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THE THREE-WAVE INTERACTION BETWEEN INTER-STRAND MODES OF THE DNA

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We consider the regime in which the bands of the torsional acoustic (TA) and hydrogen-bond-stretch (HBS) modes of the DNA interpenetrate each other. We propose a simple model accommodating the helix structure of the DNA, and, within its framework, find a three-wave interaction between the TA and the HBS modes. The phenomenon could be useful for studying the action of microwave radiation on a DNA molecule. Thus, using Zhang's mechanism of the interaction between the system of electric dipoles of a DNA molecule and the microwave radiation, we show that the latter could bring about torsional vibrations maintaining the HBS-ones. We indicate an estimate of the microwave power density necessary for generating the HBS mode, which essentially depends on the viscous properties of ambient medium.

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1. 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 10^9–10^{12} Hz [1]. According to Kim and Prohofsky [2], the region comprises 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). A local minimum of the frequency is characteristic of the HBS modes [2], its position depending on the choice of the band. Vibrations of the DNA were observed in the low-frequency Raman scattering [3, 4], and the Fourier-transform infrared absorption experiments [5]. Globus et al. [6] report the existence of internal modes generated by the interaction of artificial DNA-type molecules with electromagnetic radiation in the submillimeter range. It should be noted that the type of modes observed depends on the kind of DNA samples, i.e. in aqueous solutions, or films and filaments [6, 7]. The experimental data [1] is not conclusive as to the relative positions of the acoustic and the HBS modes.

Our work is based on the observation that if acoustic torsional bands penetrate the frequency region of 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 HBS modes. If the attenuation is small enough, the torsional acoustic band, which has the double frequency with respect to that of the HBS mode, could maintain an HBS mode through the parametric resonance. Thus, one could obtain a means for generating an HBS mode and studying the inter-helical dynamics of DNA.

2. 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 hydrogen bonds; (3) the helical symmetry. We utilize a quasi one-dimensional lattice model for the elastic properties of the DNA which accommodates these requirements.

El Hasan and Calladine [8] set up a 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 the positions of two base pairs. This is achieved by in-

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troducing local frames for the bases and the base pairs, and translation slides along their long axes. We follow the guidelines of paper [8], but aiming at a qualitative description of the DNA dynamics we use a simplified set of variables. We describe the relative position of the bases of a base pair by means of the vector $\mathbf{Y}$ directed along the long axis (the y axis in [8], see also [9]); $\mathbf{Y}$ is equal to zero when the base pair is at equilibrium. The relative position of the base pairs is described by the torsional angles ϕ_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 ϕ_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

$$\sum_n \left[\frac{I}{2}\dot{\phi}_n^2 + \frac{\tau}{2a^2}(\phi_{n+1}-\phi_n)^2\right]$$

where I is the moment of inertia, and τ is the twist coefficient, which are assumed the same for all the base pairs for simplicity and because of a qualitative picture at which we aim. Inter-strand motions should correspond to the relative motion of the bases inside the base pairs, and therefore the kinetic energy due to this degree of freedom may be cast in the form

$$\sum_n \frac{M}{2}\dot{\mathbf{Y}}_n^2,$$

where M is the effective mass of a couple.

For each base pair, we have the reference frame in which the z axis corresponds to the axis of the double helix, the y axis to the long axis of the base pair, and the x axis is perpendicular to the z and y axes (see Fig. 1 in [8]). At equilibrium, the change in position of adjacent base pairs is determined only by the twist angle Ω of the double helix. We assume that $\Omega = 2\pi/10$ 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, one may utilize the method employed by Kirchhoff for the twisted rod, that is, the covariant derivative, as was done in [10] for the DNA molecule. But a more simple and straightforward approach is possible.

