_* \), so that there are two sets of waves travelling in opposite directions of the molecule. It should be noted that the double helix has an orientation, the left or the right one, due to its screw structure. Thus, we may talk about the sign of the propagation of a wave. The value of \( \omega_1 \) at \( q_* \) is not zero, and it results in a winding motion of the vector \( \vec{Y} \) with an orientation determined by the sign of the propagation, so that for a pair of waves belonging to the eigenmode \( \omega_1 \) the windings must be of different orientation. We see that the effect depend on the polarization of a wave, in fact we have considered an eigenmode. In case we have a mixture of them, the asymmetry of the winding can be blurred or totally destroyed.

One may cast these arguments in a more quantitative form. Let us consider the first mode; its spectrum can be roughly approximated by the expression

\[ \omega = c|q - q_0| + \omega_0 \]
or

\[
\omega = \begin{cases} 
  cq - \omega_1 & \text{if } q > q_0 \\
  -cq + \omega_2 & \text{otherwise}
\end{cases}
\]

(see Fig.2), in which the frequencies \(\omega_1, \omega_2\) read

\[
\omega_1 = \omega_0 - cq_0, \quad \omega_2 = \omega_0 + cq_0
\]

It is important that for the numerical values involved, that is corresponding to the DNA data, the frequencies \(\omega_1, \omega_2\) are positive, as is seen in Fig.2.

If we are looking for a solution with the help of the Fourier transform, we may write its expression in the form of the decomposition

\[
u(x, t) = \int_{-\infty}^{\infty} dq \, u_q(t)
\]

in which \(u_q(t)\) reads

\[
u_q(t) = u_q^0 \, e^{i(\omega t - qx)}
\]

and \(\omega\) depends on \(q\). It is easy to convince oneself that the solution can be cast in the form

\[
u(x, t) = \int_{-\infty}^{q_0} dq \, [u_q^0 \, e^{-i((t+x)q)}] \, e^{i\omega_2 t} + \int_{q_0}^{\infty} dq \, [u_q^0 \, e^{-i((t-x)q)}] \, e^{-i\omega_1 t}
\]

or, otherwise

\[
u(x, t) = u_+(t + x) \, e^{\omega_2 t} + u_-(t - x) \, e^{-\omega_1 t}
\]

The latter describes the two waves travelling in opposite directions and having different windings.

We made a numerical simulation of the dynamics of our model. The asymmetry is seen in that two waves travelling from an initial disturbance in opposite direction may oscillate having equal phases of different sign. As is expected, the effect of the asymmetry depends on an initial polarization, which corresponds to a superposition of the eigenmodes indicated above, so that for a certain direction it can be totally suppressed, whereas for those belonging to the eigenmodes it is pronounced.

On considering the estimates for the values of the density per unit of length, approximately \(10^{-14} \text{gr/cm}\), and according to the papers [3], [7], the elastic constant, \(\sim 10^{-6} \text{erg/cm}\), me may suggest, therefore, that the velocity of the waves considered above is of the order \(10^3 \text{cm/sec}\). Consequently, the frequencies of the modes, even for the region of wavenumbers corresponding to the dips of the spectrum seen in Fig.1, are those of hypersonic, that is \(10^{11}\) or \(10^{12}\) or even
more, depending on the values of the elastic constant. The values are by many orders of magnitude above those involved in biological process. Their relation to the latter presents a very interesting problem. In fact, we shall investigate the influence of super-high frequency dynamics on the very low frequency one. It should be noted that so far no electronic properties have been taken into account in conjunction with the elastic ones, and in this respect the approach of elasticity theory, generally employed now, might be incomplete. Studying the elastic excitattions in the DNA could be a means for finding the answer.

Another important question is the influence of ambient media that should result in a very strong dissipation of excitations. Whether they will be overdamped, and to all practical purposes unobservable, as appears to be the case in a similar situation in proteins, remains to be seen. A strong argument in favour of their playing an important part in the dynamics of the DNA, is the rigidity of the latter displayed by its large persistence length.

At any rate, the investigation of elementary excitations should be a necessary prerequisite for investigating conformational changes due to the action of external agents, e.g. enzymes. The salient feature is that in these circumstances a preferential direction of the promoter’s action is often observed, as well as a torsional dynamics of the double helix. Thus, the anisotropy of the propagation of a disturbance due to the screw orientation of the double helix for which we make out a case in this paper, appears to be very interesting and worth further studying.

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Figure 1: Normal modes of the spectrum
Figure 2: Linear approximation