Harmonic and subharmonic resonances of microwave absorption in DNA

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We have studied theoretically the movement of large molecular groups of DNA double helices in solution, which are driven by the electromagnetic field. The longitudinal vibration of nucleotides and the torsional movement of bases are taken into account at the same time. A set of coupled nonlinear partial differential equations has been established, and we have solved these equations by the method of perturbation. The result shows that there exists resonant absorption of microwave energy for both longitudinal and torsional modes. The resonant frequencies for the former and the latter are in the region of gigahertz and subterahertz, respectively. In addition to an nth-harmonic resonance at ω_n, our theory also predicts a subharmonic resonance at $\omega_n/2$. The strength of the latter is proportional to l^{-3}, where l is the length of DNA. The necessary conditions to observe these resonances are also discussed.

I. INTRODUCTION

Edwards, Davis, Saffer, and Swicord[1] (EDSS) have reported in 1984 a very important experimental result on the demonstration of resonant absorption of microwave energy by aqueous solutions containing DNA in the region of several gigahertz. The resonances observed by EDSS have been assigned to the longitudinal acoustic waves driven by a microwave field in DNA.[2] Although their result is still controversial,[3] the work of EDSS has attracted a lot of attention theoretically. The theory of DNA lattice dynamics proposed by Prohofsky and co-workers since 1974 seems to be the most accurate and detailed theory for DNA (Ref. 4) (see also Ref. 2 and the references therein). The theory takes into account the helical conformation and all atoms besides the hydrogen in the unit cell. One of the key problems related to the EDSS experiment is the damping caused by the viscosity of water. Van Zandt and co-workers have developed a series of theories of the hydration layer around the polymer to explain the result of EDSS.[5,6] A theory of nonlinear dynamics proposed by Scott and co-workers has been used successfully to explain several outstanding experimental facts.[7–10] However, only one degree of freedom—the longitudinal displacement—was taken into account in Scott's theory. It is the purpose of this paper to consider another degree of freedom in addition to the longitudinal one. It is well known that the longitudinal vibration of nucleotides, the rotation of bases (base rotator) around the axis parallel to the helical axis, and the sugar pucker are the main degrees of freedom for B-DNA.[11] In fact, Krumhansl and Alexander have developed dynamical equations in considerable detail for these degrees of freedom.[11] We think that the sugar pucker is important for the A–B-DNA transition; however, it is less important for the microwave absorption. Therefore we shall neglect the sugar pucker in our calculation.

The rotation of bases has been studied by Englander *et al.*,[12] Yomosa,[13] Homma and Takeno,[14] and Zhang[15] in addition to the work of Krumhansl and Alexander mentioned above. It is well known that the permanent dipole moments of bases are considerably large. According to Devoe and Tinoco,[16] the permanent dipole moments for bases A, G, T, and C are (in units of D) 2.8, 6.9, 3.5, and 8.0, respectively. The coupling of the external electric field with these dipole moments may produce a moment of force for each base. So a torsional acoustic wave propagating along the DNA chain may occur. In this paper we would like to point out the possibility that a torsional acoustic wave driven by a microwave field in aqueous solution containing DNA may exhibit a series of resonances in the region of subterahertz frequencies. We shall deal with the resonances of longitudinal waves observed by EDSS and the resonances of torsional waves predicted theoretically in a unified form. This paper is organized as follows. In Sec. II we introduce the Hamiltonian and the coupled dynamic equations to be studied. In Sec. III the equations are solved by a method of perturbation. In Sec. IV the parameters in this theory are estimated. In Sec. V some discussions and conclusions are discussed.

