Solitary-wave excitation of hydrogen-bond stretching in deoxyribonucleic acid

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Abstract. A model of solitary-wave excitation for B-DNA has been proposed by taking into account the stretching of the hydrogen bonds. Using the continuum approximation we have derived a non-linear Klein–Gordon equation which has the solitary-wave solution. The stretch amplitude of the solitary wave is found to be 0.37 Å. The energy and width of the solitary wave are also estimated. It is shown by a linear stability analysis that the solitary wave is unstable. The numerical simulation of the non-linear differential-difference equation (i.e. the equation without using the continuum approximation) shows that the solitary wave is pinned by the lattice. An unstable pinned solitary wave is used to explain the opening mechanism of the bases in a DNA chain.

1. Introduction

The vibration modes of hydrogen-bond stretching in B-DNA at 10–120 cm^{-1} have been observed in both low-frequency Raman scattering [1, 2] and Fourier-transform infrared absorption [3]. According to the famous double-helix model of Watson and Crick, the base adenine (A) is always bound to the base thymine (T) with two hydrogen bonds, and the base guanine (G) to the base cytosine (C) with three hydrogen bonds. The above experimental results imply that the base and its complementary base may vibrate with each other along the direction of H bonds in a base pair. Chou [4] has developed a linear vibration theory of H-bond stretching in DNA and discussed some relevant biological functions. However, many workers (see, e.g., [5, 6]) have pointed out that the H bond is essentially non-linear. On the other hand, from theoretical studies of helix lattice dynamics of DNA, Prohofsky [7] has pointed out independently that the modes of H-bond stretching at 10–120 cm^{-1} are highly non-linear. He has also proposed a soliton model of H-bond stretching in DNA based on the Davydov solitary-wave analysis [7]. This work was stimulated by the studies of Chou and Prohofsky. I hope to improve Chou's [4] work by considering the non-linear effect of H bonds. At the same time, but different from Prohofsky's [7] theory, I hope also to establish a soliton model of H-bond stretching by assuming a concrete anharmonic potential of H bonds. The result shows that the non-linear effect of H bonds leads directly to the solitary-wave effects which are closely related to the energy concentration in DNA. Such solitary-wave or soliton effects

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are useful to explain the mechanisms of RNA transcription and of drug intercalation into DNA and more generally to elucidate the breathing motion in the DNA double helix.

2. A model of H-bond stretching

Suppose that the displacements of the nth base and its complementary base along the direction of H bonds are denoted by u_n and u'_n, respectively. For B-DNA the displacements are basically vertical to the helical axis Oz of DNA. Letting

$$Y_n = u_n - u'_n \tag{2.1}$$

Yomosa [6] has shown that the potential energy of H bonds takes the form

$$V(Y_n) = AY_n^2 - BY_n^3 \tag{2.2}$$

where A and B are two parameters, both greater than zero. On the other hand, as long as vibration of the bases takes place, a change in stacking energy of the bases occurs. Denoting the change in stacking energy for the nth base in the single strand of the DNA double helix by ΔS_n, then [8]

$$\Delta S_n = \tfrac{1}{2}S(u_n - u_{n-1})^2 + \tfrac{1}{2}S(u_{n+1} - u_n)^2 \tag{2.3}$$

where S is another parameter.

Finally, the Hamiltonian of the DNA system takes the form

$$H = \sum_n \{\tfrac{1}{2}M(\dot{u}_n^2 + \dot{u}_n'^2) + V(Y_n) + \tfrac{1}{2}S[(u_n - u_{n-1})^2 + (u'_n - u'_{n-1})^2]\} \tag{2.4}$$

where M is the effective mass of a base. The equations of motion are quickly obtained:

$$M\ddot{u}_n = -2A(u_n - u'_n) + 3B(u_n - u'_n)^2 + S(u_{n+1} - 2u_n + u_{n-1}) \tag{2.5a}$$

$$M\ddot{u}'_n = 2A(u_n - u'_n) - 3B(u_n - u'_n)^2 + S(u'_{n+1} - 2u'_n + u'_{n-1}). \tag{2.5b}$$

