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Dynamical features of deoxyribonucleic acid and configuration transition in the transcription process

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Abstract

Biological functions and genetic features of DNA, such as duplication, transcription and gene expression, are mainly determined by its structure, but depend also on the temperature and features of solution, such as salt concentration. We study the influence of temperature and salt concentration on the conformation changes and transcription of DNA by using a new dynamical model. This new model admits three degrees of freedom per base-pair: two displacement variables related to the vibrations of hydrogen atom in the hydrogen bonds and base (nucleotide), respectively, and an angular variable related to the rotation of base. The important role of motion of hydrogen atom in the hydrogen bonds is specially stressed in this model. This is helpful to reveal the mechanism of transcription of DNA. According to their properties of motion, we first give the Hamiltonian of the system, corresponding equations of motion and their soliton-solutions. The solitons are the excitation states formed by the displacements of hydrogen atoms and bases and the rotations of bases, arising from the energy absorbed by DNA, in the systems, respectively. By applying the transfer integral method we obtain the thermodynamic properties (e.g. free energy and entropy) of the thermal excitation state of DNA at the biological temperature in this model. According to the properties of these thermodynamic functions obtained we study the mechanism and processes of melting and transcription of DNA with the aid of the transforms of energy carried by the soliton in such a case. We further give the properties of the transcription of DNA with the help of the average value of the mean square of displacement of hydrogen atom, and the values of subcritical temperature and force of the phase transition are also found. Finally, we conclude that the transcription of DNA not only depends directly on the properties of its structure and of energy absorbed by it, but also is influenced by the temperature and salt concentration in the solution of DNA, which is consistent with experimental

data. Therefore this new model not only can predict the transcription of DNA, but also can give the relationship among the conformation changes and the temperature and salt concentration. Finally we discuss in simple terms the influences of water or solution around DNA on its dynamics and further point out the defects and limitations of the new model of the dynamics of DNA and its direction of development.

1. Introduction

As is known, DNA is both a genetic matter and a carrier of genetic information, and it has important biological functions in life activity, for example, duplication, transcription and gene expression. These functions are mainly determined by its particular structure [1]. DNAs work usually in a certain physiological environment with finite temperature and in water containing salt in living systems. Experimental studies show that the properties and functions of DNA depend drastically on the temperature and salt concentration of the solution. However, these dependences are not yet clear. Therefore it is quite necessary to investigate these problems. Thus, a first problem is here to establish correctly a dynamical model appropriate to DNA.

As far as the dynamics of DNA is concerned, a lot of models have been proposed in the last 30 years. Englander *et al* [2] first suggested a theory of soliton excitations as an explanation of the open state of DNA. Later, Yomosa [3] proposed another soliton model of plane base-rotator for this open state, which was further refined by Takeno, Homma [4] and Zhang [5] by taking into account some discreteness effects and introducing the base coupling. Although these models can give solitary wave solutions with a kink shape in the continuum approximation, which could show open states of DNA [4], they were not related to the thermal denaturation of DNA since no temperature effect was considered. From analyses for the vibrational normal-mode of infrared and resonant microwave absorption [5], Raman experiments [6–9], neutron scattering [10–12] and NMR measurement, etc [13, 14], we know that the features of low frequency vibrations of DNA depend on environment conditions, e.g., water content, ionic concentration and temperature of the systems. In such a case Prohofsky and co-workers [15–19] regarded that the local 'melting' of hydrogen bonds in base pairs could be achieved through breather modes, thus a self-consistent phonon theory for the 'melting' was proposed by them based on an atomistic description of a DNA molecule and a lattice dynamics. Devoting particular attention to hydrogen bond stretching modes at 85 cm^{-1}, Prohofsky and collaborators again modified the above model to study the denaturation or melting of DNA bases, arising from breaking of hydrogen bonds linking the two complementary strands of the DNA double helix [17–19]. Prohofsky and co-workers pointed out further the essential part of strong nonlinearities and analysed the results of infrared and Raman experiments in this model. Peyrard and Bishop [20] (PB model) employed a transfer integral to analyse the statistical mechanics of the model and determine the interstrand separation in the double helix as a function of temperature. Their model allows the local 'melting' of hydrogen bonds and formation of denaturation bubbles. The local 'melting' can be analytically described as breather-like objects of small amplitude [21, 22], which can be trapped by some local inhomogeneities [23]. This suggests that the breathers could allow the formation of a transcription bubble after the interaction with the bound RNA-polymerase. As far as the geometry effects on the dynamics of DNA are concerned, Barbi *et al* [24] introduced two degrees of freedom per base-pair, a radial variable related to the opening of the hydrogen bonds and an angular one related to the twisting of each base-pair responsible for the helicoidal structure of the molecules, and derived small amplitude envelope solutions made of a breather

in the radial variables combined with a kink in the angular variables. Gaeta [25] considered the helicoidal structure of DNA and its twist and proposed further a torsion model to study its dynamics and the influences of supercoiling on its vibration spectrum. Larsen *et al* [26, 27] studied the energy funnelling effect, bubble generation and its features in a twisted and bent DNA-like model with Morse oscillators of long range coupling, respectively; some interesting results were obtained. These works are helpful to study the dynamics of DNA to a certain degree. In addition, the melting process of DNA and the influences of temperature on its dynamics have been studied by many scientists, for example, Muto *et al* [28, 29], Campa *et al* [30], Bullough *et al* [31], Feng *et al* [32], Peyrard *et al* [33], Zhang *et al* [34] and Ting *et al* [35]. Muto *et al* [28, 29] calculated the thermal equilibrium number of solitons in DNA as a function of absolute temperature and the number of base-pairs by modelling DNA as a Toda lattice with parameters chosen to match experimentally measured properties of DNA, and found that a significant number of solitons is generated at physiological temperature. Campa *et al* [30] found the melting curves of short heterogeneous DNA chains on the basis of statistical thermodynamics and the PB model: in such a case it is necessary to have not only the breaking of the hydrogen bonds between single base-pairs, but also the complete dissociation of the two strands forming the double helix. Feng *et al* [32] generalized the modified self-consistent phonon approximation to calculate the critical temperature of a DNA with block inserts of different base-pair sequences. The melting-associated behaviour is predicted to initiate in major groove bonds in the inserted adenine–thymine (A–T) base pairs at 349 K, etc. These investigations of features of DNA revealed some interesting results.

Evidently, Yomosa *et al*'s rotation model of bases [3–5] focuses only on the total dynamic features, in which these hydrogen bonds or hydrogen atoms are rudely bundled together with the bases to rotate like a rigid disc; the individual peculiarities of these components are completely ignored. Prohofsky *et al*'s [17–19] vibrational model and the PB model [20] focus only on the stretching vibrations of hydrogen bonds, ignoring the dynamic effect of the bases (nucleotides); the bases are replaced by point masses. Therefore, these models cannot completely describe the dynamical properties of DNA and need to be modified and improved further. Thus, a lot of improvements have been proposed, in which some interaction potentials governing the structure and dynamical features of DNA, for example, the Morse potential, Toda lattice potential, Lennard-Jones potential, ϕ^4-field and 2–3 or 2–3–4 power potentials, and so on, have been used to replace original potentials in these models [35–40], but the shortcomings of these models are not eliminated essentially. In such a case, it is very necessary to rethink the dynamical behaviours of DNA and reconstruct its dynamical model. In this paper we propose a new model with three modes of motion, the vibrations of hydrogen atoms and bases as well as the rotation of bases, to study the dynamical behaviours of DNA and the corresponding properties of transcription and phase transition. We suppose that this model can completely describe the dynamics of DNA, and expect that it can also give some new results. The organization of this paper is as follows. The physical and biological foundations of this model, the model Hamiltonian and solutions of equations of motion are stated in sections 2 and 3, respectively. In sections 4 and 5 we discuss the influence of temperature and salt concentration in DNA on its melting or transcription and on the phase transition of the systems by using this model, respectively. Some conclusions are given in section 6.