II. HAMILTONIAN AND EQUATIONS OF MOTION

Let φ_n and φ_n' be the rotation angle of the nth base rotator and of its complementary one, respectively, as in Refs. 11–15. For simplicity the case of $|\varphi_n|=|\varphi_n'|$ will be taken into account only hereafter. In this case, the Hamiltonian H_φ related solely to φ_n takes the form

$$H_\varphi=2\sum_n\left[\tfrac{1}{2}I\dot{\varphi}_n^2+V(\varphi_n)+\tfrac{1}{2}S(\varphi_n-\varphi_{n-1})^2\right], \quad (2.1)$$

where I is the mean value of the moments of inertia of the base rotator, S is the stacking energy of bases, and $V(\varphi_n)$

is the interaction energy between the two complementary bases in a base pair. According to Ref. 15 we have

$$V(\varphi_n)=\tfrac{1}{2}B(1-\cos 2\varphi_n)+\tfrac{1}{2}\beta\sin^2\varphi_n+\lambda(1-\cos\varphi_n)\ , \tag{2.2}$$

where B is the H bond energy, β is the dipole-dipole interaction energy, and λ is a coupling constant associated with the dipole-induced dipole interaction energy.

We assume that the base pair can vibrate along the screw axis OZ (longitudinal displacement). We assume further that there is a Lennard-Jones potential between two nearest-neighbor base pairs

$$U(r)=J\left[\left(\frac{\sigma}{r}\right)^{12}-\left(\frac{\sigma}{r}\right)^{6}\right]\ , \tag{2.3}$$

where J and σ are two parameters. Suppose that a is the base spacing ($a=3.36$ Å for B-DNA), and we expand $U(r)$ at point $r=a$,

$$U(r)=U(a)+\frac{1}{2!}U''(a)(\Delta r)^2+\frac{1}{3!}U'''(a)(\Delta r)^3+\cdots\ ; \tag{2.4}$$

notice that $U'(a)=0$. From Eq. (2.3) we obtain

$$K\equiv U''(a)=18J/a^2,\quad L\equiv U'''(a)=-378J/a^3\ . \tag{2.5}$$

Let u_n be the longitudinal displacement of nth base pair. Making reference to Eqs. (2.4) and (2.5), we write the Hamiltonian H_u solely related to u_n as

$$H_u=\sum_n\left[\tfrac{1}{2}M\dot{u}_n^{\,2}+\tfrac{1}{2}K(u_n-u_{n-1})^2+\tfrac{1}{6}L(u_n-u_{n-1})^3\right]\ , \tag{2.6}$$

where M is the mean mass of the base pair; K is the longitudinal elastic constant and L is an anharmonic constant, both defined by Eq. (2.5).

To consider the coupling between φ and u, notice that, provided the longitudinal displacement of the base pair takes place, the change in stacking energy S occurs. So S is a function of u_n-u_{n-1}. Considering that u_n-u_{n-1} is generally small, we expand S as

$$S=S_0+\chi_1'(u_n-u_{n-1})\ , \tag{2.7}$$

where χ_1' is a parameter. Similarly,

$$K=K_0+\chi_2'(\varphi_n-\varphi_{n-1})\ , \tag{2.8}$$

where χ_2' is another parameter. Substituting Eqs. (2.7) and (2.8) into Eqs. (2.1) and (2.6) we obtain the coupling Hamiltonian H_c as

$$H_c=\tfrac{1}{2}\sum_n\left[2\chi_1'(u_n-u_{n-1})(\varphi_n-\varphi_{n-1})^2+\chi_2'(\varphi_n-\varphi_{n-1})(u_n-u_{n-1})^2\right]\ . \tag{2.9}$$

Then the total Hamiltonian H is

$$H=H_\varphi+H_u+H_c\ , \tag{2.10}$$

where the parameters S in H_φ and K in H_u should be replaced by S_0 and K_0, respectively.