Hereafter we shall study an important special case, i.e. the relative motion of the bases,

$$u_n = -u'_n.$$

Then equations (2.5) reduce to

$$M\ddot{u}_n = -4Au_n + 12Bu_n^2 + S(u_{n+1} - 2u_n + u_{n-1}). \tag{2.6}$$

As usual we take the continuum approximation

$$u_n(t) \to u(z, t) \qquad \sum_n \to \frac{1}{a}\int dz \tag{2.7}$$

where a is the base spacing and equals 3.4 Å for B-DNA. In this case, equation (2.6) reduces to

$$u_{tt} = c^2 u_{zz} - \omega_0^2 u + \lambda^2 u^2 \tag{2.8}$$

where u_{tt} means $\partial^2 u/\partial t^2$ and so on, and

$$c^2 = (S/M)a^2 \qquad \omega_0^2 = 4A/M \qquad \lambda^2 = 12B/M. \tag{2.9}$$

Equation (2.8) is a non-linear Klein–Gordon equation. If the last term on the right-hand

side of equation (2.8) is proportional to u^3, then it is the well known φ^4 equation. In fact, it is not. To look for the travelling solution of equation (2.8), setting

$$\xi = z - vt$$

where v is the speed of the travelling wave, we obtain

$$u_{\xi\xi} = (\omega_0^2 \gamma^2/c^2)u - (\lambda^2 \gamma^2/c^2)u^2 \tag{2.10}$$

where

$$\gamma = 1/\sqrt{1 - (v/c)^2}. \tag{2.11}$$

Multiplying both sides of equation (2.10) by u_ξ and performing the integral, we have

$$u_\xi^2 = -(2\lambda^2\gamma^2/3c^2)u^3 + (\omega_0^2\gamma^2/c^2)u^2 + C \tag{2.12}$$

where C is the integral constant. We rewrite equation (2.12) as

$$u_\xi^2 = -\alpha(u - u_1)(u - u_2)(u - u_3) \qquad (u_1 > u_2 > u_3) \tag{2.13}$$

where

$$\alpha = 2\lambda^2\gamma^2/3c^2 \tag{2.14}$$

and u_1, u_2, u_3 are the three roots of the following polynomial $P(u)$:

$$P(u) = u^3 - \tfrac{3}{2}(\omega_0^2/\lambda^2)u^2 - c/\alpha. \tag{2.15}$$

Obviously, we have

$$u_1 + u_2 + u_3 = \tfrac{3}{2}(\omega_0^2/\lambda^2)$$
$$u_1u_2 + u_2u_3 + u_3u_1 = 0 \tag{2.16}$$
$$u_1u_2u_3 = C/\alpha.$$

We have assumed that the three roots are all real. This assumption exerts a restriction on the constant C. The solution of equation (2.13) can be expressed as

$$u = u_2 + (u_1 - u_2)\,\mathrm{cn}^2\sqrt{\alpha(u_1 - u_3)/4}\,\xi \tag{2.17}$$

where cn is the Jacobian elliptic function with modulus k:

$$k = (u_1 - u_2)/(u_1 - u_3). \tag{2.18}$$

Hereafter we shall study the special boundary conditions

$$u|_{|\xi| \to \infty} = 0 \qquad u_\xi|_{|\xi| \to \infty} = 0 \tag{2.19}$$

which is reasonable for realistic DNA. In this case we have $C = 0$ and hence

$$u_1 = \tfrac{3}{2}(\omega^2/\lambda^2) \qquad u_2 = u_3 = 0 \qquad k = 1. \tag{2.20}$$