2. Model Hamiltonian of the dynamics of DNA

On carefully looking at the detailed molecular structure of bases (thymine (T), adenine (A), guanine (G) and cytosine (C)), as well as base-pairs (A–T and C–G) as shown in figure 1, we see that there are a lot of hydrogen bonds in DNA. The genetic information of DNA is

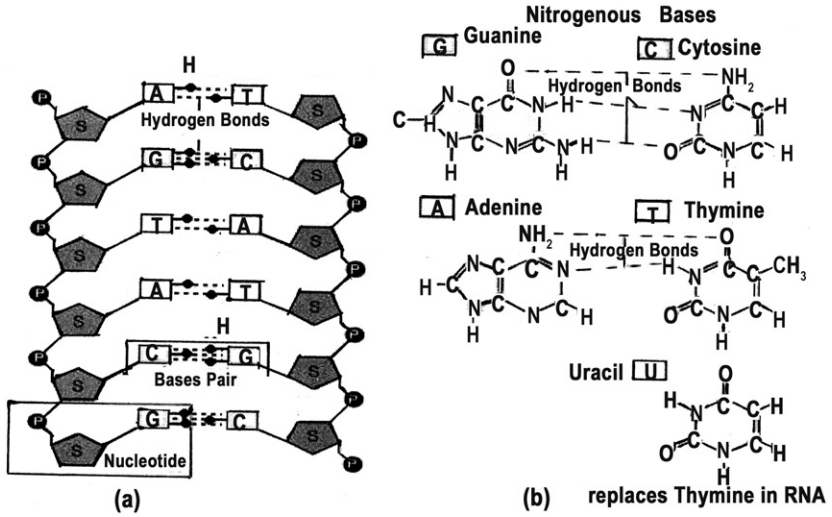

Figure 1. (a) Distribution of hydrogen bonds in DNA. (b) Hydrogen bonds for A, T, C, G bases

just carried out by the ordered arrangement of these hydrogen bonds and bases. Therefore the hydrogen bonds play an important role in the dynamics and functions of DNA, thus any changes of the order arrangement in DNA will directly influence its dynamics and functions. As is known, a hydrogen bond is made between a hydrogen atom and a strongly electronegative atom, or atom group. In DNA the hydrogen atoms associate directly with the oxygen and nitrogen atoms in the bases by hydrogen bonds. In the light of the theory of the hydrogen bond [41–44], the hydrogen atom in the hydrogen bonds is very active; it may stay around the atom on the right side or could also move to the left side under a perturbation because it interacts with not only the neighbouring base but also the complementary base in the base-pair. This motion does not change the information quantity that the DNA has. However, the hydrogen atoms can also depart from the hydrogen bonds in the form of ions and exchange further with other ions, for example, H^+, D^+ and Na^+, in the solution, when the DNA is in a solution. This feature was demonstrated in Printz *et al*'s [45] and Englander's [46–48] and Edwards *et al*'s [6] experiments (see [48–50], respectively). Meanwhile, the hydrogen atoms can also absorb infrared light or microwaves with the same frequencies as its inherent vibrations, which was verified from Martin *et al*'s and Li *et al*'s Raman and infrared spectra experiments of DNA [51, 52]. Therefore, the hydrogen atoms in the hydrogen bonds in DNA have strongly biological activity, and we cannot expect that it is the same as the motion of bases.

However, the motions of bases in DNA themselves have properties: they can both vibrate and rotate around their equilibrium positions, but cannot depart from the strands or framework of DNA to make free motion. The states of bases in B-DNA in the Watson–Crick model is schematically shown in figure 2(a), where each base attached to the strand is linked by a hydrogen bond with a complementary base in a horizontal parallel plane of distance $a_0 = 3.4$ Å; thus a base-pair is formed. In this figure each arrow shows the direction of the base, the black point denotes the hydrogen atom in the base-pairs, and the z-axis is a tenfold screw axis. In figure 2(b), each base is projected to a xy plane perpendicular to the helical axis, where B_n denotes the nth base attached to one of the two strands, and B'_n denotes the complementary base attached to the other strands. B_n and B'_n form a base-pair with a hydrogen bond in the B-DNA state. The states of hydrogen atoms are not illustrated here. In the realistic B-DNA

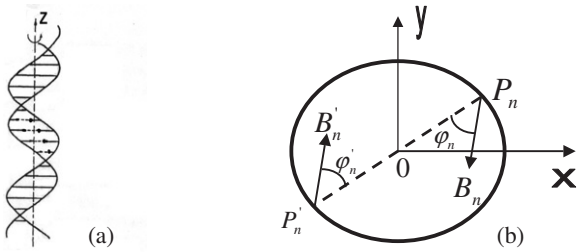

Figure 2. (a) Schematic representation of DNA in the Watson–Crick model, (b) projection of horizontal plane of the complementary pairs.

the dipole moments for the bases are larger [44]. Assuming $\mathbf{u}_A$, $\mathbf{u}_T$, $\mathbf{u}_G$ and $\mathbf{u}_C$ to be the dipole moments of the bases A, T, G and C, respectively, then they are about 5.755–6.44 Debyes for the A–T base-pair and 6.004–6.483 Debyes for the G–C base-pair, respectively. Since each base is denoted by an arrow, then the directions of these dipole moments are either parallel or antiparallel to the base arrows. According to Devoe and Tinoco's results [53], the G–C dipoles attract while the A–T dipoles repel between the coplanar bases in a base-pair. Thus, u_A and u_T are in a form of head to head, while u_G and u_C are arranged in the form of head to tail. In this physical image, the bases can both vibrate and rotate. This vibration arises from the motion of hydrogen atoms through electromagnetic interaction between them. The rotation is due to the interaction of the base with neighbouring bases, which is a foundation forming the open states or generating the duplication and transcription of DNA. This effect was proved by hydrogen–deuterium exchange measurement [54–58].