We confine ourself only to the torsional degrees of freedom of the double lattice and assume the vectors $\mathbf{Y}_n$ to be parallel to the xy plane, or two-dimensional. Consider the displacements $\mathbf{Y}_n$ and $\mathbf{Y}_{n+1}$ determined within the frames of the two consecutive base pairs, n and $n+1$. Since we must compare the two vectors in the same frame, we rotate the vector $\mathbf{Y}_{n+1}$ to the frame of the nth base pair,

$$\mathbf{Y}_{n+1}^{back} = R^{-1}(\phi)\,\mathbf{Y}_{n+1}.$$

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

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

The matrix R is 2 by 2 since the vectors $\mathbf{Y}_n$ are effectively two-dimensional. Then the strain caused by the displacements of the base pairs is determined by the difference $\mathbf{Y}_{n+1}^{back} - \mathbf{Y}_n$[1].

It is important that the angle ϕ is given by the twist angle Ω describing the double helix, in conjunction with the torsional angles ϕ_n, so that

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

Therefore, the energy due to the inter-strand stress is given by

$$\sum_n \left\{\frac{M}{2}\dot{\mathbf{Y}}_n^{\,2} + \right.$$
$$\left. + \frac{K}{2a^2}\left[R^{-1}(\Omega+\phi_{n+1}-\phi_n)\,\mathbf{Y}_{n+1} - \mathbf{Y}_n\right]^2\right\}.$$

It corresponds with the fact that the equilibrium position of the double helix is the twisted one determined by Ω and all ϕ_n being equal to zero. We suppose that the size of the DNA molecule is small enough to be visualized as a straight double helix that is not larger than the persistence length. Hence, the number of base pairs $N \le 150$, approximately. Combining the formulas given above, we can write the total energy of the DNA molecule as

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

where K and a are the torsional elastic constant and the inter-pairs distance, respectively. In summations given above n is the number of a site corresponding to the nth base pair, $n = 1, 2, \dots, N$; N being the number

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[1] For this argument, I am indebted to D. I. Tchertov.

of pairs in the segment of the DNA under consideration. The last term $(\epsilon/2)\,\mathbf{Y}_n^2$ accommodates the energy of the inter-strand separation due to the slides of the bases inside the base pairs.

It should be noted that the dynamical variables ϕ_n and $\mathbf{Y}_n$ are of the same order of magnitude, that is, the first. Consequently, preserving only terms up to the third order, we can transform Eq. (2), so that it takes on the form

$$\begin{aligned}\mathcal{H} = \sum_n \left[\frac{I}{2}\,\dot{\phi}_n^2 + \frac{\tau}{2a^2}\,(\phi_{n+1}-\phi_n)^2\right] + \\ +\sum_n \left\{\frac{M}{2}\dot{\mathbf{Y}}_n{}^2 + \frac{K}{2a^2}\left[R^{-1}(\Omega)\,\mathbf{Y}_{n+1} - \mathbf{Y}_n\right]^2 + \frac{\epsilon}{2}\,\mathbf{Y}_n^2\right\} + \\ + \frac{K}{a^2}\sum_n (\phi_{n+1}-\phi_n)\,\left[R^{-1}(\Omega)\,\mathbf{Y}_{n+1}\times\mathbf{Y}_n\right]_3 .\end{aligned} \tag{3}$$

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

Simplify Eq. (3) by diagonalizing it with the help of the unitary transformation

$$\mathbf{Y}_n = S\,\mathbf{u}_n, \quad S = \begin{bmatrix} \dfrac{1}{\sqrt{2}} & \dfrac{i}{\sqrt{2}} \\ \dfrac{i}{\sqrt{2}} & \dfrac{1}{\sqrt{2}} \end{bmatrix},$$

which is a 2 × 2-matrix, for the vectors $\mathbf{Y}_n$ and $\mathbf{u}_n$ are effectively two-dimensional, their third coordinates being equal to zero. The equation for the energy (3) becomes

