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## The influence of longitudinal vibration on soliton excitation in DNA double helices†

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**Abstract.** In this paper taking into account Takeno and Homma's model Hamiltonian we have studied the influences of the longitudinal vibration on the properties of solitons in B-DNA with infinite length. It is shown that the longitudinal vibration will influence the amplitude and the width of the soliton. However, the influences due to the longitudinal vibration may be neglected ordinarily because the corrections have the magnitude of  $O(\delta^2)$ , where  $\delta$  is a small coupling constant.

### 1. Introduction

In recent years many authors have studied the soliton excitation of DNA chains [1-5]. Yomosa [2, 3], Takeno and Homma [4, 5] have studied the soliton excitation of B-DNA by using a dynamic plane base-rotator model based on the Watson-Crick model [6]. They have considered the interstrand base-base interaction energy and the stacking energy of the intrastrand neighbouring base-base interaction, but the longitudinal vibration was neglected. Calladine has pointed out that there are repulsive forces between purine bases in consecutive base pairs but on opposite backbones. These repulsive forces between the base pairs are resisted by stresses in the helical backbones. The change of main-chain torsion angle shows that there are elastic strain forces in both strands [7]. The chain elastic constant has been obtained [8]. Thus one should ask how the soliton excitation in DNA influences the non-rigidity of the strands. On account of Takeno and Homma's model Hamiltonian we have considered the longitudinal vibration coupling with the hydrogen bond and stacking energy to study the soliton excitation in B-DNA chains with infinite length, to ascertain the soliton solution in analytic form, and to discuss the influence of the longitudinal vibration on the properties of the soliton such as the shape, amplitude, width and effective mass, etc.

### 2. The Hamiltonian and equation of motion

In the model of Homma and Takeno [5] the interstrand base-base interaction energy  $V(\varphi_n, \varphi'_n)$  of the  $n$ th base pair, the stacking energy  $U(\varphi_n, \varphi'_n)$  of the intrastrand neighbouring base-base interaction and the kinetic energy of the  $n$ th base pair are written as, respectively,

$$\begin{aligned} V(\varphi_n, \varphi'_n) &= h_n(2 - \cos \varphi_n - \cos \varphi'_n) - \lambda_n[1 - \cos(\varphi_n - \varphi'_n)] \\ U(\varphi_n, \varphi'_n) &= J_n[1 - \cos(\varphi_{n+1} - \varphi_n)] + J'_n[1 - \cos(\varphi'_{n+1} - \varphi'_n)] \\ &\quad \times \frac{1}{2} I_n \dot{\varphi}_n^2 + \frac{1}{2} I'_n \dot{\varphi}'_n{}^2. \end{aligned}$$

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The Watson-Crick model of B-DNA with helical axis taken in the  $Z$  direction is schematically shown in figure 1 in which each base is depicted by an arrow with unit length, and the complementary base pair is indicated by a conjugated arrow directed inward. Here the quantities  $h_n$  and  $\lambda_n$  are interaction constants characterising the local field energy and hydrogen-bonding energy of the  $n$ th base pair, respectively.  $J_n$  and  $J'_n$  are interaction constants associated with the  $n$ th bases in  $S$  and  $S'$ , respectively.  $I_n$  and  $I'_n$  are the moments of inertia of the  $n$ th bases in  $S$  and  $S'$ , respectively.

According to Calladine's work [7] the strand in DNA is not rigid. Instead it seems to be an elastic chain with strain forces. Thus we can assume that  $u_n$  is the longitudinal displacement from the balance position of the  $n$ th base pair. We denote the longitudinal elastic constant along the double helix main chain by  $\alpha$ . Let  $M$  be the average mass of a pair of nucleotides. Then the longitudinal vibration energy can be written as

$$\sum_n \left[ \frac{1}{2} M \dot{u}_n^2 + \frac{1}{2} \alpha (u_{n+1} - u_n)^2 \right].$$