In accordance with above different features of motion for the hydrogen atom and bases it is very necessary to distinguish the states of motion of hydrogen atoms from the those of bases, and take into account the motion of hydrogen atoms independently, instead of combining them together [59]. This is the reason why we propose here a new dynamic model of nonlinear excitation of DNA, in which we introduce three different variables (three degrees of freedom) for each base-pair, i.e., displacement of the hydrogen atom, u_n, describing its vibrations, the displacement of the base (nucleotide), R_n, denoting its harmonic state, and the rotation angle of the base, φ_n, exhibiting its rotation. The direction of B_n in the horizontal plane is just specified by the rotation angle, φ_n, around the axis L_n which passes through the point where the base B_n is attached to the strand and is parallel to the z-axis. According to these properties of motions for the three modes of motion we represent the Hamiltonian of the systems by

$$H = H_h(u_n) + H_b(R_n) + H_t(\varphi_n) + H_{\text{int}} \tag{1}$$

where H_h, H_b, H_t and H_{int} are the Hamiltonians corresponding to the motion of the hydrogen atom, linear harmonic motion and rotation of the base, as well as the coupling interactions between the vibrations of the hydrogen atom and the base, respectively. H_h, the vibrational Hamiltonian of the hydrogen atom, contains an on-site nonlinear potential and resonant or dipole–dipole interaction of the hydrogen atom in site n with that in its neighbouring base-pair, and is represented by

$$H_h = \sum_n \left[\tfrac{1}{2}mu_n^2 + \tfrac{1}{2}m\omega_0^2u_n^2 + V(u_n) - Ju_nu_{n-1}\right] \tag{2}$$

where $p_n = m\dot{u}_n$ is the momentum of the hydrogen atom at the nth site, m is its mass, and ω_0 is its frequency of harmonic vibration, $V(u_n)$ is the nonlinear potential of the hydrogen atom arising from the interaction with the complementary bases in the nth base-pair; it may be denoted by a Morse potential, double-Morse potential or double-well potential. The last term,

$-Ju_nu_{n-1}$, in equation (2) describes the resonant or dipole–dipole interaction of the hydrogen atom in the nth base-pair with those in its neighbouring base-pair [41–44], J is a constant of this interaction, and it can be denoted by $J = q^2/4\varepsilon_0\pi r'^3$, where q is the charge transfer due to the displacement of the hydrogen atom. r' is the distance between neighbouring hydrogen atoms and ε_0 is the dielectric constant of the systems.

H_b is the Hamiltonian of harmonic vibration of the nth base, and is denoted by

$$H_b = \sum_n \left[\tfrac{1}{2}M\dot{R}_n^2 + \tfrac{1}{2}W(R_n - R_{n-1})^2\right] \tag{3}$$

where $P_n = M\dot{R}_n$ is the momentum of the base at the nth site. M is its mass, and W is the spring constant of the strain mode of the sugar ring and phosphate backbone in DNA.

H_t is the Hamiltonian of rotation of bases, and is given by

$$H_t = \sum_n \{\tfrac{1}{2}I\dot{\varphi}_n^2 + \beta_1[3(1 - \cos\varphi_n\cos\varphi_{n-1}) - (1 - \cos(\varphi_n - \varphi_{n-1}))] + B[1 - \cos(\varphi_n - \varphi_{n-1})] + \lambda[(1 - \cos\varphi_n) + (1 - \cos\varphi_{n-1})]\} \tag{4}$$

where $\varphi_n(t)$ is the rotation angle of the base at the nth site, and I is the mean value of the moments of inertia of bases in the rotation around the axis L_n which is parallel to the helical axis and passes through the point where the base B_n is attached to the backbone. The second term, $\beta_1[3(1 - \cos\varphi_n\cos\varphi_{n-1}) - (1 - \cos(\varphi_n - \varphi_{n-1}))]$, represents the permanent dipole–dipole interaction between two neighbouring bases, which can be obtained from the interaction energy formula: $[\mathbf{u}_1 \cdot \mathbf{u}_2 - 3(\mathbf{u}_1 \cdot \mathbf{r})(\mathbf{u}_2 \cdot \mathbf{r})/r^2]/r^3$, where $\mathbf{u}_1$ and $\mathbf{u}_2$ are the dipole moments of the transversally neighbouring bases G and A, or C and T. $\mathbf{r}$ is the distance between them and the interaction constant β_1 can be denoted by $\beta_1 = u_1u_2/r^3$. $B[1 - \cos(\varphi_n - \varphi_{n-1})]$, which is the sum of the stacking energy between intrastrand adjacent bases and the torsional energy of the nucleotide strand [3] which is a function of the relative torsional angles between adjacent bases, where B is the interaction constant; its value in the equilibrium state of B-DNA is taken as zero. The stacking energy of the bases plays an important role for stabilizing the double helix structure of DNA. $\lambda[(1 - \cos\varphi_n) - (1 - \cos\varphi_{n-1})]$ denotes the inducting dipole–dipole interaction between transversally neighbouring bases, with λ being a coupling constant.

As is known, there is an interaction, such as electromagnetic interaction, between the hydrogen atom and the base in DNA. Thus, the displacement of the position of the hydrogen atom results necessarily in a change of position of the bases. Then, the interaction Hamiltonian between them, H_{int}, is often represented in the following form:

$$H_{\text{int}} = \sum_n [m\chi_1 u_n^2(R_n - R_{n-1})] \tag{5}$$

where χ_1 is the coupling constant. It expresses the change of relative position of neighbouring bases due to the vibration of the hydrogen atom. This amounts to assuming that the frequency of vibration of the hydrogen atom is affected by the changes of positions of bases, i.e.,

$$\omega^2(R_n - R_{n-1}) = \omega_0^2 + (\partial\omega^2/\partial R_n)\,(R_n - R_{n-1}) = \omega_0^2 + \chi_1(R_n - R_{n-1}),$$
$$\text{where } \chi_1 = \partial\omega^2/\partial R_n,$$

on using this representation to replace ω_0^2 in the second term in rhs in equation (2) we easily obtain equation (5). Hence, equation (5) has a clear physical meaning.

As far as the interaction between the vibrational and rotational modes for the base is concerned, we regard simply that this interaction results only in the change of coupling constant, λ, due to variations of the positions of the bases, i.e., $\lambda = \lambda_0 + \chi_2(R_n - R_{n-1})$, where λ_0 is the normal coupling constant of dipole–dipole interaction between neighbouring bases, which represents the dynamic contribution due to the changes of dipole–dipole interaction between neighbouring bases arising from the vibration of bases.

The above Hamiltonian differs from both the PB model and Yomosa's rotated model. In the PB model [20] the base is a point mass allowed to move only in the direction of hydrogen bonds that connects them (a Morse potential was used to describe the effects of these bonds), while neighbouring bases along the same strand are harmonically coupled. In our model the hydrogen atom in the hydrogen bond is in optical vibration in a potential field of the double potential well, providing by two neighbouring complementary bases, and is affected by resonant or dipole–dipole interaction between transversally neighbouring hydrogen atoms; the vibration of bases with a certain dipole moment is harmonic, but is influenced by the vibration of the neighbouring hydrogen atom via electromagnetic interaction; the base can also rotate under the actions of permanent dipole–dipole interaction, inducting dipole–dipole interaction and stacking energy between transversally neighbouring bases, and the rotations of bases are modulated by self-vibration. Therefore the motion of bases is also different from that in Yomosa's base-rotation model. In our model the base can not only vibrate, but also rotate, and is also coupled with the vibration of hydrogen atoms. Through the coupling between the hydrogen atom and base as well as the coupling between the vibration and rotation of bases, the three motion modes form an organic entity to perform the functions of DNA, for instance, duplication and transcription. Thus, the dynamics of DNA in this model can be described as follows. Under the stimulation of an externally applied field or energy, the hydrogen atoms in the hydrogen bonds deviate from their equilibrium position to vibrate. Thus the base vibrates also along with the vibrations of hydrogen atoms due to the electromagnetic interaction between them. Then the dipole moment of the base is changed; thus the base begins to rotate under the influences of inducting dipole–dipole interaction and stacking energy between transversal bases. In this process the base-pairs nearby the vibrational base are distorted; thus a breather bubble occurs, and the transcription begins. If the breather bubble with energy moves along the DNA chains, the complementary base-pairs at the ends of DNA can be opened. Then the duplication of DNA takes place. Hence, the dynamics of DNA is carried out by a organic combination or synthesis of three mobile modes, instead of simple vibration or rotation. Therefore this model is not a combination of Prohofsky *et al*'s [17–19] and Peyrard and Bishop's [20] vibrational model and Yomosa's plane base-rotator model, but a renovation of biophysical concept and idea. The new model has the following features: (1) the important role of hydrogen atoms in the hydrogen bonds is stressed; (2) the dynamics of DNA is a result of highly correlated interaction of the three mobile modes; (3) the model provides a more realistic description of the interactions in DNA dynamics. Thus we can expect that the model is able to predict some new dynamic properties of DNA.

