The Inter-Strand Modes of the DNA as a Probe into

MW-Radiation

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Abstract

We consider the regime in which the bands of the torsional acoustic (TA) and the hydrogen-bond-stretch (HBS) modes of the DNA interpenetrate each other. Within the framework of a model that accommodates the structure of the double helix, we find the three-wave interaction between the TA- and the HBS-modes, and show that microwave radiation could bring about torsional vibrations that could serve as a pump mode for maintaining the HBS-one. Rayleigh’s threshold condition for the parametric resonance provides an estimate for the power density of the mw-field necessary for generating the HBS-mode.

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I. INTRODUCTION

It is generally accepted that the conformational dynamics of the DNA relies essentially on elastic vibrations of the DNA molecule in the region of $10^9 \pm 10^{12}$ Hz, [1]. According to Kim and Prohofsky, [2], [3], the latter includes the two domains, which correspond with different degrees of freedom of the molecule: (1) acoustic modes, which do not involve the hydrogen bonds; (2) modes that stretch the hydrogen bonds between the base-pairs (the HBS modes). Local minimum of the frequency is characteristic for the HBS-modes, [2], [3]; its position depending on the choice of the band. The vibrations of the DNA were observed in the low-frequency Raman scattering, [4], [5], and the Fourier-transform infra-red absorption experiments, [6], to a large extent depending on the state and composition of solvent. But, the experimental data, [1], is not conclusive as to the relative positions of the TA- and HBS-modes. If the acoustic torsional bands interpenetrate the HBS-modes, the torsional vibrations of the double helix could change periodically the elastic constants of inter-strand motions, and thus provide a supply of energy for the HBS-modes. Then a torsional acoustic band, which has the double frequency with respect to that of the HBS-mode, could provide a means for maintaining an HBS-mode through the parametric resonance.

II. THE ELASTIC DYNAMICS OF TORSIONAL AND INTER-STRAND MODES

While considering the dynamics of the DNA one has to take into account: (1) the DNA having the two strands; (2) the base-pairs being linked by the hydrogen bonds; (3) the helical symmetry. We shall utilize a one-dimensional lattice model for the elastic properties of the DNA which accommodates these requirements.

El Hasan and Calladine, [7], set up the scheme for the internal geometry of the double helix of the DNA, which describes the relative position of one base with respect to the other in a Watson-Crick base-pair and also the positions of the two base-pairs. This is achieved by introducing local frames, or triads, for the bases and the base-pairs, and translation-slides along their long axes. We follow the guidelines of paper [7], but aiming at a qualitative description of the DNA dynamics use a simplified set of variables. We shall describe the relative position of the bases of a base-pair by means of the vector $\vec{Y}$ directed along the long axis ( $y$– axis of paper [7], see also paper [8]); $\vec{Y}$ being equal to zero when the base-pair is
at equilibrium. Thus, \( \vec{Y} \) describes the base-base stretch corresponding to the displacement of the two-bases that make up the base-pair away from each other along the long axis \( y \).

The relative position of the base-pairs are described by the torsional angles \( \phi_n \), which give deviations from the standard equilibrium twist of the double helix. Thus a twist of the DNA molecule, which does not involve inter-strand motion or mutual displacements of the bases inside the pairs, is determined by the torsional angles \( \phi_n \) that are the angles of rotation of the base-pairs about the axis of the double-helix. The twist energy of the molecule is given by the equation

\[
\mathcal{H}_\phi = \sum_n \left[ \frac{I}{2} \phi_n^2 + \frac{\tau}{2a^2} (\phi_{n+1} - \phi_n)^2 \right]
\]

in which \( I \) is the moment of inertia, and \( \tau \) and \( \kappa \) are the twist coefficients, which for the sake of simplicity and taking into account the qualitative picture at which we aim, are assumed the same for all the base-pairs.