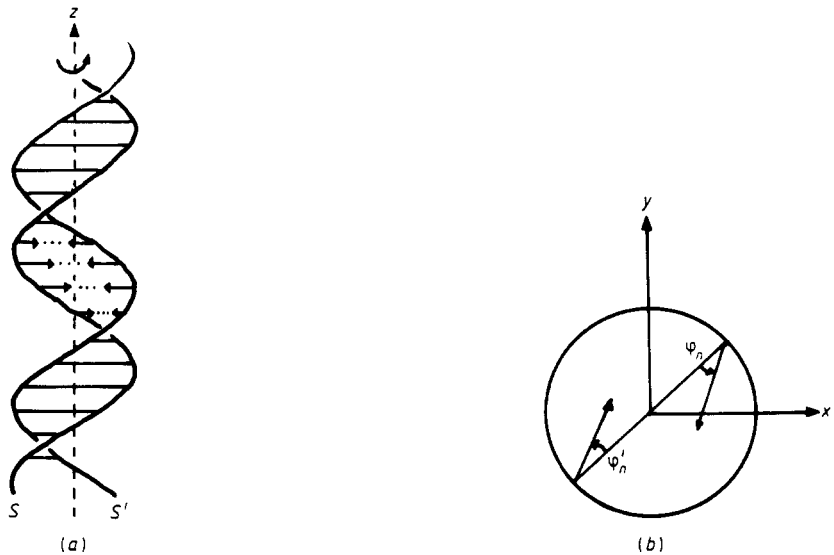
In view of the longitudinal vibration above, the Hamiltonian of the system will be changed. We assume the constants of stacking energy  $J_n, J'_n$  to be dependent on the distance between the  $n$ th and the  $(n+1)$ th base pair, but the constants of the local field energy and the hydrogen-bonding energy  $h_n, \lambda_n$  must be symmetrically dependent on the distances between the  $n$ th and the  $(n \pm 1)$ th base pair. Introducing the coupling coefficients  $\beta, \gamma, \kappa$  we expand  $J_n, J'_n$  and  $h_n, \lambda_n$  in terms of  $u_{n+1} - u_n$  and  $u_n - u_{n-1}$  up to first order

$$J_n = J'_n = S_0 + \beta(u_{n+1} - u_n)$$

$$h_n = h_0 + \gamma(u_{n+1} - u_{n-1})$$

$$\lambda_n = \lambda_0 + \kappa(u_{n+1} - u_{n-1}).$$

In fact these coupling constants  $\beta/S_0, \gamma/h_0, \kappa/\lambda_0$  must be small.



**Figure 1.** (a) Schematic feature of the B-DNA. The sugar-phosphate backbones of the double helix are represented as ribbons  $S$  and  $S'$  and the rung-like base pairs connecting them as arrows. (b) Projection of the  $n$ th pair of bases (arrows) in the  $xy$  plane.

Now we approximate  $I_n$  and  $I'_n$  by the average value  $I$ . Thus the Hamiltonian of DNA chains with infinite length can be written as

$$H = \sum_n \left\{ \frac{1}{2} M \dot{u}_n^2 + \frac{1}{2} \alpha (u_{n+1} - u_n)^2 + \frac{1}{2} I (\dot{\varphi}_n^2 + \dot{\varphi}'_n{}^2) \right. \\ \left. + [S_0 + \beta (u_{n+1} - u_n)] [2 - \cos(\varphi_{n+1} - \varphi_n) - \cos(\varphi'_{n+1} - \varphi'_n)] \right. \\ \left. + [h_0 + \gamma (u_{n+1} - u_{n-1})] [2 - \cos \varphi_n - \cos \varphi'_n] \right. \\ \left. - [\lambda_0 + \kappa (u_{n+1} - u_{n-1})] [1 - \cos(\varphi_n - \varphi'_n)] \right\}. \quad (2.1)$$