The equations of motion for φ_n and u_n are soon obtained:

$$I\ddot{\varphi}=-(2B+\beta+\lambda)\varphi_n+S_0(\varphi_{n+1}-2\varphi_n+\varphi_{n-1})+\chi_1'[(u_{n+1}-u_n)(\varphi_{n+1}-\varphi_n)-(u_n-u_{n-1})(\varphi_n-\varphi_{n-1})]+\tfrac{1}{4}\chi_2'[(u_{n+1}-u_n)^2-(u_n-u_{n-1})^2]\ , \tag{2.11}$$

$$M\ddot{u}_n=K_0(u_{n+1}-2u_n+u_{n-1})+\tfrac{1}{2}L[(u_{n+1}-u_n)^2-(u_n-u_{n-1})^2]+\chi_1'[(\varphi_{n+1}-\varphi_n)^2-(\varphi_n-\varphi_{n-1})^2]+\chi_2'[(\varphi_{n+1}-\varphi_n)(u_{n+1}-u_n)-(\varphi_n-\varphi_{n-1})(u_n-u_{n-1})]\ , \tag{2.12}$$

where we have assumed $\sin\varphi_n\simeq\varphi_n$, since φ_n is small in this study. Next we shall take the continuum approximations $\varphi_n(t)\to\varphi(z,t)$, $u_n(t)\to u(z,t)$ and expand $\varphi(z\pm a,t)$ and $u(z\pm a,t)$ as

$$\varphi(z\pm a,t)=\varphi\pm\frac{1}{1!}\varphi_z a+\frac{1}{2!}\varphi_{zz}a^2\pm\frac{1}{3!}\varphi_{zzz}a^3+\frac{1}{4!}\varphi_{zzzz}a^4+\cdots\ , \tag{2.13a}$$

$$u(z\pm a,t)=u\pm\frac{1}{1!}u_z a+\frac{1}{2!}u_{zz}a^2\pm\frac{1}{3!}u_{zzz}a^3+\frac{1}{4!}u_{zzzz}a^4+\cdots\ . \tag{2.13b}$$

Substituting Eqs. (2.13) into Eqs. (2.11) and (2.12) we obtain

$$\varphi_{tt}=v^2\varphi_{zz}-\omega_0^2\varphi+s\chi_2(u_z^2)_z+4s\chi_1(\varphi_z u_z)_z\ , \tag{2.14}$$

$$u_{tt}=c^2u_{zz}+\epsilon u_{zzzz}+\delta(u_z^2)_z+\chi_1(\varphi_z^2)_z+\chi_2(\varphi_z u_z)_z\ , \tag{2.15}$$

where we have neglected the term φ_{zzzz} in Eq. (2.14) and the terms φ_{zzz}, u_{zzz}, . . . , in the nonlinear parts of Eqs. (2.14) and (2.15). In Eqs. (2.14) and (2.15) the parameters v and c are the torsional and longitudinal acoustic velocity of DNA, respectively,

$$v=(S_0/I)^{1/2}a,\quad c=(K_0/M)^{1/2}a\ . \tag{2.16}$$

The frequency parameter ω_0 and the parameter for dimension transform s are

$$\omega_0=[(2B+\beta+\lambda)/I]^{1/2}\ , \tag{2.17}$$

$$s=M/8I\ , \tag{2.18}$$

respectively. The parameters ϵ and δ are called the dispersive and anharmonic parameters, respectively, by Scott,[9] and determined from Eqs. (2.5) and (2.15) to be

$$\epsilon/c^2=a^2/12,\quad \delta/c^2=-\tfrac{21}{2}\ . \tag{2.19}$$

The two coupling constants χ_1 and χ_2 are defined by

$$\chi_1=\chi_1'a^3/M,\quad \chi_2=\chi_2'a^3/M\ . \tag{2.20}$$

If $\chi_1=\chi_2=0$, Eqs. (2.14) and (2.15) reduce to

$$\varphi_{tt}=v^2\varphi_{zz}-\omega_0^2\varphi\ , \tag{2.21}$$

$$u_{tt}=c^2u_{zz}+\epsilon u_{zzzz}+\delta(u_z^2)_z\ . \tag{2.22}$$

Equation (2.21) is the Klein-Gordon equation and Eq. (2.22) is the Ostrovskii-Sutin equation.[17] Considering a circularly cylindrical homogeneous elastic rod, Ostrovskii and Sutin have derived Eq. (2.22) for the longitudinal displacement u. Defining the longitudinal strain as $Q=u_z$, Eq. (2.22) becomes