3. Equation of motion and corresponding solutions

Utilizing the formulae $\partial H/\partial u_n(t) = -p_n(t)$, $\partial H/\partial R_n(t) = -P_n(t)$ and $\partial H/\partial \varphi_n(t) = -I\ddot{\varphi}_n(t)$, and using equations (1)–(5), we can find the equations of motion for $u_n(t)$, $R_n(t)$ and $\varphi_n(t)$. They are

$$m\ddot{u}_n = -m\omega_0^2 u_n + J(u_{n+1} + u_{n-1}) - \frac{\partial V(u_n)}{\partial u_n} - 2m\chi_1 u_n(R_n - R_{n-1}) \tag{6}$$

$$M\ddot{R}_n = W(R_{n+1} + R_{n-1} - 2R_n) - m\chi_1(u_{n+1}^2 - u_n^2) \tag{7}$$

$$I\ddot{\varphi}_n = (B - \beta_1)(\varphi_{n+1} + \varphi_{n-1} - 2\varphi_n) - 3\beta_1(\cos\varphi_{n-1}\sin\varphi_n + \cos\varphi_{n+1}\sin\varphi_n) - \lambda(\sin\varphi_n + \sin\varphi_{n+1}) \tag{8}$$

respectively. In the continuum approximation, the above equations become

$$m\ddot{u}(z,t) = (-2J - m\omega_0^2)u + Jr_0^2\frac{\partial^2 u}{\partial z^2} - \frac{\partial V(u)}{\partial u} - 2mr_0\chi_1 u\frac{\partial R}{\partial z} \tag{9}$$

$$M\ddot{R}(z,t) = r_0^2 W \frac{\partial^2 R}{\partial z^2} - r_0 m \chi_1 \frac{\partial u^2}{\partial z} \tag{10}$$

$$I\ddot{\varphi}(z,t) = r_0^2(B-\beta_1)\frac{\partial^2 \varphi}{\partial z^2} - 3\beta_1 \sin 2\varphi - 2\left(\lambda_0 + r_0\chi_2 \frac{\partial R}{\partial z}\right)\sin\varphi. \tag{11}$$

If let $\xi = z - vt$, then from equation (10) we can get

$$\frac{\mathrm{d}R}{\mathrm{d}\xi} = \frac{\partial R}{\partial z} = -\frac{mr_0\chi_1}{Mv_0^2(1-s^2)}u^2 + g \tag{12}$$

where $s = v/v_0$, $v_0 = r_0(W/M)^{1/2}$, r_0 is the distance between neighbouring base-pairs in the z-direction and g is the integration constant. Substituting equation (12) into equations (9) and (11) we can get

$$m\ddot{u}(z,t) = -C_0 u + Jr_0^2 \frac{\partial^2 u}{\partial z^2} - \frac{\partial V(u)}{\partial u} + D_0 u^3 \tag{13}$$

and

$$I\ddot{\varphi}(z,t) = r_0^2(B-\beta_1)\frac{\partial^2 \varphi}{\partial z^2} - 3\beta_1 \sin 2\varphi - 2(gr_0\chi_1 + \lambda_0)\sin\varphi + N_0 u^2 \sin\varphi \tag{14}$$

where $C_0 = (m\omega_0^2 + 2J + 2gmr_0\chi_1)$, $D_0 = 2m^2 r_0^2 \chi_1^2 / Mv_0^2(1-s^2)$, $N_0 = 2m\chi_1\chi_2 r_0^2 / Mv_0^2(1-s^2)$.

We can find the solutions of equations (13) and (14), when the $V(u)$ in equations (9)–(13) is known. We here give two kinds of different potentials to discuss the features of solutions of above equations.

(1) $V(u_n)$ is the following double-Morse potential with two different well-depths,

$$V(u) = U_1[1 - \exp(-\alpha u_n)]^2 + U_2\{1 - \exp[-\alpha(u_n - b)]\}^2 \tag{15}$$

where U_1 and $U_2 < U_1$ are the depths of the two wells at $u = 0$ and $u = b$ ($b > 0$), respectively. $\alpha = 1.8$ Å^{-1} and $U_1 = 0.15$ eV for a hydrogen bond. This potential is appropriate to the hydrogen atoms in the hydrogen bonds, because they stay usually in the side of the base, but may move to another side of a complementary base, which is only a metastable state of hydrogen atom. This amounts to the double-well potential having two wells with different depths: the hydrogen atoms stay usually in the potential well with large depth. However, the resulting equations are very difficult to solve in such a case. To make the equations solvable, we expand the above double-Morse potential as a power series and keep only a finite number of terms in this expansion. Using up to the fourth-order term in the power series, then equation (13) can be written, in the continuum approximation, as

$$\ddot{u}(z,t) = A_1 + C_1 u + B_1 u^2 + v_1^2 \frac{\partial^2 u}{\partial z^2} + D_1 u^3 \tag{16}$$

with $A_1 = bU_2\alpha^2(6\alpha b - 2 - \alpha^2 b^2)/m$, $C_1 = \{[U_1 + U_2(1 - 3b\alpha + 3b^2\alpha^2/2)] - C_0\}/m$,

$v_1 = r_0(J/m)^{1/2}$, $B_1 = \alpha^3(U_2 - U_1 - U_2 b\alpha)/m$, $D_1 = (\alpha^4(U_1 + U_2) - D_0)/m$.

This is a 2–3–4 equation, and can be solved by a multiple scale expansion [17–20], but here we solve it directly by the following method. Making the variable transformation $\xi = (\sqrt{D_1}\gamma/v_1)(z - vt)$, and assuming $\gamma = (1 - v^2/v_1^2)^{-1/2}$, and

$$F(u) = -\frac{\partial V'(u)}{\partial u} = A_1/D_1 - (C_1/D_1)u + (B_1/D_1)Qu^2 + u^3,$$

where $F(u)$ has two or three different real roots, which implies that $V'(u)$ has one maximum and one reflection point, or two maxima and one minimum, then equation (16) has the solutions

of a solitary wave [41–44]. Through an appropriate transformation, equation (16) can be denoted by

$$\frac{\mathrm{d}^2u}{\mathrm{d}\xi^2} = F(u) = (u-u_1)(u-u_2)(u-u_3) \tag{17}$$

where u_1, u_2 and u_3 are three roots of $F(u)$. The soliton solution can be represented by [59, 60]

$$u(z,t) = \frac{(u_j-u_i)}{\{1+\exp[(k\gamma\sqrt{D_1}/v_1)(z-vt-z_0)]\}+u_i} \tag{18}$$

where $k = (\varepsilon'/\sqrt{2})(u_i-u_j)$, $v = \varepsilon'(u_i+u_j-2u_k)$, $\varepsilon' = \pm 1$, z_0 is constant, $i, j, k = 1, 2, 3$, but $u_i \neq u_j$, $u_3 \neq 0$, and u_k is the third solution of u in $F(u)$. The above solution can be written by

$$u(z,t) = u_0\{1-\tanh[(k\gamma\sqrt{D_1}/v_1)(z-vt-z_0)/2]\}, \qquad u_0 = (u_i-u_j)/2. \tag{19}$$

Thus

$$R(z,t) = \left[\frac{mr_0\chi_1u_0^2}{Mv_0^2(1-s^2)k}\right]\{(-\tanh[(\gamma\sqrt{D_1}k/v_1)(z-vt-z_0)] - \operatorname{Ln}\cosh^2[(\gamma\sqrt{D_1}k/v_1)(z-vt-z_0)]\} \tag{20}$$

where the integrating constants are set to be zero.