$$\begin{aligned}\mathcal{H} = \sum_n \left[\frac{I}{2}\,\dot{\phi}_n^2 + \frac{\tau}{2a^2}\,(\phi_{n+1}-\phi_n)^2\right] + \\ +\sum_n \left[\frac{M}{2}\,\dot{\mathbf{u}}_n\cdot\dot{\mathbf{u}}_n^* + \frac{\epsilon}{2}\,\mathbf{u}_n\cdot\mathbf{u}_n^* + \right. \\ \left. + \frac{K}{2a^2}\,\left(|e^{i\Omega}\,u_{n+1}^1 - u_n^1|^2 + |e^{-i\Omega}\,u_{n+1}^2 - u_n^2|^2\right)\right] - \\ - \frac{K}{a^2}\sum_n (\phi_{n+1}-\phi_n)\,\left[-ie^{i\Omega}u_{n+1}^1\,u_n^{*1} + ie^{-i\Omega}u_{n+1}^2\,u_n^{*2}\right],\end{aligned}$$

where $*$ signifies complex conjugation.

We can further simplify the equation for the energy by applying the Fourier transformation given by the equations

$$f_n = \frac{1}{\sqrt{N}}\sum_q e^{-inaq}\,f_q,$$

$$f_q = \frac{1}{\sqrt{N}}\sum_{n=-N/2}^{n=+N/2} e^{inaq}\,f_n, \quad q = \frac{2\pi}{Na}\,m,$$

$$m = 0, \pm 1, \ldots, \pm\frac{N}{2}.$$

It is important that after the Fourier transformation the variables $\mathbf{u}_n$ satify the following equations for their complex conjugates

$$u_q^{*1} = iu_{-q}^2, \quad u_q^{*2} = iu_{-q}^1. \tag{4}$$

The equation for the energy can be written as

$$\begin{aligned}\mathcal{H} = \sum_q \left[\frac{I}{2}\,\dot{\phi}_q\,\dot{\phi}_q^* + \frac{\tau}{2a^2}\,\sin^2\,\frac{aq}{2}\,\phi_q\,\phi_q^*\right] + \\ +\sum_q \left[\frac{M}{2}\,\dot{\mathbf{u}}_q\cdot\dot{\mathbf{u}}_q^* + \frac{\epsilon}{2}\,\mathbf{u}_q\cdot\mathbf{u}_q^* + \right. \\ \left. + \frac{2K}{a^2}\,\left(\sin^2\,\frac{\Omega - aq}{2}\,u_q^1 u_q^{*1} + \sin^2\,\frac{\Omega + aq}{2}\,u_q^2 u_q^{*2}\right)\right] + \\ + \frac{K}{a^2}\sum_{q'\,q''} i\,\frac{e^{-iaq}}{\sqrt{N}}\,\times \\ \times\,\phi_{q'}\,\left[-e^{i\Omega}u_{q''}^1\,u_{q'+q''}^{*1} + e^{-i\Omega}u_{q'}^2\,u_{q'+q''}^{*2}\right].\end{aligned} \tag{5}$$

The interaction term in Eq. (5) corresponds to the three-wave process and may result in a resonance. We use this fact for deriving the parametric maintenance of the u_q modes, i.e., the HBS modes (see below).

In the usual way, one can obtain the equations of motion for u_q^α, $\alpha = 1, 2$ and ϕ_q from the equation for the energy given 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 [11]. The dissipation can be accommodated by writing down terms linear in $\dot{u}_q^\alpha$ and $\dot{\phi}_q$. We take the external force, or torque $\mathcal{T}_q$ into account only in the equation for ϕ_q, because it corresponds to external degrees of freedom of our model. Thus, the equations of motion can be cast in the form

$$\begin{aligned}\ddot{u}_q^\alpha + \omega_{\alpha\,q}^2 u_q^\alpha + \gamma_u\,\dot{u}_q^\alpha + \\ + \frac{4K\sin\Omega}{Ma^2\,\sqrt{N}}\sum_{q'} e^{-iaq'}\,\phi_{q'}\,u_{q-q'}^\alpha = 0,\end{aligned} \tag{6}$$