$$Q_{tt}=c^2Q_{zz}+\epsilon Q_{zzzz}+\delta(Q^2)_{zz}\ , \tag{2.23}$$

which is the Boussinesq equation. Scott and co-workers have used Eqs. (2.22) and (2.23) to study the resonant absorption of DNA.[7–9] The dispersion relations for Eqs. (2.21) and (2.22) ($\delta=0$) are

$$\omega^2=\omega_0^2+v^2q^2,\quad \omega^2=c^2q^2-\epsilon q^4\ , \tag{2.24}$$

respectively, where q is the wave number.

Suppose that an external electric field is exerted to the DNA chain. Let Ie_φ and Me_u represent the moment of force and force produced by the electric field, respectively. Let $-\alpha\varphi_t$ and $-\gamma u_t$ represent the damping of water to the torsional and longitudinal movement, respectively. Then Eqs. (2.14) and (2.15) become

$$\varphi_{tt}=v^2\varphi_{zz}-\omega_0^2\varphi-\alpha\varphi_t+s\chi_2(u_z^2)_z+4s\chi_1(\varphi_zu_z)_z+e_\varphi\ , \tag{2.25}$$

$$u_{tt}=c^2u_{zz}+\epsilon u_{zzzz}+\delta(u_z^2)_z-\gamma u_t+\chi_1(\varphi_z^2)_z+\chi_2(\varphi_zu_z)_z+e_u\ , \tag{2.26}$$

where α and γ are damping constants. Equations (2.25) and (2.26) are the complete equations to be studied in this paper.

III. SOLUTIONS OF EQUATIONS OF MOTION

To solve Eqs. (2.25) and (2.26) we have to give the detailed expressions of e_φ and e_u. Suppose that a microwave of linear polarization with wave number k and angular frequency ω is exerted to a linearized DNA of length l. Since $kl\simeq 0$, the electric field E takes the form

$$E=\mathcal{E}\cos\omega t\ , \tag{3.1}$$

where $\mathcal{E}$ is the amplitude. Let the angle between the vector of external electric field and the Z axis be denoted by ψ. Then the electric field will exert a moment of force to each of the bases. Let the moment of force for the nth base be denoted by T_n; we have

$$T_n=-P_nE\sin\psi\sin\theta_n\ , \tag{3.2}$$

where P_n is the dipole moment of the nth base, and θ_n is the angle between the vector of the projection of electric field (perpendicular to the Z axis) and the vector of dipole moment. The symmetry of double helix demands

$$\theta_{n+m}=\theta_n+m\pi/5=\theta_m+n\pi/5\ .$$

So we can always set $\theta_n=n\pi/5$ without losing generality. Then Eq. (3.2) becomes

$$T_n=-\mathcal{E}P_n\sin\psi\sin(n\pi/5)\cos\omega t\ . \tag{3.3}$$

Taking the continuum approximation for Eq. (3.3) we have

$$e_\varphi=T(z)/I=-\mathcal{E}I^{-1}P(z)\sin\psi\sin(\pi z/5a)\cos\omega t\ . \tag{3.4}$$

The driven force for the base pair is $-2eE\cos\psi$, where e is the proton charge. So

$$e_u=-2eM^{-1}\cos\psi\mathcal{E}\cos\omega t\ . \tag{3.5}$$

Equations (2.25) and (2.26) are a set of nonlinear and coupled partial differential equations. We use a method of perturbation to solve it. Since the external electric field is weak, we expand φ and u by a series of $\mathcal{E}$. Setting

$$\varphi=\mathcal{E}\varphi^{(0)}+\mathcal{E}^2\varphi^{(1)}+\cdots\ , \tag{3.6}$$

$$u=\mathcal{E}u^{(0)}+\mathcal{E}^2u^{(1)}+\cdots\ , \tag{3.7}$$

and substituting Eqs. (3.6) and (3.7) into Eqs. (2.25) and (2.26), we have

$$\varphi_{tt}^{(0)}=v^2\varphi_{zz}^{(0)}-\omega_0^2\varphi^{(0)}-\alpha\varphi_t^{(0)}+e_\varphi\ , \tag{3.8}$$