If we insert equation (19) into (14), then equation (14) becomes very difficult to solve. At present, we first find an approximate solution for it, i.e., we replace the u with its amplitude u_0. Thus equation (14) becomes the following double sine–Gordon equation [59, 60]:

$$I\ddot{\varphi}(z,t) = r_0^2(B-\beta_1)\frac{\partial^2\varphi}{\partial z^2} - 3\beta_1\sin 2\varphi - 2(gr_0\chi_1+\lambda_0-N_0u_0^2/2)\sin\varphi \tag{21}$$

$Z = (\gamma_1/q)(z-ct)$, $q^2 = r_0^2(B-\beta_1)/(gr_0\chi_1+\lambda_0-N_0u_0^2/2)$, $\gamma_1 = (1-c^2/c_0^2)$, let

$$c = [(B-\beta_1)/I]^{1/2}r_0, \qquad \rho = 3\beta_1/[4gr_0\chi_1+4\lambda_0-2N_0u_0^2] \tag{22}$$

and then equation (21) becomes

$$\frac{\partial^2\varphi}{\partial z^2} - \frac{1}{c_0^2}\frac{\partial^2\varphi}{\partial t^2} - \frac{1}{q^2}[2\rho\sin 2\varphi+\sin\varphi]. \tag{23}$$

Its soliton solution is of the form

$$\varphi(Z,t) = 2\tan^{-1}\{\pm(1-4\rho)^{-1/2}\operatorname{cosech}[(1+4\rho)^{1/2}Z]\} \tag{24}$$

where $+$ and $-$ correspond to the kink and antikink, respectively. The profiles of the solitary waves, equations (19), (20) and (24), are shown in figure 3.

(2) The following double-well potential with different well-depth also is often adopted:

$$V(u) = A[(a-u(z,t))(b-u(z,t))]^2. \tag{25}$$

Its two minimum values are at a and b, and the height of barrier is $(ab)^2A$. Inserting this potential into equation (13), we find that it becomes equation (16), except its coefficients have some differences. Thus it is not necessary to study the solutions of the equations further. On letting $a = -b$, we can get

$$\ddot{u}(z,t) = -C_2u + v_1^2\frac{\partial^2u}{\partial z^2} + D_2u^3 \tag{26}$$

with $C_2 = [C_0-(4a^4A)]/m$, $v_1 = r_0\,(J/m)^{1/2}$, $D_2 = (D_0-4Aa^4)/m$. The soliton solution of equation (26) can be easily found. If let $\xi = z-vt$, the solution is of the form [59, 60]

$$u(z,t) = (C_2/D_2)^{1/2}\tanh[\mu(z-vt)], \qquad \mu = [C_2/2(v_1^2-v^2)]^{1/2}. \tag{27}$$

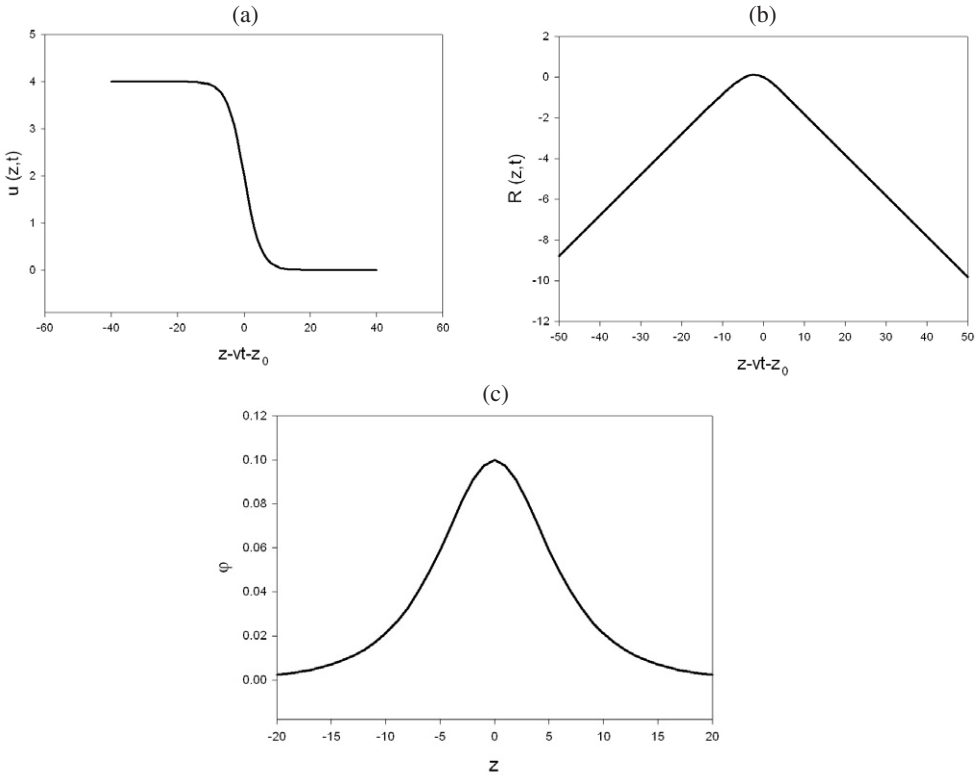

Figure 3. Plots of the solutions for equations (19) (a), (20) (b) and (24) (c), respectively.

From equation (12) we get

$$R(z,t) = -\{[\sqrt{2}m\chi_1 r_0/Mv_0^2(1-s^2)][C_2(v_1^2-v_0^2)/D_2^2]^{1/2}\}\tanh[\mu(z-vt)], \tag{28}$$

where $g = r_0 m C_2 \chi_1 / M v_0^2 (1-s^2) D_2$.

On inserting equation (27) directly into (14), the solution of equation (14) is found to be very difficult. If still adopting the above method, we can first seek an approximate solution. Now replacing the u^2 with its amplitude (C_2/D_2) in equation (14), equation (14) becomes the following double sine–Gordon equation:

$$I\ddot{\varphi}(z,t) = r_0^2(B-\beta_1)\frac{\partial^2\varphi}{\partial z^2} - 3\beta_1 \sin 2\varphi - 2(gr_0\chi_1 + \lambda_0 - N_0C_1/2D_1)\sin\varphi. \tag{29}$$

This equation is the same as equation (21) except for its coefficients. Therefore its solution can be immediately written by [59, 60]

$$\varphi(Z,t) = 2\tan^{-1}\{\pm(1-4\rho_1)^{-1/2}\,\mathrm{cosech}[(1+4\rho_1)^{1/2}Z]\} \tag{30}$$

where + and − correspond to the kink and antikink, respectively.