Substituting (2.1) into the Hamilton equation, then the differential equations of the motion may be obtained:

$$M \ddot{u}_n = \alpha [(u_{n+1} - u_n) - (u_n - u_{n-1})] - \beta [\cos(\varphi_{n+1} - \varphi_n) - \cos(\varphi_n - \varphi_{n-1}) \\ + \cos(\varphi'_{n+1} - \varphi'_n) - \cos(\varphi'_n - \varphi'_{n-1})] \\ - \gamma [\cos \varphi_{n+1} - \cos \varphi_{n-1} + \cos \varphi'_{n+1} - \cos \varphi'_{n-1}] \\ + \kappa [\cos(\varphi_{n+1} - \varphi'_{n+1}) - \cos(\varphi_{n-1} - \varphi'_{n-1})] \quad (2.2)$$

$$I \ddot{\varphi}_n = [S_0 + \beta (u_{n+1} - u_n)] \sin(\varphi_{n+1} - \varphi_n) - [S_0 + \beta (u_n - u_{n-1})] \sin(\varphi_n - \varphi_{n-1}) \\ - [h_0 + \lambda (u_{n+1} - u_{n-1})] \sin \varphi_n + [\lambda_0 + \kappa (u_{n+1} - u_{n-1})] \sin(\varphi_n - \varphi'_n) \quad (2.3)$$

$$I \ddot{\varphi}'_n = [S_0 + \beta (u_{n+1} - u_n)] \sin(\varphi'_{n+1} - \varphi'_n) - [S_0 + \beta (u_n - u_{n-1})] \sin(\varphi'_n - \varphi'_{n-1}) \\ - [h_0 + \gamma (u_{n+1} - u_{n-1})] \sin \varphi'_n - [\lambda_0 + \kappa (u_{n+1} - u_{n-1})] \sin(\varphi_n - \varphi'_n). \quad (2.4)$$

According to [5], we can employ a continuum approximation

$$n \rightarrow \xi \\ \left. \begin{array}{l} u_n(t) \\ \varphi_n(t) \\ \varphi'_n(t) \end{array} \right\} \rightarrow \left\{ \begin{array}{l} u(\xi, t) \\ \varphi(\xi, t) \\ \varphi'(\xi, t) \end{array} \right\} \quad (2.5)$$

and take a transformation of variable

$$\zeta = \xi - Vt. \quad (2.6)$$

Thus (2.3), (2.4) and (2.5) are reduced to

$$\frac{d^2 u}{d\zeta^2} = \frac{1}{M(V^2 - V_0^2)} \frac{d}{d\zeta} \left\{ \frac{\beta}{2} \left[ \left( \frac{d\varphi}{d\zeta} \right)^2 + \left( \frac{d\varphi'}{d\zeta} \right)^2 \right] - 2\gamma (\cos \varphi + \cos \varphi') + 2\kappa \cos(\varphi - \varphi') \right\} \quad (2.7)$$

$$V^2 \frac{d^2 \varphi}{d\zeta^2} = \left( S_0 + \beta \frac{du}{d\zeta} \right) \frac{d^2 \varphi}{d\zeta^2} + \beta \frac{d^2 u}{d\zeta^2} \frac{d\varphi}{d\zeta} - \left( h_0 + 2\gamma \frac{du}{d\zeta} \right) \sin \varphi + \left( \lambda_0 + 2\kappa \frac{du}{d\zeta} \right) \sin(\varphi - \varphi') \quad (2.8)$$

$$V^2 \frac{d^2 \varphi'}{d\zeta^2} = \left( S_0 + \beta \frac{du}{d\zeta} \right) \frac{d^2 \varphi'}{d\zeta^2} + \beta \frac{d^2 u}{d\zeta^2} \frac{d\varphi'}{d\zeta} - \left( h_0 + 2\gamma \frac{du}{d\zeta} \right) \sin \varphi' \\ - \left( \lambda_0 + 2\kappa \frac{du}{d\zeta} \right) \sin(\varphi - \varphi') \quad (2.9)$$

where

$$V_0^2 = \alpha / M. \quad (2.10)$$

For the infinite long chain the boundary conditions may take the form

$$\begin{aligned} \zeta = \pm\infty & \quad \frac{du}{d\zeta} = \frac{d\varphi}{d\zeta} = \frac{d\varphi'}{d\zeta} = 0 \\ \zeta = 0 & \quad \varphi = \varphi' = \pi \end{aligned} \tag{2.11}$$

if we assume that the centre of soliton is at  $\zeta = 0$ .

Equations (2.7)–(2.11) are motion equations of B-DNA with infinite length.