Then the solution (2.17) reduces to the following solitary wave:

$$u(z, t) = \tfrac{1}{2}(A/B)\,\mathrm{sech}^2[\gamma(z - vt)/2d] \tag{2.21}$$

where

$$d = c/\omega_0. \tag{2.22}$$

It is interesting to see that the amplitude of the solitary wave in equation (2.21) is

determined solely by the H-bond potential. We can define the width of the solitary wave by the width at half-maximum:

$$W \simeq 4d. \tag{2.23}$$

We have also seen that the vibration of the H-bond stretching seems to support the energy concentration due to the non-linear effect of the H-bond potential. For a continuum approximation, the energy E_s of the solitary wave can be calculated from the following integral:

$$E_s = \frac{1}{a} \int_{-\infty}^{\infty} (Mu_t^2 + 4Au^2 - 8Bu^3 + aSu_z^2) \, dz. \tag{2.24}$$

Substituting equation (2.21) into (2.24) and performing the integral, we obtain

$$E_s = \tfrac{2}{15}(A/B)^2(M/ad)v^2 + \tfrac{16}{15}(A/B)^2(d/a)A \tag{2.25}$$

where the first and second terms on the right-hand side of equation (2.25) correspond to the kinetic and potential energies, respectively, of the solitary wave.

When the displacement u is small, equation (2.8) approximately reduces to

$$u_{tt} = c^2 u_{zz} - \omega_0^2 u \tag{2.26}$$

which is the famous Klein–Gordon equation. We obtain the phonon mode solution

$$u(z, t) = \exp[i(\beta z - \omega t)] \tag{2.27}$$

where β is the wavenumber. Substituting equation (2.27) into equation (2.26), we obtain the dispersion relation

$$\omega^2 = \omega_0^2 + c^2 \beta^2. \tag{2.28}$$

It should be noted that in the case of some boundary conditions the solution of equation (2.26) is a standing wave which is the theoretical basis of Chou's [4] work.

3. The linear stability analysis of the solitary wave

We shall study the stability of the solitary-wave solution (2.21) by a technique presented by Scott *et al* [9], which is called the analysis of linear stability. For the reason explained later, we first assume that the speed of the solitary wave is equal to zero, i.e. $v = 0$; then equation (2.21) reduces to

$$u_s(z) = \tfrac{1}{2}(A/B) \operatorname{sech}^2(z/2d). \tag{3.1}$$

Now write the solution $u(z, t)$ of equation (2.8) as the sum of $u_s(z)$ and a perturbation term $u_p(z, t)$, which will be assumed to be small in some sense. That is,

$$u(z, t) = u_s(z) + u_p(z, t). \tag{3.2}$$

Substituting equations (3.1) and (3.2) into equation (2.8), we find a non-linear equation for $u_p(z, t)$:

$$u_{p,tt} - c^2 u_{p,zz} + \omega_0^2 u_p = \lambda^2[(u_s + u_p)^2 - u_s^2] \tag{3.3}$$

and note that $u_s(z)$ is a known function. Since u_p is small, the linear assumption is such that equation (3.3) approximately reduces to a linear equation

$$u_{p,tt} - c^2 u_{p,zz} = (-\omega_0^2 + 2\lambda^2 u_s)u_p. \tag{3.4}$$

To solve equation (3.4) we further assume the product solution

$$u_p(z, t) = \psi(z) \exp(st) \tag{3.5}$$

where s is a parameter. According to Scott *et al* [9], 'The basic problem of linear stability

is to determine whether or not for any such product solution, with reasonable boundary conditions on ψ as $z \to \pm \infty$, the real part of s is greater than zero.' In particular, if any product solution has $\text{Re}(s) > 0$, the solitary-wave solution is said to be unstable. Substituting equation (3.5) into equation (3.4), we obtain

$$-\psi_{zz} - (2\lambda^2/c^2)u_s\psi = -(s'^2 + \omega_0^2/c^2)\psi \qquad s' = s/c. \tag{3.6}$$