$$u_{tt}^{(0)}=c^2u_{zz}^{(0)}+\mathcal{E}u_{zzzz}^{(0)}-\gamma u_t^{(0)}+e_u\ , \tag{3.9}$$

$$\varphi_{tt}^{(1)}=v^2\varphi_{zz}^{(1)}-\omega_0^2\varphi^{(1)}-\alpha\varphi_t^{(1)}+e_\varphi^{(1)}\ , \tag{3.10}$$

$$u_{tt}^{(1)}=c^2u_{zz}^{(1)}+\mathcal{E}u_{zzzz}^{(1)}-\gamma u_t^{(1)}+e_u^{(1)}\ , \tag{3.11}$$

where

$$e_\varphi^{(1)}=s\chi_2((u_z^{(0)})^2)_z+4s\chi_1(\varphi_z^{(0)}u_z^{(0)})_z\ , \tag{3.12}$$

$$e_u^{(1)}=\delta((u_z^{(0)})^2)_z+\chi_1((\varphi_z^{(0)})^2)_z+\chi_2(\varphi_z^{(0)}u_z^{(0)})_z\ . \tag{3.13}$$

After getting Eqs. (3.8)–(3.11) we then set $\mathcal{E}=1$ in Eqs. (3.6) and (3.7). It is pleasant to point out that Eqs. (3.8)–(3.11) are all linear. To solve these equations we assume the boundary conditions and the initial conditions as

$$\varphi(0,t)=\varphi(l,t)=u(0,t)=u(l,t)=u_{zz}(0,t)=u_{zz}(l,t)=0, \quad t>0 , \tag{3.14a}$$

$$\varphi(z,0)=\varphi_t(z,0)=u(z,0)=u_t(z,0)=0, \quad 0<z<l . \tag{3.14b}$$

We have used Duhamel's method[18] to solve these equations. Since the derivations are trivial, we neglect the detailed calculations here. The exact solution of Eq. (3.8) under conditions (3.14) takes the form

$$\varphi^{(0)}(z,t)=\sum_{n=1}^{\infty}\sum_{m=0}^{1}A_n(z)\left[\frac{(-1)^m\alpha\sin\omega t/2-(-1)^m[\omega-(-1)^m\Omega_n]\cos\omega t}{2\{[\omega-(-1)^m\Omega_n]^2+\alpha^2/4\}}\right], \tag{3.15a}$$

$$A_n(z)=\sqrt{2/l}\,\sin\left[\frac{n\pi z}{l}\right]\frac{F_n}{\Omega_n}, \tag{3.15b}$$

$$F_n=\sqrt{2/l}\int_0^l F(z)\sin\left[\frac{n\pi z}{l}\right]dz , \tag{3.15c}$$

$$F(z)=-\mathcal{E}I^{-1}P(z)\sin\psi\sin(\pi z/5a) , \tag{3.15d}$$

$$\Omega_n^2=\omega_0^2+n^2v^2\pi^2/l^2-\alpha^2/4, \quad n=1,2,3,\ldots . \tag{3.15e}$$

It is easy to see that when $\omega\to\Omega_n$ a resonance occurs

$$\varphi^{(0)}(z,t)=\sqrt{2/l}\,\sin\left[\frac{n\pi z}{l}\right]\frac{\alpha F_n}{4\Omega_n}\frac{\sin\omega t}{(\omega-\Omega_n)^2+\alpha^2/4}, \quad \omega\to\Omega_n, \quad n=1,2,3,\ldots , \tag{3.16}$$

where the resonant frequency Ω_n is determined by Eq. (3.15e). The full width at half maximum (FWHM) is found to be equal to α. Similarly, the exact solution of Eq. (3.9) under conditions (3.14) takes the form