$$\begin{aligned}\ddot{\phi}_q + \omega_q^2\,\phi_q + \gamma_\phi\dot{\phi}_q + \\ + i\,\frac{4K\sin\Omega\,e^{iaq}}{Ia^2\,\sqrt{N}}\sum_{q'} u_{q'}^1 u_{q-q'}^2 = \mathcal{T}_q,\end{aligned} \tag{7}$$

where

$$\begin{aligned}\omega_{\alpha q}^2 = \frac{4K}{Ma^2}\,\sin^2\frac{\Omega + (-1)^\alpha aq}{2} + \frac{\epsilon}{M}, \\ \omega_q^2 = \frac{4\tau}{Ia^2}\,\sin^2\frac{aq}{2}\end{aligned} \tag{8}$$

are the dispersion laws for the fields u_q^α, $\alpha = 1, 2$, and ϕ_q. We see that the spectrum of ϕ_q has a typical acoustic character, whereas that for u_q^α has a local minimum determined by the helical twist Ω. Thus, the spectrum of our model is in qualitative agreement with the conclusions in [2]. The specific nature of the torque is to be specified elsewhere (see Sec. 3). For the moment, we consider the general dynamical phenomena to which the torque may be conducive.

Suppose that on the one hand, the amplitudes of the HBS modes given by u_q^α are so small that the quadratic term in Eq. (7) can be neglected, and on the other hand, the external torque $\mathcal{T}_q$ is appreciable enough to maintain the vibration of the torsional mode ϕ_q. Thus, we can visualize the torsional mode as a pump mode that interacts with the HBS mode u_q^α through the nonlinearity in Eq. (6). We confine ourself to the case of the torque $\mathcal{T}_q$ being nonzero only at $q = q_*$ and having the frequency 2ω. Therefore, the forced wave, or the pump wave for the HBS mode, has the form

$$\phi_{q^*} = e^{i2\omega t}\,\Phi\,\delta_{qq^*}, \quad \phi_{-q^*} = e^{-i2\omega t}\,\Phi^*\,\delta_{-qq^*}. \tag{9}$$

To obtain larger values for the pump wave ϕ_q, the resonance condition

$$\omega_{q^*} = 2\omega, \quad q_* = \Omega/a,$$

should be satisfied, even though the resonance behavior of the torsional ϕ_q-mode itself could be attenuated by dissipation, i.e., may be a mode of small amplitude.

The equations of motion for u_q^α in the pumping regime are

$$\ddot{u}_q^\alpha + \omega_{\alpha q}^2 u_q^\alpha + \gamma_u \dot{u}_q^\alpha + \frac{2K}{Ma^2}\,\frac{\sin\Omega}{\sqrt{N}} \times \\ \times \left(A\,e^{i2\omega t}\,u^\alpha_{q-q*} + A^*\,e^{-i2\omega t}\,u^\alpha_{q+q*}\right) = 0,$$

where

$$A = e^{-i\Omega}\,\Phi.$$

Note that the momentum conservation in the q-values is preserved, as required by the three-wave interaction. The equations given above can be rewritten in the matrix form as

$$\ddot{\mathbf{u}}_\alpha + \hat{\omega}_\alpha^2 \mathbf{u}_\alpha + \gamma_u \dot{\mathbf{u}}_\alpha = \left(e^{i2\omega t}\,\mathcal{K} + e^{-i2\omega t}\,\mathcal{K}^+\right)\mathbf{u}_\alpha, \tag{10}$$

where $\mathcal{K}$ and $\mathcal{K}^+$ are Hermitian conjugate, and

$$\mathcal{K}^+\mathcal{K} = \mathcal{I}\left(\frac{2K}{Ma^2}\,\frac{\sin\Omega}{\sqrt{N}}\right)^2 |A|^2, \quad \mathcal{I}_{ij} = \delta_{ij}$$