Interstrand motions should correspond to the relative motion of the bases inside the base-pairs, therefore the kinetic energy due to this degree of freedom may be cast in the form

\[
\sum_n \frac{M}{2} \dot{\vec{Y}}_n^2
\]

where \( M \) is the effective mass of a couple. For each base-pair we have the reference frame in which (1) \( z \)-axis corresponds to the axis of the double helix, (2) \( y \)-axis to the long axis of the base-pair, (3) \( x \)-axis perpendicular to \( z \)- and \( y \)- axes (see Fig. 1 of paper [7]). At equilibrium the change in position of adjacent base-pairs is determined only by the twist angle \( \Omega \) of the double helix. We shall assume \( \Omega = 2\pi/10 \) as for the B-form of DNA. To determine the energy due to the inter-strand displacements we need to find the strain taking into account the constraint imposed by the helical structure of our system. For this end one may utilize the covariant derivative, as is done in paper [11], but a simpler approach is possible.

Let us confine ourself only to the torsional degrees of freedom of the double lattice and assume the vectors \( \vec{Y}_n \) being parallel to x-y plane, or two-dimensional. Consider the displacements \( \vec{Y}_n, \vec{Y}_{n+1} \) for the two consecutive base-pairs, \( n, n+1 \). Since we must compare the two vectors in the same frame, we shall rotate the vector \( \vec{Y}_{n+1} \) to the frame of the n-th base pair,

\[
\vec{Y}_{n+1}^{\text{back}} = R^{-1}(\phi) \vec{Y}_{n+1}
\]

Here \( R^{-1}(\phi) \) is the inverse matrix of the rotation of the n-th frame to the \( (n+1) \)-one given
by the equation

$$R(\phi) = \begin{bmatrix} \cos \phi - \sin \phi \\ \sin \phi & \cos \phi \end{bmatrix}$$  \hspace{1cm} (1)$$

The matrix $R$ is 2 by 2 since the vectors $\vec{Y}_n$ are effectively two-dimensional. Then the strain caused by the displacements of the base-pairs is determined by the difference

$$\vec{Y}_{n+1}^{\text{back}} - \vec{Y}_n$$

For this argument I am indebted to D.I.Tchertov.

It is important that the angle $\phi$ is given by the twist angle, $\Omega$, describing the double helix, in conjunction with the torsional angles $\phi_n$, so that

$$\phi = \Omega + \phi_{n+1} - \phi_n$$

Therefore, the energy $\mathcal{H}_Y$ due to the base-base stretch, or the *inter-strand* stress, reads

$$\mathcal{H}_Y = \sum_n \left\{ \frac{M}{2} \dot{\vec{Y}}_n^2 + \frac{K}{2a^2} \left[ R^{-1}(\Omega + \phi_{n+1} - \phi_n) \vec{Y}_{n+1}^{\text{back}} - \vec{Y}_n \right]^2 + \frac{\epsilon}{2} \vec{Y}_n^2 \right\}$$

in which $K$ and $a$ are the torsional elastic constant and the inter-pairs distance, correspondingly. In summations given above $n$ is the number of a site corresponding to the $n$-th base-pair, and $n = 1, 2, \ldots, N$, $N$ being the number of pairs in the segment of the DNA under consideration. The constant $K$ is assumed to be the same for all the base-pairs. In fact, it differs from the situation in real life, but we are aiming at a rough qualitative picture. Besides it is possible to manufacture artificial double helices of the form $(\text{poly}X). (\text{poly}Y)$, in which the elastic constants shall not depend on the choice of the base-pair. The last term, $\epsilon/2 \vec{Y}_n^2$ accommodates the energy of the inter-strand separation due to the slides of the bases inside the base-pairs. The form of $\mathcal{H}_Y$ corresponds with the fact that the equilibrium position of the double helix is the twisted one determined by $\Omega$, all $\phi_n$ being equal to zero. We suppose that the size of DNA molecule is small enough that it can be visualized as a straight double helix, that is not larger than the persistence length. Hence the number of base-pairs, $N \leq 150$, approximately. The total energy $\mathcal{H}_{\text{elastic}}$ of the DNA molecule reads

$$\mathcal{H}_{\text{elastic}} = \mathcal{H}_\phi + \mathcal{H}_Y$$ \hspace{1cm} (2)$$