$$u^{(0)}(z,t)={\sum_{n=1}^{\infty}}'\sum_{m=0}^{1}B_n(z)\left[\frac{(-1)^m\gamma\sin\omega t/2-(-1)^m[\omega-(-1)^m\omega_n]\cos\omega t}{2\{[\omega-(-1)^m\omega_n]^2+\gamma^2/4\}}\right], \tag{3.17a}$$

where $\sum'$ means the summation is performed for $n=1,3,5,\ldots$ and

$$B_n(z)=\sqrt{2/l}\,\sin\left[\frac{n\pi z}{l}\right]\frac{G_n}{\omega_n}, \tag{3.17b}$$

$$G_n=-4\sqrt{2l}\,e\mathcal{E}M^{-1}\cos\psi/n\pi , \tag{3.17c}$$

$$\omega_n^2=c^2n^2\pi^2/l^2-\mathcal{E}n^4\pi^4/l^4-\gamma^2/4 , \quad n=1,3,5,\ldots . \tag{3.17d}$$

When $\omega\to\omega_n$ a resonance occurs,

$$u^{(0)}(z,t)=\sqrt{2/l}\,\sin\left[\frac{n\pi z}{l}\right]\frac{\gamma G_n}{4\omega_n}\frac{\sin\omega t}{(\omega-\omega_n)^2+\gamma^2/4}, \quad \omega\to\omega_n, \quad n=1,3,5,\ldots , \tag{3.18}$$

where the resonant frequency ω_n is determined by Eq. (3.17d). In this case FWHM$=\gamma$.

Next we substitute Eqs. (3.15) and (3.17) into (3.12) and (3.13) and then solve Eqs. (3.10) and (3.11). However, the resulting expressions are too complicated to write down here. Now we give the result for $u^{(1)}$ approximately and briefly

$$u^{(1)}=\frac{\delta(e\mathcal{E}M^{-1}\cos\psi)^2\gamma^3}{l^3}\sum_{n=1}^{\infty}\sin\left[\frac{n\pi z}{l}\right]\frac{M_n}{\omega_n}\frac{\cos 2\omega t}{(2\omega-\omega_n)^2+\gamma^2/4}+f(\chi_1)+f(\chi_2) , \tag{3.19a}$$

$$M_k={\sum_{n=1}^{\infty}}'{\sum_{m=1}^{\infty}}'\frac{J_{m,n,k}}{\omega_m\omega_n}\frac{1}{(\omega-\omega_n)^2+\gamma^2/4}\frac{1}{(\omega-\omega_m)^2+\gamma^2/4} , \tag{3.19b}$$

f is the terms of the argument and they have similar structure and $J_{m,n,k}$ is a number of dimensionless.

It is seen from Eqs. (3.19) that when $\omega \to \omega_n/2$ another resonance occurs. We shall call the resonance at $\omega=\omega_n$ the main resonance or the harmonic resonance, and at $\omega=\omega_n/2$ the subharmonic resonance. Of course, the former is stronger than the latter. This implies that a mechanism of double frequency exists in DNA, because the DNA in our theory is a nonlinear system. That is to say, if the forced frequency is ω, then the vibrators will vibrate in frequency ω and 2ω at the same time. When $\omega=\omega_n$ or $2\omega=\omega_n$ a resonance may occur. It is also seen that $u^{(1)}$ contributes a resonant factor at $\omega=\omega_n$, too. So the FWHM at $\omega=\omega_n$ is not simply equal to γ, it is also dependent on δ and χ_2 terms. Since $u^{(1)} \propto l^{-3}$, both effects discussed above are remarkable for DNA chain with short length l. A similar conclusion can be obtained for $\varphi^{(1)}$.