It is worth noting that Eq. (10) is a kind of the matrix Mathieu equation. In fact, we can apply Rayleigh's method to it for studying parametric resonance [12]. For this, we look for the solution to Eq. (10) in the form of a series

$$\mathbf{u}(t) = \mathbf{A}_1\,e^{i\omega t} + \mathbf{B}_1\,e^{-i\omega t} + \mathbf{A}_3\,e^{i3\omega t} + \mathbf{B}_3\,e^{-i3\omega t} + \ldots$$

Substituting the expression given above into Eq. (10) and preserving only the terms corresponding to $e^{\pm i\omega t}$, we obtain the equations

$$\left[(-\omega^2 + i\gamma_u\omega)\,\mathcal{I} + \hat{\omega}_\alpha^2\right]\,\mathbf{A}_1 + \mathcal{K}\,\mathbf{B}_1 = 0,$$

$$\left[(-\omega^2 - i\gamma_u\omega)\,\mathcal{I} + \hat{\omega}_\alpha^2\right]\,\mathbf{B}_1 + \mathcal{K}^+\,\mathbf{A}_1 = 0.$$

The compatibility condition of the equations given above can be cast in the form of determinant for the block matrix,

$$\det\begin{bmatrix} \hat{\omega}_\alpha^2 - \omega^2 + i\gamma_u\,\omega & \mathcal{K} \\ \mathcal{K}^+ & \hat{\omega}_\alpha^2 - \omega^2 - i\gamma_u\,\omega \end{bmatrix} = 0, \tag{11}$$

where $\hat{\omega}^2$ is the matrix of frequencies given by Eq. (8), and ω^2 and $\gamma_u\,\omega$ are the scalar frequences. We can transform Eq. (11) into a more amenable form. Note that it is equivalent to the equation

$$\det\left\{\begin{bmatrix} \hat{\omega}_\alpha^2 - \omega^2 + i\gamma_u\omega & \mathcal{K} \\ \mathcal{K}^+ & \hat{\omega}_\alpha^2 - \omega^2 - i\gamma_u\omega \end{bmatrix} \times \\ \times \begin{bmatrix} \mathcal{I} & -(\hat{\omega}_\alpha^2 - \omega^2 + i\gamma_u\omega)^{-1} \\ 0 & \rho^2\mathcal{K}^+ \end{bmatrix}\right\} = 0,$$

where

$$\rho = \frac{Ma^2}{2K}\,\frac{\sqrt{N}}{\sin\Omega} \tag{12}$$

and the matrices $\mathcal{K}^+$ and $\mathcal{K}$ satisfy the equation

$$-\mathcal{I} + \rho^2\,\mathcal{K}\,\mathcal{K}^+ = 0.$$

We have used the fact that for the range of frequencies under consideration, the matrix

$$\hat{\omega}_\alpha^2 - \omega^2 + i\gamma_u\,\omega$$

is nondegenerate. Therefore, the equation given above is equivalent to

$$\det\left[-\mathcal{I} + \rho^2\,(\hat{\omega}_\alpha^2 - \omega^2 + i\gamma_u\,\omega) \times \\ \times \mathcal{J}(\hat{\omega}_\alpha^2 - \omega^2 - i\gamma_u\,\omega)\mathcal{J}^+\right] = 0,$$

where the matrix $\mathcal{J}$ is given by $\mathcal{J}_{qq'} = \delta_{q'\,q-q_*}$. We may rewrite the last equation as

$$(\omega_{\alpha q}^2 - \omega^2 - i\gamma_u\,\omega)(\omega_{\alpha\,q-q_*}^2 - \omega^2 + i\gamma_u\,\omega) - \\ - \left(\frac{2K}{Ma^2}\,\frac{\sin\Omega}{\sqrt{N}}\right)^2 |A|^2 = 0, \tag{13}$$

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

$$\omega^2_{\alpha q - q_*} = \omega^2_{\alpha q}, \quad q = q_{res}. \tag{14}$$

Thus, we may cast the condition for parametric resonance in the familiar form [12]

$$(\omega^2 - \omega^2_{\alpha q_{res}})^2 + \gamma^2\omega^2 - \left(\frac{2K}{Ma^2}\frac{\sin\Omega}{\sqrt{N}}\right)^2 |A|^2 = 0. \tag{15}$$