### 3. Soliton solution

Considering the boundary conditions (2.11), (2.7) can be integrated directly. Then we obtain

$$\frac{du}{d\zeta} = \frac{1}{M(V^2 - V_0^2)} \left\{ \beta \left[ \left( \frac{d\varphi}{d\zeta} \right)^2 + \left( \frac{d\varphi'}{d\zeta} \right)^2 \right] - 2\gamma(\cos \varphi + \cos \varphi') + 2\kappa \cos(\varphi - \varphi') + A \right\} \tag{3.1}$$

where integrating constant  $A \sim 4\gamma - 2\kappa$ . According to [5] we substitute (3.1) into (2.8) and (2.9). We limit our solution for two special cases.

In the first case let  $\varphi = \varphi'$ , from (2.8) and (3.1) we have

$$\begin{aligned} \frac{d^2\varphi}{d\zeta^2} = & a^2 \sin \varphi + b \left\{ \left[ \beta \left( \frac{d\varphi}{d\zeta} \right)^2 - 4\gamma \cos \varphi + 2\kappa + A \right] \left( \beta \frac{d^2\varphi}{d\zeta^2} - 2\gamma \sin \varphi \right) \right. \\ & \left. + \beta \frac{d\varphi}{d\zeta} \frac{d}{d\zeta} \left[ \beta \left( \frac{d\varphi}{d\zeta} \right)^2 - 4\kappa \cos \varphi + 2\kappa \right] \right\} \end{aligned} \tag{3.2}$$

where

$$\begin{aligned} a^2 &= \frac{h_0}{I(V_1^2 - V^2)} \\ b^2 &= \frac{1}{MI(V_0^2 - V^2)(V_1^2 - V^2)} \\ V_1^2 &= \frac{S_0}{I} \end{aligned} \tag{3.3}$$

Using the successive approximation by iterations to solve (3.2) we assume that  $\beta = \gamma = \kappa = 0$  for the zero-order approximation, i.e. the longitudinal vibration can be neglected. Equation (3.2) can be reduced to

$$d^2\varphi/d\zeta^2 = a^2 \sin \varphi. \tag{3.4}$$

Equation (3.4) is a classical sine-Gordon equation. Considering (2.11) its solution is [5]

$$\varphi_0 = 4 \tan^{-1} \exp(\pm a\zeta). \tag{3.5}$$

For the positive kink we substitute the solution of the zero approximation  $\varphi_0$  into the right-hand side of (3.2) and obtain

$$\frac{d^2\varphi}{d\zeta^2} = -2a^2 \frac{\sinh(a\zeta)}{\cosh^2(a\zeta)} + 8b^2(4\gamma^2 - 4a^2\beta\gamma - 3a^4\beta^2) \frac{\sinh(a\zeta)}{\cosh^4(a\zeta)}. \tag{3.6}$$

Integrating (3.6) and using boundary conditions (2.11) we obtain the solution of the first-order approximation  $\varphi_1$  of (3.2)

$$\varphi_1 = \varphi_0 + \frac{4b^2}{3a^2} (3a^4\beta^2 + 4a^2\gamma\beta - 4\gamma^2) \left( \frac{\sinh(a\zeta)}{\cosh^2(a\zeta)} + \tan^{-1}[\sinh(a\zeta)] \right). \quad (3.7)$$

In the second case let  $\varphi = -\varphi'$ , then from (2.8), (2.9), (3.1) and (3.2) we can obtain

$$\begin{aligned} \frac{d^2\varphi}{d\bar{Z}^2} = & \sin\varphi - \eta \sin 2\varphi \\ & + \frac{b^2}{a^2} \left\{ \left[ \beta a^2 \left( \frac{d\varphi}{d\bar{Z}} \right)^2 - 4\gamma \cos\varphi + 2\kappa \cos 2\varphi + 4\gamma - 2\kappa \right] \right. \\ & \times \left( \beta a^2 \frac{d^2\varphi}{d\bar{Z}^2} - 2\gamma \sin\varphi + 2\kappa \sin 2\varphi \right) \\ & \left. + \beta a^2 \left( \frac{d\varphi}{d\bar{Z}} \right)^2 \left( 2\beta a^2 \frac{d^2\varphi}{d\bar{Z}^2} + 4\gamma \sin\varphi - 4\kappa \sin 2\varphi \right) \right\} \end{aligned} \quad (3.8)$$

where

$$\bar{Z} \equiv a\zeta \quad \eta \equiv \lambda_0/h_0. \quad (3.9)$$

Similarly, we can obtain the different solutions of the zero-order approximation of (3.8) with different values of  $\eta$ . For example, when  $|\eta| < \frac{1}{2}$ , we have [5]

$$\varphi_0 = 2 \tan^{-1}[\pm(1-2\eta)^{1/2} \operatorname{cosech}(1-2\eta)^{1/2} \bar{Z}]. \quad (3.10)$$