Equation (3.6) is the Schrödinger equation and hence is an eigenvalue problem. Since the 'potential' is proportional to $-u_s$, we conclude that there are at most a finite number of bound-state solutions for which $\psi \to 0$ as $z \to \pm \infty$. The eigenvalue is $-(s'^2 + \omega_0^2/c^2)$ and the corresponding eigenfunction is ψ. We shall show that at least one solution of the Schrödinger equation (3.6) is already found. In fact, since u_s satisfies

$$c^2 u_{s,zz} = \omega_0^2 u_s - \lambda^2 u_s^2 \tag{3.7}$$

and on differentiation with respect to z, we have

$$c^2 (\mathrm{d}u_s/\mathrm{d}z)_{zz} = \omega_0^2 (\mathrm{d}u_s/\mathrm{d}z) - 2\lambda^2 u_s(\mathrm{d}u_s/\mathrm{d}z) \tag{3.8}$$

which is the same as the Schrödinger equation (3.6) when $s = 0$. Therefore one eigenfunction is

$$\psi(z)|_{s=0} = \mathrm{d}u_s/\mathrm{d}z = -(1/2d)(A/B)\,\text{sech}^2(z/2d)\tanh(z/2d) \tag{3.9}$$

and the corresponding eigenvalue is $-\omega_0^2/c^2$. Note that there is one crossing of the eigenfunction in equation (3.9), we know that the solution in equation (3.9) is not the solution of the 'ground state'. In fact, it is the solution of the 'first excitation state'. The solution of the ground state must have a lower eigenenergy than $-\omega_0^2/c^2$. That is to say, the eigenenergy of the ground state is $-(s'^2 + \omega_0^2/c^2)$ with s'^2 or $s^2 > 0$. According to the definition of the instability mentioned above, we thus conclude that, with respect to the boundary condition $\psi \to 0$ as $z \to \pm \infty$, the linear stability analysis shows that the solitary wave in equation (2.21) is unstable. In fact, it is shown by direct observation that the ground-state eigenfunction of the Schrödinger equation (3.6) is

$$\text{constant} \times \text{sech}^3(z/2d) \tag{3.10}$$

with an eigenvalue $-9A/S$, which corresponds to

$$s^2 = 5A/M. \tag{3.11}$$

Defining

$$\tau' = 1/s = \sqrt{M/5A} \tag{3.12}$$

we calculate the value of τ' from the data given later:

$$\tau' = 7.4 \times 10^{-14}\,\text{s}. \tag{3.13}$$

When $t \gg \tau'$, $u_p(z, t)$ and hence the $u(z, t)$-values diverge quickly.

It should be pointed out that the stability analysis discussed above is still valid for the solitary-wave solution in the case of $v \neq 0$. For $v \neq 0$, we perform the Lorentz transformation

$$z \to \eta = \gamma(z - vt) \tag{3.14}$$

$$t \to \sigma = \gamma(t - vz/c^2) \tag{3.15}$$

$$\partial/\partial z \to \gamma[\partial/\partial\eta - (v/c^2)(\partial/\partial\sigma)] \tag{3.16}$$

$$\partial/\partial t \rightarrow \gamma[\partial/\partial\sigma - \upsilon(\partial/\partial\eta)] \tag{3.17}$$

and equation (2.8) is invariant to this transformation:

$$u(z, t) \rightarrow \bar{u}(\eta, \sigma) = u \tag{3.18a}$$

$$\bar{u}_{\sigma\sigma} = c^2\bar{u}_{\eta\eta} - \omega_0^2\bar{u} + \lambda^2\bar{u}^2. \tag{3.18b}$$

In the new coordinate system we may regard the speed of the solitary wave as zero. For any $\upsilon < c$ and any fixed position in z, an increase in σ implies an increase in t. Therefore the conclusion of an instability remains valid for $\upsilon \neq 0$. Note that it is quite different from the situation of the sine–Gordon and Korteweg de Vries (KDV) equations, in which the solitary waves or solitons are stable according to the linear stability analysis.