3. MICROWAVE IRRADIATION AND THE HBS MODES

We may use the results of the previous section for assessing the action of microwave (mw) radiation on a DNA molecule. 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 Zhang who suggested a mechanism to overcome this difficulty [13]. The main point of Zhang's argument is that the helical configuration of the electric dipoles corresponding to the base pairs makes the interaction of the dipole **P** and the field **E**

$$U = -\mathbf{P}\cdot\mathbf{E}$$

angle-dependent. Therefore, different torsional momenta are applied at the base pairs. The equation for the energy of interaction between the DNA dipoles and an incident microwave is given by

$$-\sum_n \mathbf{E}\cdot R(n\Omega + \phi_n)\mathbf{P}_0,$$

where $R(n\Omega + \phi_n)$ is the rotation matrix given by Eq. (1), and $\mathbf{P}_0$ is the dipole at the site $n = 0$. Consequently, even though the radiation has a plane wave configuration at the molecular scale, it still twists the DNA molecule about the double helix axis. Since the momenta change 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 that takes up initial torsion excitations and transforms them into longitudinal acoustic vibrations.

In the present paper, we try to combine Zhang's mechanism [13] and the excitations of the double helix studied by Prohofsky and Kim [2] 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. (5).

The main point is that by expanding the rotation matrix $R(n\Omega + \phi_n)$ in the angles ϕ_n and keeping only the first-order terms, we can write Zhang's interaction as

$$\begin{aligned} \mathcal{H}_Z &= -\sum_n \phi_n(\mathbf{E}\times\mathbf{P}_n)_3 + \text{const}, \\ \mathbf{P}_n &= R(n\Omega)\,\mathbf{P}_0, \end{aligned} \tag{16}$$

where $\mathbf{P}_0$ is the dipole vector at site $n = 0$. Next, using Eq. (1) for the matrix $R(n\Omega)$ and neglecting the constant term, we rewrite Eq. (16) as

$$\begin{aligned} \mathcal{H}_Z = \frac{1}{2}\sum_n \phi_n \{ & e^{in\Omega}[(\mathbf{E}\times\mathbf{P}_0)_3 - i(\mathbf{E}\cdot\mathbf{P}_0)] + \\ & + e^{-in\Omega}[(\mathbf{E}\times\mathbf{P}_0)_3 + i(\mathbf{E}\cdot\mathbf{P}_0)]\}. \end{aligned}$$

Applying the Fourier transform for the ϕ_n and using 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:

$$\begin{aligned} \mathcal{H}_Z = \frac{N}{2}\{ & \phi_{q=\Omega/a}[(\mathbf{E}\times\mathbf{P}_0)_3 - i(\mathbf{E}\cdot\mathbf{P}_0)] + \\ & + \phi_{q=-\Omega/a}[(\mathbf{E}\times\mathbf{P}_0)_3 + i(\mathbf{E}\cdot\mathbf{P}_0)]\}. \end{aligned}$$

Hence, the torque $\mathcal{T}_q$ in Eq. (7) corresponding to $\mathcal{H}_Z$ is given by

$$\mathcal{T} = \frac{\mathcal{Z}}{I}\delta_{q,-q^*} + \frac{\mathcal{Z}^*}{I}\delta_{q,q^*}, \quad q_* = \frac{\Omega}{a}, \tag{17}$$

where

$$\mathcal{Z} = \frac{N}{2}[(\mathbf{E}\times\mathbf{P}_0)_3 + i(\mathbf{E}\cdot\mathbf{P}_0)].$$