$$\begin{aligned} &Z = (\gamma_1/q)(z-ct), \qquad q_1^2 = r_0^2(B-\beta_1)/(gr_0\chi_1 + \lambda_0 - N_0C_1/2D_1), \\ &\gamma_1 = (1-c^2/c_0^2), \\ &c = [(B-\beta_1)/I]^{1/2}r_0, \qquad \rho_1 = 3\beta_1/[4gr_0\chi_1 + 4\lambda_0 - 2N_0C_1/D_1]. \end{aligned} \tag{31}$$

These solutions, equations (27) and (28), are shown in figure 4, but the shape of solution (30), which is not shown here, is similar to that of equation (24). From the above results we know that

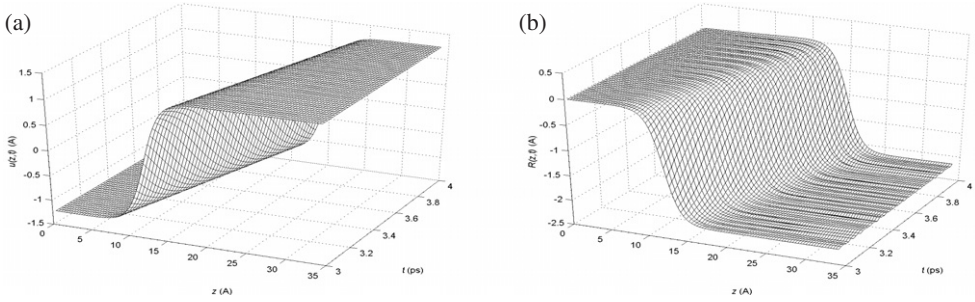

Figure 4. Images of soliton solutions equations (27) (a) and (28) (b).

the states and properties of motions of hydrogen atoms and of bases are different for different potential forms of hydrogen atom. The main features of their motions can be summarized as follows. The vibrational motions of hydrogen atoms can be easily stimulated. When influenced by an external field or the energy released in ATP hydrolysis, the hydrogen atoms will leave their equilibrium positions, which results in a propagation of solitary waves or the motion of kink-like solitons carrying the vibrational energy along the DNA chains. Due to the interbase interaction, in such a case the vibrations and rotations of the base occur, which can result in collective reversal of bases in the DNA double helix and promote the opening of the base-pairs at the ends of DNA double helix. These motions not only provide a mechanism for the transportation of energy and information in DNA for performing its biological functions, but also serve as a precursor for biological processes such as the denaturation or melting, duplication and transcription of DNA. In the following we apply the above results to discuss these important processes in more detail.

4. Transcription of DNA and influences of temperature on the transcription

What is the transcription of DNA? In the light of molecular biology, it is the process in which the genetic information of DNA is transcribed into mRNA, which in turns instructs the arrangement of amino acid molecules on the protein molecules through translation of RNA. The total process is referred to as gene expression of DNA. This chain law of genetic information is called the central rule of life. Therefore, the transcription is an elementary and main process and it has an important role in life activity. As is known, the first and key step of the transcription is the denaturation or melting of DNA, i.e., the double helix chains of DNA open and separate further into two single chains; subsequently mRNA with one chain comes into the middle of the opening DNA and incorporates with a single chain in DNA. This single chain of DNA serves as a template of transcription to transcribe itself genetic information into the mRNA. In this process, a basic 'step' is to fuse a DNA nucleotide to the growing RNA transcription. In each step a DNA base-pair is split on the downstream side, and a DNA–RNA hybrid base-pair is then formed. A DNA–RNA hybrid base-pair is split, a DNA base-pair upstream is reformed, and a polymerization event in the RNA backbone occurs. As mentioned in the introduction, many scientists [26–34] have studied the properties of the melting or transcription of DNA in some models; however, it is very difficult to explain this process completely. Here we will use the above model to study the essence and properties of this phenomenon.

Obviously, the opening process of double chains of DNA is due to the fact that the hydrogen atoms in the base-pairs leave their normal positions. The so-called 'melting' of DNA is just a highly cooperative thermal disruption of hydrogen bonds between complementary

bases in the double helix at the biological temperature [1, 18, 19]. As a result of the backbone chemistry, a pyrophosphate group is removed from the nucleoside triphosphate which is the source of the added RNA section. The pyrophosphate group is later hydrolysed but not at the site directly connected to the other operations. The overall energy flow in the transcription complex is such that on average 0.5 kcal mol^{-1} transcribed energy must be absorbed by the complex from its surroundings. The free energy needed to melt a G–C base-pair is accepted to be 3.5 kcal mol^{-1} and that for an A–T base pair is 1 kcal mol^{-1} [61]. In general, this energy is provided by the bio-energy released in ATP hydrolysis which is transported through the protein molecules in the chromatins, or by the external applied field such as infrared and ultraviolet light absorbed. The question is how the energy is absorbed by the DNA molecule. Obviously, it can be only accepted by the hydrogen atoms in the hydrogen bonds because its intrinsic frequencies of vibration match those of ATP hydrolysis or infrared and ultraviolet light [50–52]. Therefore, above new model benefits in understanding and explaining this process, and it can exactly reveal the mechanism of denaturation and melting of DNA. More precisely, when an externally applied energy is accepted by the hydrogen atoms in DNA working at biological temperature, they leave their equilibrium positions to vibrate thermally. Then the bases, which associate the hydrogen atoms through the hydrogen bonds, vibrate correspondingly due to the interaction between them. The vibrations of these bases change their dipole moments and induce dipole–dipole interaction between neighbouring bases on the same strand. The rotation of bases is then initiated. The electromagnetic interaction between the hydrogen atoms in neighbouring base-pairs makes the solitary waves to propagate along DNA chains. This results in more hydrogen atoms deviating from their equilibrium positions. At the same time, more bases rotate and a rotation wave is generated due to the stacking and dipole–dipole interactions between neighbouring bases. Thus these hydrogen atom leave their normal positions, the double helix chains of DNA open and separate further into two single chains; thus the melting occurs, and the transcription of DNA begins. This phenomenon is generated, in general, at the ends of a DNA double helix. Very clearly, this melting or transcription is initiated and motivated due to the fact that the hydrogen atoms in the base-pairs leave their normal positions to move thermally. Hence the above melting of DNA arising from the energy absorbed is a biomolecular dissociation process, wherein the initial state is a duplex and the final state is the separated single strands. Therefore the above model is very helpful in explaining the transcription of DNA. However, since DNA lies always in physiological solution and works at the biological temperature, we can think that DNA's melting is like a first-order phase transition, in which there are increases of volume and changes of thermodynamic features of DNA including the increase of entropy and release of latent heat. Thus, we must further study the states and thermodynamic features of DNA working at the biological temperature and the influences of temperature on the motion of hydrogen atoms in the base-pairs by the above theory in order to understand the transcription.

From the above analysis we know that for the melting and transcription we should mainly pay attention to and study the states of hydrogen atoms and their changes at the biological temperature (here we have not especially studied the influence of motion of bases, which are always attached to the strands and cannot move freely, on the transcription; however, we do not ignore their effects on the states and motion of hydrogen atoms because these effects were considered and embodied already through the interaction Hamiltonian in our model). However, the effect of temperature of medium on the solitons is not considered in the above model, thus we now have to generalize this model into the DNA systems at physiological temperatures to study the influences of the temperature of medium on the states of hydrogen atoms and corresponding changes of thermodynamic features of the systems.