Preserving only terms up to the third order in $\phi_n$, and $\vec{Y}_n$, we may transform $\mathcal{H}_{\text{elastic}}$ given by Eq.(2), so that it takes on the form

$$\mathcal{H}_{\text{elastic}} = \sum_n \left\{ \frac{I}{2} \dot{\phi}_n^2 + \frac{\tau}{2a^2} (\phi_{n+1} - \phi_n)^2 \right\}$$
\[
+ \sum_n \left\{ \frac{M}{2} \ddot{Y}_n^2 + \frac{K}{2a^2} \left[ R^{-1}(\Omega) \dot{Y}_{n+1} - \dot{Y}_n \right]^2 + \frac{\epsilon}{2} \dot{Y}_n^2 \right\} \\
+ \frac{K}{a^2} \sum_n (\phi_{n+1} - \phi_n) \left[ R^{-1}(\Omega) \dot{Y}_{n+1} \times \dot{Y}_n \right]^3
\]

We have used the fact that the axis of the double-helix is directed along Oz-axis.

Let us simplify the equation for \( H_{\text{elastic}} \) with the help of the unitary transformation

\[
Y_n^1 = \frac{1}{\sqrt{2}} (u_n^1 + iu_n^2), \quad Y_n^2 = \frac{1}{\sqrt{2}} (iu_n^1 + u_n^2)
\]

Note that the vectors \( \tilde{Y}_n \) and \( \tilde{u}_n \) are effectively two-dimensional, their third coordinates being equal to zero. On applying the Fourier transform

\[
f_n = \frac{1}{\sqrt{N}} \sum_q e^{-iaq} f_q
\]

where \( q = \frac{2\pi}{N a} m, \quad m = 0, \pm 1, \ldots, \pm \frac{N}{2} \) we cast the equation for the energy \( H_{\text{elastic}} \) in the form

\[
H_{\text{elastic}} = \sum_q \left[ \frac{I}{2} \dot{\phi}_q \dot{\phi}_q^* + \frac{\tau}{2a^2} \sin^2 \frac{aq}{2} \phi_q \dot{\phi}_q^* \right] \\
+ \sum_q \left[ \frac{M}{2} \ddot{u}_q \cdot \ddot{u}_q^* + \frac{\epsilon}{2} \dot{u}_q \cdot \dot{u}_q^* + \frac{2K}{a^2} \left( \sin^2 \frac{\Omega - aq}{2} u_q^1 \dot{u}_q^1 \dot{u}_q^1 + \sin^2 \frac{\Omega + aq}{2} u_q^2 \dot{u}_q^2 \dot{u}_q^2 \right) \right] \\
+ \frac{K}{a^2} \sum_{q'q''} i e^{-iaq} \dot{\phi}_{q'} \left[ -e^{i\Omega} u_{q'}^1 \dot{u}_{q'+q''}^1 + e^{-i\Omega} u_{q'}^2 \dot{u}_{q'+q''}^2 \right]
\]

It is important that after the Fourier transform the variables \( \tilde{u}_n \) verify the following equations for their complex conjugates

\[
\dot{u}_q^1 = i u_{-q}^2, \quad \dot{u}_q^2 = i u_{-q}^1
\]

The interaction term in the last equation corresponds to the three-wave process, and may result in resonance. We shall utilize the fact for deriving the parametric maintenance of the \( u_q \) modes, i.e. the HBS modes, (see below).