4. Numerical estimate of parameters and a study of the H-bond energy

There are three parameters A, B and S in this model, where A and B were given by Yomosa [6]:

$$A = 0.62\,\text{eV Å}^{-2} \qquad B = 0.83\,\text{eV Å}^{-3}. \tag{4.1}$$

We know that the G–C base pair has three H bonds while the A–T base pair has two H bonds. For the naturally occurring DNA molecule, the ratio of A + T to G + C is in the range 0.98–1.12 to 1 [4], i.e. very close to 1 to 1. Therefore, instead of A and B, we should use A' and B' in the calculation hereafter, where $A' = 2.5A$, $B' = 2.5B$. According to equation (2.21) the amplitude of the solitary wave is

$$A_m = \tfrac{1}{2}(A'/B') = \tfrac{1}{2}(A/B) = 0.37\,\text{Å}. \tag{4.2}$$

Note that the equilibrium distance of H bonds is about 2.9 Å; so the amplitude of the solitary wave is only 12.8% of that distance. Note also that this quantity is independent of the structure of DNA and is dependent only on the character of H bonds.

Let us take the effective mass M as [4]

$$M = 307.3\,\text{g}/N \tag{4.3}$$

where N is the Avogadro constant. From equation (2.9) we find that

$$\omega_0/2\pi = (1/2\pi)\sqrt{4A'/M} = 74.4\,\text{cm}^{-1} \tag{4.4}$$

which falls in the range 10–120 cm^{-1}.

It is difficult to estimate the parameter S. From the phonon mode solution (2.27) we know that c is the acoustic velocity associated with the motion of H-bond stretching. The acoustic velocity associated with the longitudinal motion of the bases was measured by Hakim *et al* [10] as 1.69 km s^{-1} for B-DNA. The acoustic velocity associated with the torsional motion of the bases was estimated to be 1.3 km s^{-1} [11]. If we take $c \simeq 1.5$ km s^{-1}, we obtain

$$S = A = 0.62\,\text{eV Å}^{-2}. \tag{4.5}$$

Then according to equation (2.25) the rest energy ($\upsilon = 0$) of the solitary wave is

$$E_s^{(0)} = \tfrac{16}{15}(A'/B')^2(d/a)A' = 0.29\,\text{eV} = 6.78\,\text{kcal mol}^{-1}. \tag{4.6}$$

At the same time

$$d = 0.32a \tag{4.7}$$

and so the width of the solitary wave is given by

$$W = 4d = 1.28a \simeq 1 - 2bp. \tag{4.8}$$

Turning to equation (3.12), where A should be replaced by A', we obtain the result in equation (3.13).
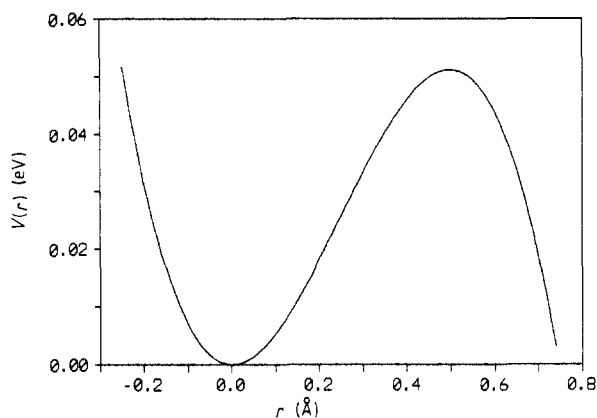
Figure 1. Plot of $V(r)$ against r.

Table 1. The theoretical and experimental values of energy required to melt a base pair.

| | Energy (kcal mol^{-1}) | | D |
	G–C	A–T	(Å^2)
Theoretical	3.55	2.37	0.0625
Experimental	3.5	1	0.040

The instability of the solitary wave (2.21) discussed above is directly related to the potential energy form of H bonds (equation (2.2)). Now we pay some attention to the potential

$$V(r) = Ar^2 - Br^3. \tag{4.9}$$

$V(r)$ is shown in figure 1 as a function of r. It is seen that V has a maximum value at $r = r_0$:

$$V_{\max} = V(r_0) = \tfrac{4}{27}(A/B)^2 A = 0.05 \text{ eV} \tag{4.10a}$$

$$r_0 = \tfrac{2}{3}(A/B) = 0.498 \text{ Å}. \tag{4.10b}$$

Prohofsky [7] has defined a quantity called the vibrational fluctuation D on each H bond, where $D = \langle uu \rangle$, and he has found that, when the H bond attains a vibrational state at $D = 0.040$ Å^2, melting occurred. In this paper we are studying only the relative vibration of the complementary bases, i.e. $u = -u'$; so, when $r = r_0$, $u = -u' = r_0/2$, and $D = r_0^2/4 = 0.0625$ Å^2. That is to say, when the vibration is beyond r_0, the H bond is broken. Since the G–C base pair has three H bonds, and the A–T base pair two H bonds, we obtain the values of energy to melt a G–C or A–T base pair by simply multiplying by 3 or 2 respectively, in equation (4.10a). The results are listed in table 1, where the experimental results [7] are also shown.

The amplitude of the solitary wave (2.21) is determined from equation (4.2), corresponding to $r = 0.74$ Å $> r_0$. Therefore, in the centre of the solitary wave, at least one H bond is melted. This is closely related to the instability of the solitary wave.

Finally, as pointed out by Yomosa [12], when $r \geq r_0$, the potential (4.9) is only valid approximately and, when $r \gg r_0$, it is incorrect. Only when $r < r_0$ is the formula justified.

5. Numerical simulation

Since the numerical simulation of sine–Gordon soliton dynamics by Currie *et al* [13], much similar work has been done [14–18]. If the kink width is of the order of the lattice spacing, a lattice-pinning effect has been observed by these researchers. The pinning effect means that the kink is pinned by the lattice. In this case the continuum approximation is no longer valid. Note that the width of the solitary wave (2.21) is of the same order as the base spacing (equation (4.8)); it is reasonable to conclude that the continuum approximation (2.7) is also no longer valid. This conclusion has been confirmed by the following numerical simulation.

Let us consider the non-linear differential-difference equation (2.6). Let u_n be in ångströms, n in units of a ($a = 3.4$ Å) and t in units of t', where

$$t' = \sqrt{M/S} = 2.27 \times 10^{-13} \text{ s}. \tag{5.1}$$

Letting $T = t/t'$, then equation (2.6) reduces to

$$d^2 u_n / d T^2 = -10u_n + 40.16(u_n)^2 + (u_{n+1} - 2u_n + u_{n-1}). \tag{5.2}$$

Let the time T be divided into $1\tau, 2\tau, 3\tau, \ldots, j\tau, \ldots$, and let $u_n(j\tau)$ be denoted by u_n^j. Taking the approximation

$$d^2 u_n / d T^2 = (u_u^{j+1} - 2u_n^j + u_n^{j-1})/\tau^2 \tag{5.3}$$

we obtain

$$u_n^{j+1} = 2u_n^j + \tau^2[u_{n+1}^j - 12u_n^j + 40.16(u_n^j)^2 + u_{n-1}^j] - u_n^{j-1}. \tag{5.4}$$

It is shown by the difference scheme that, if the displacements in the present time $T = j\tau$ and the past time $T = (j - 1)\tau$ are known, then the displacements in the future time $T = (j + 1)\tau$ can be calculated. The value of τ should be small enough to avoid possible numerical instability. Typical values of τ that we use are $0.05, 0.01, 0.001$, etc.

We use the solitary-wave solution (2.21) as the initial conditions for equation (5.4). Setting $v = c/2$, we take

$$u_n^0 = u(na, 0) = 0.37 \text{ sech}^2(n/0.55) \tag{5.5a}$$

$$u_n^1 = u_n^0 + u_t(na, t)|_{t=0}\tau \tag{5.5b}$$

$$n = -20, \ldots, 0, \ldots, +20. \tag{5.5c}$$

The evolution of u_n^j with respect to the time is shown in figure 2, where $\tau = 0.05$. The result shows that:

    (i) the solitary wave is really pinned by the lattice;

    (ii) the width of the solitary wave remains unchanged when the time increases; and

    (iii) the amplitude of the solitary wave increases quickly when the time increases and, in particular, when $T = 13\tau$, i.e. $t = 13\tau t' = 1.48 \times 10^{-13}$ s, the amplitude becomes infinite (i.e. overflow in the computer).