IV. ESTIMATION OF PARAMETERS

There are ten parameters in our theory: ω_0, v, c, ϵ, δ, s, γ, α, χ_1, and χ_2. We shall estimate them in due course. Using the values of parameters in Ref. 15, from Eq. (2.17) we have

$$\omega_0/2\pi = 1.2\times 10^{11}\ \mathrm{s}^{-1} = 0.12\ \mathrm{THz}\ . \tag{4.1}$$

The torsional force constant $C \equiv S_0 a$ was estimated from the free energy of superhelical winding to be nearly 2×10^{-19} erg cm[12]. Substituting this datum into Eq. (2.16) we find

$$v = 1.3\ \mathrm{km/s}\ . \tag{4.2}$$

The longitudinal acoustic speed c was measured by Hakim *et al.* as[19]

$$c = 1.69\ \mathrm{km/s}\ . \tag{4.3}$$

According to Eqs. (2.19) the dispersive and anharmonic parameters ϵ and δ are

$$\epsilon/c^2 = a^2/12 = 0.96\times 10^{-20}(3.6\times 10^{-20})\ \mathrm{m}^2\ , \tag{4.4}$$

$$\delta/c^2 = -10.5(-9.2)\ , \tag{4.5}$$

respectively, where the data within the parentheses are those estimated by Scott and co-workers.[9,10] The parameter s is

$$s = M/8I = 1.56\times 10^{18}\ \mathrm{m}^{-2}\ . \tag{4.6}$$

Now we use the resonant data of EDSS (Ref. 1) to estimate the damping constant γ. A linearized DNA of length $l = 948$ bp has been found to have a fundamental resonance at $f_1 = 2.65$ GHz. Setting $n=1$ in Eq. (3.17d), we have

$$f_1 = \frac{c}{2l}\left[1 - \frac{\epsilon\pi^2}{c^2 l^2} - \frac{l^2\gamma^2}{4\pi^2 c^2}\right]^{1/2}\ . \tag{4.7}$$

Using the value of c in Eq. (4.3) and taking $a = 3.36$ Å, we obtain

$$\gamma = 1.53\times 10^9\ \mathrm{s}^{-1}\ , \tag{4.8}$$

$$\tau \equiv 1/\gamma = 6.5\times 10^{-10}\ \mathrm{s} = 650\ \mathrm{ps}\ , \tag{4.9}$$

which is in agreement with the estimation of EDSS (Ref. 1) in order of magnitude. Lacking direct experimental data of α, we assume that

$$\alpha \simeq \gamma\ . \tag{4.10}$$

According to Eqs. (2.7) and (2.8)

$$\chi_1' = \left[\frac{\partial S}{\partial z}\right]_{z=a}\ ,\quad \chi_2' = \left[\frac{\partial K}{\partial \varphi}\right]_{\varphi=\pi/5}\ . \tag{4.11}$$

Lacking better data of S and K we shall estimate these parameters very roughly by the data of A-DNA. The base spacing a' and twist angle φ' of A-DNA are 2.92 Å and 33°, respectively. So

$$\begin{aligned}\Delta z &= a' - a = -0.44\ \text{Å}\ ,\\ \Delta\varphi &= \varphi' - \varphi = -3° = -\pi/60\ \mathrm{rad}\ .\end{aligned} \tag{4.12}$$

The longitudinal acoustic speed c' of A-DNA was measured by Hakim *et al.* as[19]

$$c' = 2.22\ \mathrm{km/s}\ . \tag{4.13}$$

Considering Eqs. (2.16) and (2.20) and (4.11)–(4.13) we have

$$\chi_2 = -\frac{60a^3}{\pi}\left[\left[\frac{c'}{a'}\right]^2 - \left[\frac{c}{a}\right]^2\right]\ . \tag{4.14}$$

So

$$\chi_2 \sim -10^{-2}\ \mathrm{m^3 s^{-2} rad^{-1}}\ . \tag{4.15}$$

The torsional force constant $C \equiv S_0 a$ was estimated to be 2×10^{-19} erg cm for B-DNA.[12] Lacking the corresponding constant C' for A-DNA, we assume $C' \sim 10^{-19}$ erg cm in order of magnitude. Taking $M = 260 M_{\mathrm{proton}}$ and considering Eqs. (2.20), (4.11), and (4.12) we obtain

$$\chi_1 \sim -10^{-13}\ \mathrm{m^4 s^{-2}}\ . \tag{4.16}$$

The overestimations in Eqs. (4.15) and (4.16) are so rough that we regard them as an upper limit for χ_1 and χ_2 in order of magnitude only.