One can obtain, in the usual way, the equations of motion for \( u_q^\alpha, \alpha = 1, 2 \) and \( \phi_q \), from the equation for the energy indicated above. The essential point is the effects of dissipation, which are due to ions in the close neighborhood of the molecule and water effects, see \[12\]. The dissipation can be accommodated by writing down terms linear in \( \dot{u}_q^\alpha, \dot{\phi}_q \). We shall take into account external force, or torque \( T_q \), only in the equation for \( \phi_q \), for it corresponds to
external degrees of freedom of our model. Thus, the equations of motion can be cast in the form

\[ \ddot{u}_q^\alpha + \omega_{aq}^2 u_q^\alpha + \gamma_u \dot{u}_q^\alpha + 4K \sin \Omega \frac{1}{Ma^2 \sqrt{N}} \sum_{q'} e^{-i\alpha q'} \Phi_{q-q'}^{\alpha} u_{q-q'}^\alpha = 0, \]  

(6)

\[ \ddot{\phi}_q + \omega_q^2 \phi_q + \gamma_\phi \dot{\phi}_q + \frac{4K \sin \Omega e^{i\alpha q}}{Ia^2 \sqrt{N}} \sum_{q'} u_{q-q'}^1 u_{q-q'}^2 = T_q \]  

(7)

in which the dispersion laws for the fields \( u_{q,q}^\alpha, \alpha = 1, 2 \), and \( \phi_q \) are given by the equations

\[ \omega_{aq}^2 = \frac{4K}{Ma^2} \sin^2 \Omega + \frac{(-1)^\alpha aq}{2} + \frac{\epsilon}{M}, \]  

(8)

\[ \omega_q^2 = \frac{4\tau}{Ia^2} \sin^2 \frac{aq}{2} \]  

(9)

We see that the spectrum of \( \phi_q \) has a typical acoustic character, whereas that for \( u_{q,q}^\alpha \) has a local minimum determined by the helical twist, \( \Omega \). Thus, the spectrum of our model is in qualitative agreement with conclusions of [2], [3]. The nature of the torque is to be specified elsewhere (see Section III). For the moment, we shall consider general dynamical phenomena to which the torque may be conducive.

Let us suppose that for one thing the amplitudes of the HBS-modes given by \( u_{q,q}^\alpha \) be so small that the quadratic term in Eq.(7) can be neglected, and for another the external torque \( T_q \) be appreciable enough to maintain the vibration of the torsional mode \( \phi_q \). Thus, we can visualize the latter as a pump mode that interacts with the HBS-mode \( u_{q,q}^\alpha \) through the non-linearity in Eq.(6). Since we aim at studying the problem of mw-radiation (see next section), we shall confine ourself to the case of the torque \( T_q \) being non-zero only at \( q = q_* = \Omega/a \), and having the frequency \( 2\omega \). Therefore, the forced wave, or the pump wave for the HBS-mode, has the form

\[ \phi_{q_*} = e^{i2\omega t} \Phi \delta_{qq_*}, \quad \phi_{-q_*} = e^{-i2\omega t} \Phi^* \delta_{-qq_*} \]  

(10)

To obtain larger values for the pump wave, \( \phi_{q_*} \), the resonance condition

\[ \omega_{q_*} = 2\omega \]

should be verified. The equations of motion for \( u_{q,q}^\alpha \) in the pumping regime read
\[ u''_{q} + \omega_{a}^{2} u'_{q} + \gamma_{u} u_{q} + \frac{2K \sin \Omega}{M a^{2} \sqrt{N}} \left( A e^{i2\omega t} u_{q-q_{*}} + A^* e^{-i2\omega t} u_{q+q_{*}} \right) = 0 \]

Here
\[ A = e^{-i\Omega \Phi} \]

Note that the momentum conservation in the \( q \)-values is preserved, as required by the three-wave interaction. The equation indicated above can be cast in the matrix form
\[ \ddot{\bar{u}}_{\alpha} + \dot{\omega}_{\alpha}^{2} \bar{u}_{\alpha} + \gamma_{u} \dot{u}_{\alpha} = \left( e^{i2\omega t} \mathcal{K} + e^{-i2\omega t} \mathcal{K}^{+} \right) \bar{u}_{\alpha} \quad (11) \]

where \( \mathcal{K} \) and \( \mathcal{K}^{+} \) are hermitian conjugate, and
\[
\mathcal{K}^{+} \mathcal{K} = \mathcal{I} \left( \frac{2K \sin \Omega}{M a^{2} \sqrt{N}} \right)^{2} |A|^2, \quad \mathcal{I}_{ij} = \delta_{ij}
\]