It should be noted that $\pm q_*$ are the local minima of the HBS modes. From Eq. (8), we infer that q satisfies the constraint given by Eq. (14),

$$q_{res} = \frac{3}{2}q_*. \tag{18}$$

It is worth noting that the wave numbers q_* and q_{res} correspond to the wavelengths of one and 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 $\mathcal{T}$ has the size

$$\mathcal{T} \propto e^{2i\omega t} E\, P,$$

where E and P are the external field and the dipole moment of the base pair, respectively. Next, suppose that the resonance condition

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

be true, so that the action of the radiation on the torsional modes should be the largest possible. Then the amplitude of the pumping wave, ϕ_{q_*}, according to Eq. (7), is of the order

$$\Phi \propto \frac{\sqrt{N}}{I} \frac{EP}{2\omega\gamma_\phi}. \tag{19}$$

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

$$(\omega^2 - \omega^2_{\alpha q_*})^2 + \gamma_u^2 \omega^2 \approx 4 \left(\frac{K \sin\Omega}{Ma^2} \frac{EP}{I\gamma_\phi} \right)^2 .$$

Hence we have the threshold

$$\gamma_u \gamma_\phi \le \frac{2K \sin\Omega}{Ma^2\omega^2} \frac{EP}{I}, \tag{20}$$

which is the condition that the energy supplied to a DNA molecule is greater than that dissipated, such that the maintaining of the HBS mode can take place. We suppose that the frequency of the HBS modes, given by Eq. (8), is generally determined by the gap term ϵ/M in the equation for $u_{\alpha q}$ and 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 and the twist of the relative positions of the two adjacent base pairs should be comparable. At any rate, the hypothesis appears not to contradict the data reproduced in [2]. If so, we could have the estimate for the dissipative constants, at least by orders of magnitude,

$$\gamma_u \gamma_\phi \le \frac{EP}{I}. \tag{21}$$

Using the relation

$$E \propto 2\sqrt{\frac{\pi S}{c}},$$

which follows from the expression for the Pointing vector

$$\mathbf{S} = \frac{c}{4\pi} \mathbf{E} \times \mathbf{H},$$

where c is the velocity of light, we rewrite Eq. (21) as

$$\gamma_u \gamma_\phi \le 2 \frac{P}{I} \sqrt{\frac{\pi S}{c}}, \tag{22}$$

where S is the power density of the interaction. If we assume

$$P \sim 1 \text{ D} \quad \text{or} \quad 10^{-18} \text{ CGS}$$

and the inertia coefficient $I \propto 10^{-36}$ g·cm^2, corresponding to the mass of the base pair $\sim 10^{-22}$ g and the size ~ 10 Å, then for the power density $S \sim 100$ mW/cm^2, we have $\gamma_u \gamma_\phi \le 10^{16}$ Hz^2 or $\gamma_u, \gamma_\phi \le 10^8$ Hz. The estimate suggests that the effect produced by mw-radiation is to be looked for at the edge of the GHz zone, because 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 the ambient solvent and ions contained in it. In fact, the irradiation may result in just heating the solvent, such 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 VanZandt [11] put forward arguments that the ions contained in a layer close to the DNA molecule should have an influence small enough to allow the survival of the effect due to mw-irradiation. The part played by the dissipation caused by water is more subtle.

The current arguments [14] about the overdamping of the DNA elastic modes rely on the Stokes law for the friction force, $F = 6\pi\eta R v$, for a sphere of radius R moving in a fluid of viscosity η at a speed v; and in the specific case of the DNA, it should involve the GHz region of frequencies. But the classical hydrodynamics, that is, the Navier – Stokes theory, breaks down in the region, as can be inferred from the phenomenon of light scattering in liquids, which is characterized by the triplet structure: the central Rayleigh line ν due to the elastic scattering and the Mandelstam – Brillouin doublet $\nu \pm f$ of the inelastic one, with f being the frequency of elastic waves in the liquid. The classical hydrodynamics gives the width of a line in the Mandelstam – Brillouin doublet larger than the distance between this line and the maximum of the central line of the triplet, so that the discrete triplet structure should not be observable; in fact, it is [15]. Mandelstam and Leontovich [15] brought about the solution to this problem by using the relaxational theory of hydrodynamics in which liquid is considered as a viscous elastic medium characterized by a viscosity coefficient η and a shear modulus G, the so-called Maxwell model. In fact, the theory also takes anisotropy effects into account [15]. It predicts that in the region of hypersound, a few GHz or more, the attenuation coefficient for sound waves, α_η, ceases to depend on the frequency ω, whereas in the low frequency classical region, in which the Stokes law is valid, the dependence is $\alpha_\eta \sim \omega^2$. Davis and VanZandt [11] used the approach of the Maxwell theory to find estimates for the damping of the DNA elastic modes, taking the first and the second hydration layers and the quasi-crystallin structure of water in a neighborhood of the DNA into account. They found the attenuation to be two orders of magnitude smaller than that given by the Stokes law.