Here we also ascertain the solution of the first-order approximation of (3.8), but only for the special case above. For the positive kink we substitute  $\varphi_0$  of (3.10) into the right-hand side of (3.8) and obtain

$$\begin{aligned} \frac{d^2\varphi}{d\bar{Z}^2} = & \sin\varphi - \eta \sin 2\varphi \\ & + \sinh[(1-2\eta)^{1/2} \bar{Z}] \left( \frac{B}{\{\sinh^2[(1-2\eta)^{1/2} \bar{Z}] + (1-2\eta)\}^2} \right. \\ & + \frac{C}{[\sinh^2[(1-2\eta)^{1/2} \bar{Z}] + (1-2\eta)]^3} \\ & \left. + \frac{D}{[\sinh^2[(1-2\eta)^{1/2} \bar{Z}] + (1-2\eta)]^4} \right) \end{aligned} \quad (3.11)$$

where

$$\begin{aligned} B = & \frac{8b^2(1-2\eta)^{3/2}}{a^2} [3a^4\beta^2(1-2\eta)^2 + 4a^2\beta(\gamma-2\kappa)(1-2\eta) - 4(\gamma-2\kappa)^2] \\ C = & \frac{32b^2(1-2\eta)^2}{a^2} [a^2(1-2\eta)^{3/2}\beta(3\eta\beta a^2 + 2\kappa) + 2(1-2\eta)^{1/2}(\gamma-2\kappa)(a^2\eta\beta - 2\kappa)] \\ D = & \frac{32b^2(1-2\eta)^{7/2}}{a^2} (6\eta^2\beta^2 a^4 + 8\eta\kappa\beta a^2 - 8\kappa^2). \end{aligned} \quad (3.12)$$

Integrating (3.11) and using conditions (2.11) we can obtain the solution of the first-order approximation

$$\begin{aligned} \varphi_1 \approx & \varphi_0 - R \tan^{-1}[(1-2\eta)^{-1/2} \sinh[(1-2\eta)^{1/2} \bar{Z}]] \\ & + Q \frac{\sinh[(1-2\eta)^{1/2} \bar{Z}]}{[\sinh^2[(1-2\eta)^{1/2} \bar{Z}] + (1-2\eta)]^2} + SW(\bar{Z}) \\ & + P \frac{\sinh[(1-2\eta)^{1/2} \bar{Z}]}{\sinh^2[(1-2\eta)^{1/2} \bar{Z}] + (1-2\eta)} + SW_0 \end{aligned} \tag{3.13}$$

where

$$\begin{aligned} R = & -\frac{1}{4\eta(1-2\eta)^{3/2}} \left[ B - \frac{1}{8\eta} \left( \frac{7}{3} C - D \right) - \frac{5D}{16\eta^2} \right] \\ Q = & -\frac{D}{12(1-2\eta)^2 \eta} \\ P = & -\frac{1}{24\eta(1-2\eta)^2} \left[ C + D \left( \frac{3}{4(1-2\eta)} - \frac{5}{8\eta} \right) \right] \\ S = & -\frac{1}{4\eta(1-2\eta)^{1/2}} \left( B - \frac{3C}{8\eta} + \frac{5D}{32\eta^2} \right) \end{aligned} \tag{3.14}$$

$$W(\bar{Z}) = \begin{cases} \frac{1}{(-2\eta)^{1/2}} \int_0^{\bar{Z}} \left[ \tan^{-1} \left( \frac{\cosh[(1-2\eta)^{1/2} x]}{(-2\eta)^{1/2}} \right) - \frac{\pi}{2} \right] dx & (\eta < 0) \\ \frac{1}{(2\eta)^{1/2}} \int_0^{\bar{Z}} \left[ \tan^{-1} \left( \frac{\cosh[(1-2\eta)^{1/2} x]}{-(2\eta)^{1/2}} \right) + 1 \right] dx & (\eta > 0) \end{cases}$$

$$W_0 = \lim_{\bar{Z} \rightarrow \infty} W(\bar{Z}).$$

A similar solution can be obtained for the case of  $\eta > \frac{1}{2}$  and  $\eta < -\frac{1}{2}$ .