It is worth noting that Eq.(11) is a kind of matrix Mathieu equation. In fact, we can apply to it Rayleigh’s method for studying parametric resonance, \[10\]. For this end let us look for the solution to Eq.(11) in the form of a series
\[ \bar{u}(t) = \bar{A}_{1} e^{i\omega t} + \bar{B}_{1} e^{-i\omega t} + \bar{A}_{3} e^{i3\omega t} + \bar{B}_{3} e^{-i3\omega t} + \ldots \]

On substituting the expression given above into Eq.(11) and preserving only the terms corresponding to \( e^{\pm i\omega t} \), we obtain the equations
\[
\begin{bmatrix}
(\omega^{2} + i\gamma_{u}\omega) \mathcal{I} + \dot{\omega}_{\alpha}^{2} & \mathcal{K} \\
\mathcal{K}^{+} & \mathcal{K}^{+} \mathcal{K}
\end{bmatrix}
\begin{bmatrix}
\bar{A}_{1} \\
\bar{B}_{1}
\end{bmatrix}
= 0
\]

The compatibility condition of the equations indicated above can be cast in the form of determinant for the block matrix
\[ \det \begin{bmatrix}
\dot{\omega}_{\alpha}^{2} - \omega^{2} + i\gamma_{u} \omega & \mathcal{K} \\
\mathcal{K}^{+} & \dot{\omega}_{\alpha}^{2} - \omega^{2} - i\gamma_{u} \omega
\end{bmatrix} = 0 \quad (12) \]

Here \( \dot{\omega}^{2} \) is the matrix of frequencies given by Eq.(8), and \( \omega^{2} \) and \( \gamma_{u} \omega \) are the scalar ones. Using the fact that for the range of frequencies we are considering, the matrix
\[ \dot{\omega}_{\alpha}^{2} - \omega^{2} + i\gamma_{u} \omega \]

is not degenerate, we may cast Eq.(12) in a more amenable form given by the equation
\[(\omega_{\alpha q}^2 - \omega^2 - i\gamma_u \omega)(\omega_{\alpha q-q_\ast}^2 - \omega^2 + i\gamma_u \omega) - \left(\frac{2K \sin \Omega}{Ma^2 \sqrt{N}}\right)^2 |A|^2 = 0 \quad (13)\]

which is quite similar to the usual condition for parametric resonance. Solutions to Eq.\(13\) are generally complex and therefore correspond to attenuated regimes. But there is a specific wave number, \(q_{\text{res}}\), for which the solution gives the real frequency \(\omega\), and it is easy to see that it should satisfy the constraint

\[\omega_{\alpha q-q_\ast}^2 = \omega_{\alpha q}^2, \quad q = q_{\text{res}} \quad (14)\]

Thus, we may cast the condition for parametric resonance in the familiar form, \[10\],

\[\left(\omega^2 - \omega_{\alpha q_{\text{res}}}^2\right)^2 + \gamma^2 \omega^2 - \left(\frac{2K \sin \Omega}{Ma^2 \sqrt{N}}\right)^2 |A|^2 = 0 \quad (15)\]

### III. MICRO-WAVE IRRADIATION AND THE HBS-MODES

We may use the results of the previous section for assessing the action of mw-radiation on the molecule of the DNA. The key point is accommodating the fact that the wavelength of radiation is by many orders of magnitudes larger than the characteristic size of the region of the molecule involved in the process. It was Chun-Ting Zhang, \[13\], who suggested a mechanism to overcome this difficulty. The main point of Zhang’s argument is that the helical configuration of the electric dipoles corresponding with the base-pairs makes the interaction \(U = -\vec{P} \cdot \vec{E}\) of the dipole \(\vec{P}\) and the field \(\vec{E}\) dependent on angle, and therefore, different torsional momenta are applied at the base-pairs. For our model the equation for the energy of interaction between the dipoles of DNA and an incident micro-wave reads

\[-\sum_n \vec{E} \cdot R(n\Omega + \phi_n)\vec{P}_o\]