In fact, there is a further reason for rejecting the approach based on the Stokes law. The water molecules form hydration shells of DNA [16]. The primary hydration shell comprises the water molecules immediately adjacent to the DNA, about 20 molecules per nucleotide pair, which constitute a medium different from bulk water. The secondary hydration shell is generally considered to be similar to bulk water. But at the spatial scale of the diameter of the DNA molecule, that is, several tens Å, the water in the second hydration shell is hardly a condensed medium. Indeed, in this case, one should have accommodated its local quasicrystalline structure, described by the icosahedral model [17, 18], which is to result in sophisticated dynamical equations. The conclusion is that, presently, it is difficult, if possible at all, to construct accurate theoretical estimates for the attenuation of DNA modes.

From the experimental standpoint, the situation is more advanced. The DNA helical modes were observed in the experiments on the Raman [3, 4, 16] and far-infrared [5] scattering. Therefore, one may suggest that the attenuation effects due to viscosity should not preclude elastic modes of the DNA. At the same time, small relaxation times for damping between the DNA and the first hydration layer, of the order of several tens ps (see [19]) should result in the double helix of the DNA concerted motion with the surrounding layer of water. The circumstance could be accommodated within the framework of the semi-phenomenological model in the present paper. In fact, the DNA molecule and its first hydration layer still form a helix structure, and the mutual motion of constituent bases of a pair together with hydration water molecules could be described with the field $\mathbf{Y}$. Of course, the values of the model constants, K, τ, should be changed, and for the time being there is lack of information as to their size.

It is also worth noting that the effects of dissipation in aqueous solutions, where a certain form of the Stokes law could be possible, and in films, or fibers, should be quite different. So far, there has been no comprehensive theoretical analysis of the dissipation that would allow comparing the DNA dynamics in solutions and in films. Nonetheless, the interplay of internal vibration modes and submillimeter electromagnetic irradiation was registered in paper [6], using Fourier transform spectroscopy and films of the double-stranded homopolymers poly[A]–poly[U] and poly[C]–poly[G]. Employing the concept of normal modes, or oscillators, of macromolecules, developed earlier for proteins [20] and used later for DNA [21], Globus et al. [6] made a numerical simulation of their experimental results and thus obtained an estimate for the relaxational parameter γ, which has the meaning of oscillators dissipation. It turned out that in the range of frequencies several 10 cm^{-1}, the best fit for γ is less than 1 cm^{-1}, depending on the conformation of the external electric field and the sample. This value of γ is too large for Eq. (22), but the region of frequencies studied in [6] is far from the edge of the GHz region, and therefore one may consider the question of the acceptable dissipation rate still open, and suggest that studying the effects of mw-radiation on the DNA modes may be instrumental for understanding the phenomenon.

4. CONCLUSIONS

We have shown that 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 maintenance of the HBS modes could be expected at the edge of the HBS zone. The best technique for studying the H-bond stretching still remains the Raman spectroscopy, on which certain improvements have been made (see [22] and the references therein). Thus, the HBS modes and also the breathing modes are well accessible from the experimental standpoint.

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, the 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. At this point, 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. 0.1–0.2 mW/cm^2.

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