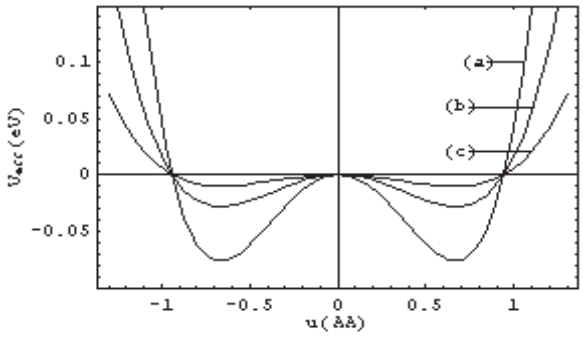

Figure 5. The effective potential of a hydrogen atom and its change versus the salt concentration. Here a, b and c represent the values at $\eta = 0$, 1 and 2 respectively.

From equation (26) or (16) we get the following effective potential of the hydrogen atom in this model:

$$U_{\text{eff}}[u(z,t)] = -\tfrac{1}{2}C_2u^2 + \tfrac{1}{4}D_2u^4. \tag{32}$$

It has two ground states at $u_{\min} = \pm(C_2/D_2)^{1/2}$; the ground state energy is $E_0 = -(C_2^2/4D_2)$, which is shown in figure 5. This is, in general, the lowest energy state of DNA, which corresponds to the B-DNA form with high order. However, the soliton state mentioned above is an excitation state because the energy of the soliton, equation (27), is [59, 60]

$$E_{\text{sol}} = \frac{1}{r_0}\int_{-\infty}^{\infty} \mathrm{d}zm\left[\frac{1}{2}u_t^2 + \frac{1}{2}v_1^2u_z^2 + \frac{D_2}{4}u^4 - \frac{C_2}{2}u^2\right] = \frac{4mv_1C_2^{3/2}}{3\sqrt{2}D_2r_0(1-s_1^2)^{1/2}} > 0,$$
$$(s_1 = v/v_1). \tag{33}$$

This result means that the above soliton is formed, when the DNA absorbs the energy

$$\Delta E = E_{\text{sol}} - E_0 = \frac{mC_2^{3/2}}{D_2}\left[\frac{4v_1}{3\sqrt{2}r_0(1-s_1^2)^{1/2}} + \frac{C_2^{1/2}}{4}\right] > 0 \tag{34}$$

from the environment. Thus we can also say from this result that the hydrogen atoms, or the DNA system, lies in an excitation state after the solitons appear. If we choose the values of parameters for the systems to be [17–24] $m = m_{\text{p}}$, $M = 300m_{\text{p}}$, $J = (0.11\text{–}0.25)$ eV Å^{-2}, $\omega_0 = (10 - 300)$ cm^{-1}, $(a^4A) = (0.15\text{–}0.33)$ eV, $W = (0.11\text{–}0.31)$ eV Å^{-2}, $a = 1$ Å, $r_0 = (3.4 - 6)$ Å and $\chi_1 = (1 - 3) \times 10^{37}$ (S^2 m)$^{-1}$, then the dependence of the energy difference, ΔE, on the velocity of hydrogen atom, v, can be found, which is shown in figure 6(a). From this figure we see that the absorbed energy increases with increasing velocity of hydrogen atom; in other words, the larger its velocity, the more the energy absorbed by the DNA. Because the DNA works at the biological temperature, these hydrogen atoms are essentially in a thermal excitation state: namely, the absorbed energy increases the displacements of hydrogen atoms, then also enhances their energies of thermal motion; thus the temperature of the DNA system increases. This is necessary to result in the melting of DNA. In this condition, the thermodynamic features of the system, containing free energy and entropy, will be changed. Thus we have to generalize the above model into a thermal DNA system to study the changes of thermodynamic features on melting. We treat these problems by using a transfer integral method and statistical physical method [62–64] and the theory of first-order phase transitions.

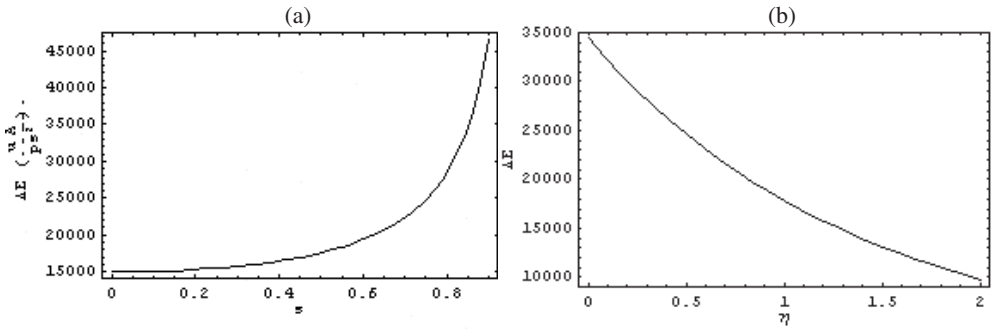

Figure 6. The excitation energy of a soliton with respect to the ground state and its changes along with the velocity in (a) and the variations of salt concentration in (b), respectively.

We now write the effective Hamiltonian of hydrogen atoms corresponding to equation (26) by

$$H_{\text{eff}} = \frac{1}{r_0}\int \mathrm{d}zm\left[\frac{1}{2}u_t^2 + \frac{1}{2}v_1^2u_z^2 + \frac{D_2}{4}u^4 - \frac{C_2}{2}u^2\right] \tag{35}$$

(the functions of motion of bases on the hydrogen atoms were already considered in this formula). The discrete form corresponding to it can also be written. In accordance with statistical physics methods, the classical partition function corresponding to equation (35) in the field variables $u(z,t)$ and $p(z,t) = mu_t(z,t)$ can be expressed by

$$Z(\beta, L) = \int \mathrm{d}p \int \mathrm{d}u e^{-\beta H_{\text{eff}}} = Z_p Z_u, \qquad \beta = 1/K_{\text{B}}T \tag{36}$$

where L is the length of the systems, T is the temperature of the systems, K_{B} is the Boltzmann constant, and

$$Z_p = \int \mathrm{d}p\, \mathrm{e}^{-\beta E_p} = (2\pi m K_{\text{B}}T)^{N/2}, \qquad Z_u = \int \mathrm{d}u\, \mathrm{e}^{-\beta E_u} \tag{37}$$

with $E_p = \int_0^L \mathrm{d}z(p^2/2)$, $E_u = \int_0^L \mathrm{d}zm[v_1^2u_z^2/2 + D_2u^4/4 - C_2u^2/2]$, $H_{\text{eff}} = E_p + E_u$.