Here \(R(n\Omega + \phi_n)\) is the rotation matrix given by Eq.\[11\], and \(\vec{P}_o\) is the dipole at site \(n = 0\). Consequently, even though at the molecular scale the radiation has a plane wave configuration, it still twists the DNA molecule about the axis of the double-helix. Since the momenta changes periodically in time with the incident wave, the irradiation results in a periodic stress that may produce elastic vibrations in the DNA molecule. Zhang suggested that the force may generate resonance vibrations, resulting in a cross-over mechanism which takes up initial torsion excitations and transforms them into longitudinal acoustic vibrations.
In the present paper we will try to combine Zhang’s mechanism, and the excitations of the double-helix studied by Prohofsky and Kim, with the view of generating inter-strand waves in the DNA by mw-irradiation. In contrast to the original idea by Zhang, we do not utilize a cross-over into longitudinal acoustic vibrations, but employ the interaction between torsional oscillations and the inter-strand ones, i.e. the three-wave, given by Eq. 14.

The main point is that by expanding the rotation matrix \( R(n\Omega + \phi_n) \) in the angles \( \phi_n \) and keeping only the first order terms, we may cast Zhang’s interaction in the form

\[
\mathcal{H}_Z = -\sum_n \phi_n (\vec{E} \times \vec{P}_n)_3 + \text{const}, \quad \vec{P}_n = R(n\Omega) \vec{P}_o
\] (16)

in which \( \vec{P}_o \) is the dipole vector at site \( n = 0 \). Next, by using Eq. (1) for the matrix \( R(n\Omega) \) and neglecting the constant term we may cast Eq. (16) in the form

\[
\mathcal{H}_Z = \frac{1}{2} \sum_n \phi_n \left\{ e^{i\Omega n} \left[ (\vec{E} \times \vec{P}_o)_3 - i(\vec{E} \cdot \vec{P}_o) \right] + e^{-i\Omega n} \left[ (\vec{E} \times \vec{P}_o)_3 + i(\vec{E} \cdot \vec{P}_o) \right] \right\}
\]

On applying the Fourier transform for the \( \phi_n \), and utilizing the equation

\[
\frac{1}{N} \sum_n e^{i(\Omega \pm aq)n} = \delta_{\Omega \pm aq}
\]

we obtain the following expression for Zhang’s interaction

\[
\mathcal{H}_Z = \frac{\sqrt{N}}{2} \left\{ \phi_{q = \frac{\Omega}{a}} [(\vec{E} \times \vec{P}_o)_3 - i(\vec{E} \cdot \vec{P}_o)] + \phi_{q = -\frac{\Omega}{a}} [(\vec{E} \times \vec{P}_o)_3 + i(\vec{E} \cdot \vec{P}_o)] \right\}
\]

Hence, the torque \( T_q \) in Eq. (17) corresponding to \( \mathcal{H}_Z \) is given by the equation

\[
T = \frac{Z}{I} \delta_{q_* - q^*} + \frac{Z^*}{I} \delta_{q^* - q_*} \quad \text{for} \quad q_* = \Omega / a
\] (17)

in which

\[
Z = \frac{\sqrt{N}}{2} \left[ (\vec{E} \times \vec{P}_o)_3 + i(\vec{E} \cdot \vec{P}_o) \right]
\]

It should be noted that \( \pm q_* \) are the local minima of the HBS-modes; \( q_{\text{res}} \) given by Eq. (14) reads

\[
q_{\text{res}} = \frac{3}{2} q_*
\] (18)

It is worth noting that the wave numbers \( q_* \) and \( q_{\text{res}} \) correspond to the wavelengths of one and \( \frac{2}{3} \) turns of the double-helix.
Equations given above provide an opportunity for making numerical, order of magnitude, estimates, which enable us to assess the effect of mw-radiation on the HBS-modes. From Eq. (17) we infer that the torque $T$ has the size

$$T \propto e^{2i\omega t} \sqrt{N} E P$$

where $E$ and $P$ are the external field and the dipole moment of the base-pair, respectfully.