Note that when the amplitude is greater than r_0 (0.498 Å), the solution becomes meaningless, since the potential in equation (4.9) is incorrect in this case. In order to
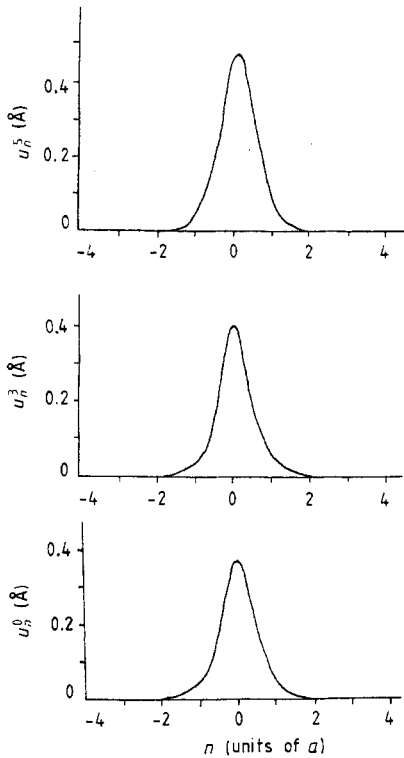
Figure 2. The evolution of the solitary wave with respect to time.

estimate the lifetime of a solitary wave more precisely, we should study the case in which the amplitude is less than r_0. Instead of equation $(5.5a)$, if we use the initial condition

$$u_n^0 = 0.24 \operatorname{sech}^2(n/0.55) \tag{5.6}$$

then the solution of equation (5.4) is really no longer divergent. We have observed an unstable breather solution, which decays into the acoustic vibration distributed in both sides of the breather. The lifetime and the frequency of the breather are 'measured' to be about 10^{-11} s and 10^{12} Hz, respectively. The lifetime τ_b of the breather is defined as usual, i.e. $|u_0^t(t = \tau_b)/u_0^0| = 1/e$. Note that the lifetime estimated by the numerical analysis under the condition $r < r_0$ is much longer than that of the analytical study. Again note that equation (2.2) is only an approximate formula describing the H-bond potential. When $r > r_0$ the potential is meaningless. We think that the Lennard-Jones potential or the Toda lattice potential may be more suitable for describing the H-bond interaction. Study of the solitary excitation of H-bonds using these potentials is in progress.

6. Discussion and conclusion

In this paper we have proposed a model for the opening motion of the bases by taking the stretching of H bonds into account. Since the potential of the H bond is non-linear, it leads to solitary-wave excitation. The solitary wave in our model looks like a 'hole' in a DNA chain, extending several base pairs long. In the centre of the solitary wave the H

bonds are broken or melted. Because of the lattice-pinning effect the velocity of the solitary wave is zero, i.e. a pinned soliton. The energy of the solitary wave is only 0.2–0.3 eV; so it can be excited by the thermokinetic energy of the surrounding molecules or by the hydrolysis of the ATP molecules (releasing an energy of 0.49 eV each time). The solitary wave in our model is unstable; it leads to the melting of several H bonds within the solitary wave. The width of the solitary wave is estimated to be one to two base pairs only. This implies that the continuum approximation in equation (2.7) is no longer valid. The numerical solution of the non-linear differential-difference equation (2.6) in fact shows a pinning effect, i.e. the solitary wave is pinned by the lattice. Such a localized solitary wave provides a suitable mechanism for transcription and drug intercalation. A localized and an unstable solitary wave means a local melting of the DNA double helix, which yields a good opportunity for drug intercalation into DNA or the transcription of the information from DNA to mRNA.

In conclusion, we have proposed a solitary-wave model of DNA, based on the stretching motion of the H bonds and its non-linear effect. The solitary wave is unstable and is pinned by the lattice. The energy of the solitary wave is so small that it can be excited by the thermokinetic energy of the surrounding molecules or by hydrolysis of the ATP molecules. The pinned solitary wave provides a suitable mechanism to explain the transcription process and drug intercalation into DNA, etc.

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