#### 4. Discussion

From the above discussion, by considering the longitudinal vibration we find that at the first approximation the soliton solution of DNA chains can be written as

$$\varphi_1 \approx \varphi_0 + \Delta\varphi \tag{4.1}$$

where the correction term  $\Delta\varphi$  is

$$\Delta\varphi \approx N \left( \frac{\sinh(a\zeta)}{\cosh^2(a\zeta)} + \tan^{-1}[\sinh(a\zeta)] \right) \tag{4.2}$$

when  $\varphi = \varphi'$  and

$$\begin{aligned} \Delta\varphi \approx & -R \tan^{-1}\{(1-2\eta)^{-1/2} \sinh[(1-2\eta)^{1/2} a\zeta]\} \\ & + Q \{ \sinh^2[(1-2\eta)^{1/2} a\zeta] + (1-2\eta) \}^{-2} \sinh[(1-2\eta)^{1/2} a\zeta] + \dots \end{aligned} \tag{4.3}$$

when  $\varphi = -\varphi'$ .

The coefficients in the above expression have been given by (3.7) and (3.14). These can easily be estimated. By defining  $\delta = \max(\beta/S_0, \gamma/h_0, k/\lambda_0)$  the coefficient  $N$  in (4.2) can be written as

$$N \sim V^2 O(\delta^2) \tag{4.4}$$

where  $O(\delta^2)$  represents the second-order correction of  $\delta$  and  $V$  is the velocity of the soliton. This correction consists of two parts: the correction to the amplitude and to the width of the soliton. However our calculation shows that these corrections are very small. Similar corrections can be obtained for the case of  $\varphi = -\varphi'$ . These results, which are different from (4.4), are independent of the velocity  $V$ . We may therefore conclude that the influence of the longitudinal vibration on the soliton in the case of  $\varphi = \varphi'$  increases with the increase of soliton velocity.

Moreover we can calculate the kinetic energy of longitudinal motion along the helix of the DNA chain. It is

$$E_k = \frac{1}{2} \sum_n M \dot{u}_n^2 = \frac{1}{2L} \int_{-\infty}^{\infty} M V^2 \left( \frac{du}{d\zeta} \right)^2 d\zeta \quad (4.5)$$

where  $n$  denotes the label of the  $n$ th nucleotide,  $L$  the distance between the nearest-neighbouring nucleotide,  $M$  the mass of unit DNA,  $x$  is the coordinate along the helix axis and  $\zeta = x - Vt$ . As we know that (4.5) can be integrated using (3.1), if we are interested in the lowest correction we can substitute the solution without longitudinal coupling into the right-hand side of (3.1) and substitute  $du/d\zeta$  obtained from (3.1) into (4.5) and perform the integral. For example, we have obtained the following approximate expression of  $E_k$  at low velocity by straight calculation for the case of  $\varphi = \varphi'$ :

$$E_k \approx (a^2\beta + 2\gamma)^2 \frac{32}{3MLaV_0^2} V^2. \quad (4.6)$$

If the soliton is regarded as a quasiparticle, the contribution to the soliton is

$$m_s \approx O(\delta^2)M. \quad (4.7)$$

Similarly we can show that another contribution to the soliton due to the correlation between the longitudinal motion and the motion of the rotational angles are also quantities of the second order.

Similar results can be obtained for the case of  $\varphi = -\varphi'$ . This shows that the corrections of the longitudinal coupling to the effective mass of the soliton are small quantities of the second order.

Conclusively, the above results show that corrections of the longitudinal vibration on the behaviour of the soliton in the long chain of DNA are always to second order of the coupling constant. Therefore these can be neglected ordinarily, and it also explains the exact reason why the results obtained by neglecting the longitudinal vibration in the early theories are reasonable.

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