Next, suppose that the resonance condition

$$\omega_q = 2\omega, \quad q = q_s = \frac{\Omega}{a}$$

be true, so that there is the resonance of the incident mw-radiation and the acoustic torsional mode $\phi_{q_s}$. Therefore, we may expect that the action of the radiation on the torsional modes should be the largest possible. Then the amplitude of the pumping wave, $\phi_{q_s}$, according to Eq. (7), is of the order

$$\Phi \propto \sqrt{N} E P I \sqrt{\frac{\gamma}{\omega}}$$

(19)

Next, we turn to Rayleigh's condition for the parametric resonance of the HBS-mode given by Eq. (15). For the pumping wave corresponding to Eq. (19), it gives

$$(\omega^2 - \omega_{aq_s}^2)^2 + \gamma_u^2 \omega^2 \approx 4 \left( \frac{K \sin \Omega}{M a^2} \frac{EP}{I\gamma \omega} \right)^2$$

Hence we have the threshold condition

$$\gamma_u \gamma \phi \leq \frac{2K \sin \Omega}{M a^2 \omega^2} \frac{EP}{I}$$

(20)

We suppose that the frequency of the HBS-modes be determined by the first term in Eq. (8), so that the first factor in Eq. (20) does not differ much from unity. It signifies that the energies of the inter-strand separation per base-pair is approximately of the same order as that due to the twist of the relative positions of the two adjacent base-pairs. If so, we could have the estimate for the dissipative constants, at least by orders of magnitude,

$$\gamma_u \gamma \phi \leq \frac{EP}{I}$$

(21)

On utilizing the expression

$$\vec{S} = \frac{c}{4\pi} \vec{E} \times \vec{H},$$
for Pointing’s vector, we cast the estimate given by Eq. (21) in the form

\[ \gamma_u \gamma_\phi \leq \frac{2 P}{I} \sqrt{\frac{\pi S}{c}} \]  

(22)

in which \( S \) is the power density of the interaction and \( c \) the light velocity. If we assume \( \propto 1 \) Debye and the inertia coefficient \( I \propto 10^{-36} \text{ gr cm}^2 \), corresponding to the mass of the base-pair \( \propto 10^{-22} \text{ gr} \), and the size \( \propto 10 \text{ Å} \), then for the power density \( S \propto 100 \text{ mW/cm}^2 \), we have

\[ \gamma_u \gamma_\phi \leq 10^{16} \text{ Hz}^2 \]

The estimate suggests that the effect produced by mw-radiation is to be looked for at the edge of the GHz zone, for in this case the requirement on the line-width is less stringent. It should be noted that the crucial point in assessing the feasibility of experiments on mw-irradiation of the DNA, and its possible influence, is the part played by ions in ambient solvent. In fact, the irradiation may result in just heating the solvent, so that the dissipation due to the ions takes up all effects on the molecules of DNA. Generally, the thin boundary layer of water and ions close to the DNA-molecule may have an important bearing on the dynamics initiated by the incident mw-radiation and result in the overdamping of the molecule’s torsional oscillations. Davis and VanZhandt, [12], put forward arguments that nonetheless the influence of the boundary layer could be effectively small so as to allow the survival of the effect caused by the mw-irradiation. But, so far there have been no definite arguments in this respect, and studying the mw-effect may turn out to be helpful for its understanding.

IV. CONCLUSIONS : IMPLICATIONS FOR THE DNA BIOPHYSICS

The elastic dynamics of the double helix could have enough structure for providing a means for stretching the hydrogen bonds of the base-pairs of DNA, or generating the HBS-modes. If the vibrational modes of the DNA are not overdamped by the ambient solvent, and the balance between energies supplied and dissipated is favorable, the “optimistic” forecast is that sufficiently developed resonance instabilities could bring about the breaking of the relatively weak H-bonds (with free energy of less than \( 2k_B T \), see [14]), and even result in the denaturation of the molecule. On the contrary, if the dissipation is strong, which is quite likely, the maintenance of the HBS-modes could be expected only at the edge of the HBS-zone and for sufficiently strong pumping. It is important that in the range of frequencies less
than 10$GHz$, the absorption due to water is small, whereas close to 100$GHz$ the permittivity of water changes drastically.