We should point out that only few parameters discussed above are most important for this model. In fact, by carefully examining the model we have found that there are two key parameters among the whole, i.e., the damping constant γ and α which will strongly influence the general conclusion of this study. The numerical calculation of Eqs. (3.17) shows that when γ is larger than $10\times 10^9\ \mathrm{s}^{-1}$, the FWHM (height) of the resonances are so wide (short) that it is difficult to regard this absorption as resonances. A similar situation occurs for the damping constant α. We think that the water is subjected to a shearing motion when the torsional or longitudinal displacement takes place. So the assumption $\alpha \simeq \gamma$ seems to be reasonable. Finally, our theory depends on estimating the γ sensibly. However, the precise estimation or measurement of γ is still an unsolved problem. Nowadays the EDSS experiment is a rather controversial issue in molecular biophysics. The key problem may be the viscosity of water to the biopolymers. Recently, Sokoloff studied the coupling of water to the surface atoms of the macromolecules.[20] It was found that the acoustic modes are completely overdamped by using the viscosity of water at room temperature and zero frequency. However, if the viscosity were half of its zero-frequency, room temperature value, the acoustic modes would be underdamped. That is, the acoustic vibration sensibly depends on the viscosity of water. Our result is consistent with this.

V. DISCUSSIONS AND CONCLUSIONS

As for the so-called subharmonic resonance discussed in Sec. III we hope to see some experimental evidence. Making reference to the experimental result of EDSS,[1] a linearized DNA of length 2734 bp has resonant frequencies near 2.75, 4.15, and 5.60 GHz. Noticing that 5.60: 2.75=2.04, we think that the weaker resonance at 2.75 GHz may be a subharmonic resonance for the harmonic resonance at 5.60 GHz. According to the resonance assignment of EDSS,[1] for a constant acoustic velocity the above ratio should be 7:3=2.33. Edwards *et al.* have explained this contradiction by an effect of wavelength-dependent acoustic velocities.[2] The above two explanations both seem to be possible.

We should point out the limitation of our Hamiltonian to include only the nearest-neighbor interactions. In fact, before 1981 Mei *et al.* discussed the need for long-range interactions far beyond the nearest neighbors.[4] Using the measured values of the longitudinal acoustic velocity by the Brillouin scattering, they found that the long-range forces are needed for A conformation and are likely to dominate in B conformation as well.[4] With this conclusion in mind, we examine our whole derivation again. In this case Eqs. (2.5) and (2.19) are no longer valid. That is, the values of the two parameters ϵ and δ estimated previously should be revised. However, since ϵ and δ are not the key parameters in our model, i.e., the change in values of ϵ and δ will not change our general conclusion basically, this problem remains a topic for further study.

There are two important control parameters in this study. The first one is ω—the angular frequency of microwave; the second one is ψ—the angle between the vector of electric field and the helical axis OZ. In fact, the two parameters constitute a plane (ω,ψ). The longitudinal or the torsional resonances are possible only for the control parameters ω,ψ falling into the particular area in this plane. For example, when $\psi=\pi/2$ no longitudinal resonances can take place according to Eqs. (3.17)–(3.19). In our opinion it is possible to observe the longitudinal resonances for a linearized DNA by arranging all DNA chains with the same length parallel with each other in solution and setting $\psi=0$.

In conclusion we have shown that the resonant absorption of microwave energy is possible for both longitudinal and torsional modes. The resonant frequencies are expressed in Eqs. (3.17d) and (3.15e), respectively. The former is in the region of gigahertz; the latter is in the region of subterahertz. For both modes the so-called subharmonic resonances at $\omega_n/2$ or $\Omega_n/2$ are possible. It is pointed out that the two control parameters ω and ψ are important for the observation of these resonances experimentally.

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