The best technique for studying the H-bond stretching still remains the Raman spectroscopy on which certain improvements have been made (see [15] and references therein). The choice of specific means for generating torsional excitations of the DNA is important and interesting. In this paper we have envisaged mw-irradiation of the DNA. In case the interpenetration of the acoustic and the HBS-modes takes place, we come to the conclusion that mw-radiation could maintain the HBS-modes, if the power density is sufficiently large, 100 $mW/cm^2$ or more. It is important that there is no need for long exposures of the sample to the radiation. Thus, the double helix could be a kind of mw-parametric amplifier for the HBS-modes, which are always present due to heat fluctuations; the torsional vibrations serving a pump beam for the HBS-modes. It is worthwhile to take into account that the parametric resonance can take place also for the frequencies $p$ of the pumping wave that verify the equation $p = 2\omega/n$, $n = 1, 2, 3, \ldots$. Therefore, the constraint imposed on the frequencies of the AT- and HBS-modes is less stringent than it appears at first sight. If the effect be sufficiently pronounced, it may result in the formation of the bubbles of broken H-bonds. In this respect it is worth noting that our estimate for the critical power density, 100 $mW/cm^2$, is by orders of magnitude larger than that officially prescribed, i.e. $0.2 - 1 mW/cm^2$.

The whole range of problems related to the direct action of mw-radiation on the DNA is highly controversial (see H. Lai’s discussion of the subject, [16]). For one thing there is enough evidence for the conclusion that it has a bearing upon the functioning of living organisms; for another, ”micro-wave” effect, considered as the resonance absorption of radiation, is difficult to distinguish from accompanying phenomena, for example heating, as well as to assess its real implications. In this respect utilizing the HBS-mode, which can be maintained by short pulses of radiation and detected and registered by the experimental methods currently employed in condensed matter physics, could be a valuable probe into the action of mw-irradiation on the DNA molecule.
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[1] E. B. Starikov, Physics Reports, 284, 1 (1997).
[2] Y. Kim and E. W. Prohofsky, Phys. Rev. B36, 3449 (1987).
[3] E. W. Prohofsky, Comments Mol. Cell. Biophys. 2, 65 (1983).
[4] H. Urabe, Y. Sugawara, M. Tsukakoshi and T. Kasuya, J. Chem. Phys. 95, 5519 (1991).
[5] H. Urabe and Y. Tominaga, J. Phys. Soc. Jpn., 50, 3543 (1981).
[6] W. Powell, G. S. Edwards, L. Genzel, and A. Wittlin, Phys. Rev. A35, 3929 (1987).
[7] M. E. El Hassan and C. R. Calladine, J. Mol. Biol. 251, 648 (1995).
[8] Ch. A. Hunter, J. Mol. Biol., 230, 1025 (1993).
[9] R. J. Isaacs and H. P. Spielmann, J. Mol. Biol. 307, 525 (2001).
[10] J. W. Rayleigh, The Theory of Sound, vol. I, MacMillan, London (1926).
[11] V. L. Golo, E. I. Kats, and Yu. M. Yevdokimov, Pisma ZhETF 70, 766 (1999).
[12] M. E. Davis and L. L. VanZandt, Phys. Rev. A 37, 888 (1987).
[13] C. T. Zhang, Phys. Rev. A40, 2148 (1989).
[14] J. Santa Lucia, Jr., Proc. Natl. Acad. Sci. USA 95, 1460 (1998).
[15] L. Moliveanu, J. M. Benevides, and G. J. Thomas, Jr., Nucl. Acids Res. 30, 3767 (2002).
[16] H. Lai, Neurological effects of radiofrequency electromagnetic radiation, the Workshop on possible biological and health effects of RF electromagnetic fields, University of Vienna, Austria, October 25 - 28, 1998.