The above integrals can be evaluated exactly in the thermodynamic limit of a large system containing N base-pairs ($N \to \infty$) using the eigenfunctions and eigenvalues of a transfer integral operator [62–64]

$$\int \mathrm{d}z_{i-1}\, \mathrm{e}^{-\beta m C_2 F_u(u_i, u_{i-1})}\psi_i(u_{i-1}) = \mathrm{e}^{-\beta m C_2 \varepsilon_i}\psi_i(u_i) \tag{38}$$

where $F(u_i, u_{i-1})$ relates to the potential-energy component E_u. This calculation is similar to the one performed by Krumhansl and Schrieffer [62] and Schneider and Stoll [64], where the $\psi_i(u)$ and ε_i satisfy the following equation:

$$\left[-u^2 + (D_2/C_2)u^4 - (r_0^2/2\beta^2m^2C_2v_1^2)\frac{\mathrm{d}^2}{\mathrm{d}u^2}\right]\psi_i(u) = (\varepsilon_i - h_0)\psi_i(u) \tag{39}$$

with $h_0 = (1/2mC_2\beta)\ln(mv_1^2\beta/2\pi)$. We here assume that $m^* = m^2C_2v_1^2/r_0^2K_{\text{B}}^2T^2)$. Since the single-site potential in equation (39) is bounded from below, the eigenspectrum is also bounded from below; then we denote the lowest eigenvalue of the above Schrödinger equation by ε_0, which is

$$\varepsilon_0 = h_0 + (2m^*)^{-1/2}\left\{1 \pm \frac{1}{2}\exp\left[-\frac{w_0\beta}{r_0}(m^2v_1^2C_2^2/2D_2)^{1/2}\right]\right\}, \qquad \beta = 1/K_{\text{B}}T. \tag{40}$$

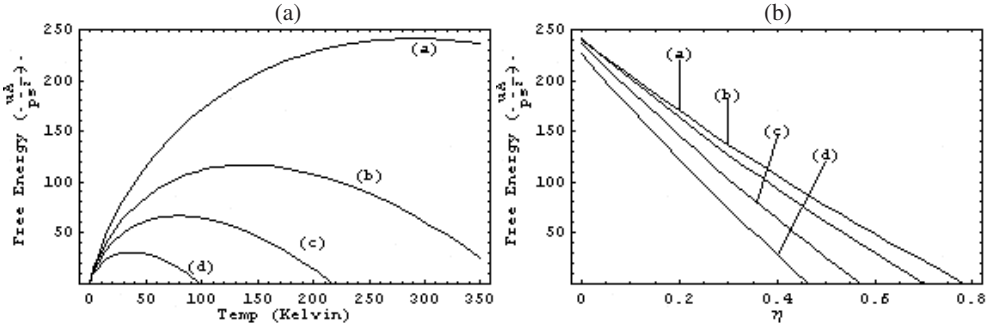

Figure 7. Dependences of free energy on the temperature (a) and salt concentrations (b) in the melting state of DNA. In (a), a, b, c and d are the values at $\eta = 0$, 0.5, 1 and 2, respectively. In (b), a, b, c, and d, are the values at $T = 273$, 300, 350, and 400 K, respectively.

Then, in the thermodynamic limit we can approximately get

$$Z_u = \exp[-\beta N m C_2 \varepsilon_0]. \tag{41}$$

Thus

$$Z = (2\pi m K_B T)^{N/2} (2\pi/\beta m v_1^2)^{N/2} (2q_1 \cosh g_0)^{N/2} \tag{42}$$

where

$$\begin{aligned} q_1 &= \exp[-4q_4], \qquad & g_0 &= q_4 \exp[-\beta q_3], \\ q_4 &= r_0\sqrt{2C_2}/4v_1, \qquad & q_3 &= \frac{w_0}{r_0}(m^2 v_1^2 C_2^2/2D_2)^{1/2}, \end{aligned} \tag{43}$$

where w_0 is the width of the barrier of the double-well potential. Then the free energy per particle for the DNA can be found, and it is of the form

$$f = -\tfrac{1}{2} K_B T \{\mathrm{Ln}[2^2\pi^2 (K_B T)^2/v_1^2] + \mathrm{Ln}(2q_1 \cosh g_0)\}. \tag{44}$$

Evidently, the free energy increases with increasing temperature, but there is a maximum at a certain temperature as shown in figure 7(a). What does this free energy mean for the DNA system with high order? The free energy can enhance the thermal motion of hydrogen atoms. Thus when the hydrogen bonds are destroyed, the temperature of the system increases, and the melting effect of DNA occurs successively. At the same time, the entropy of the system increases also. According to the thermodynamic theory we can find the entropy of the system in such a case, which is as follows:

$$S/K_B = \mathrm{Ln}[2\pi(K_B T)/v_1] + \tfrac{1}{2}\mathrm{Ln}(2q_1 \cosh g_0) + 1 + \tfrac{1}{2}\beta q_3 q_0 \tanh g_0. \tag{45}$$

From this formula we see that the above free energy and entropy, arising from the displacements of hydrogen atoms and bases, always exist in the DNA, if the temperature is not equal to zero. The entropy increases with increasing temperature, which is shown in figure 8(a). This means that the structural disorder of DNA or the displacements of hydrogen atoms and bases are enhanced in the melting state. This shows clearly that in the transcription processes, the B-DNA lies in the excitation state, the displacements of hydrogen atoms and bases increase with increasing temperature of the systems, the double-helix chains can naturally open, DNA base-pairs are split, the duplex DNA separates into two single strands, and the DNA–RNA hybrid base-pairs are formed in such a case. At the same time, the energy carried by the above soliton in DNA is partially transferred to the RNA segment to form the new RNA chain. Once the energy carried by the soliton has been fully transferred to the RNA, the soliton terminates,

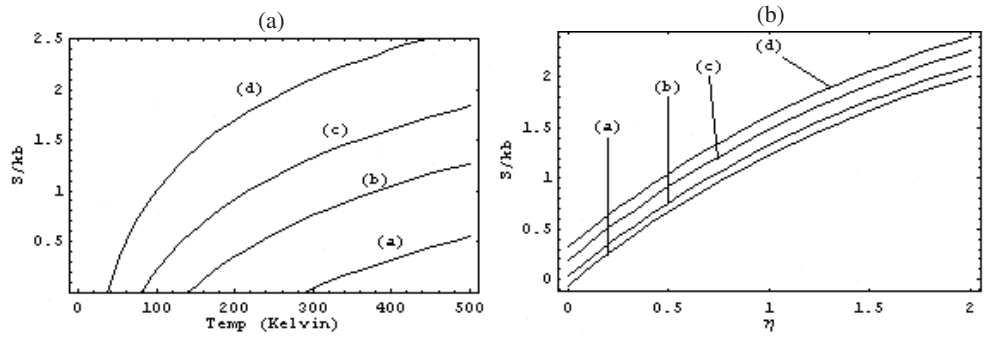

Figure 8. The entropy in the melting state of the DNA system and its variations with varying of temperature and salt concentrations. (a) shows the changes with varying of temperature, T, where a, b, c, and d are the values at $\eta = 0$, 0.5, 1, and 2, respectively. (b) shows the changes with varying of η where a, b, c and d are the values at $T = 273$, 300, 350 and 400 K, respectively.

the displacements or vibrations of hydrogen atoms and bases cease and the DNA–RNA hybrid is split. Thus the DNA restores itself again to its original B-DNA form. Finally, a new and complete RNA is born and the transcription of DNA is finished. Therefore, the DNA lies always in the B-DNA state before and after the transcription process. This is simply all the process of transcription of DNA. Thus we explain the melting and transcription of DNA by this model. This is an advantage of this model. Certainly, its visualized process is very complicated and it has been not delineated in detail here.

From above studies we know that the duplex DNA separates into two single strands in the melting or phase transition process. At present, a key problem is how we judge quantitatively that DNA is separated. Hence the displacement of hydrogen ions was introduced, which plays an important role in the melting of DNA in the new model. It can result in the self-consistent 'softening' of frequency of hydrogen atoms and 'thermal expansion' of the hydrogen bond (or in other words, the softening and expansion lead to a melting of hydrogen bonds). Thus, we can use the average value of the mean square of the displacement to represent the melting effects of DNA. It can be defined by [64] $\langle u^2\rangle = -\frac{1}{m}\frac{\partial f_u}{\partial C_2}$. If $\langle u^2\rangle = 0$, this means that there is no melting effect in DNA. If $\langle u^2\rangle > 0$, the melting phenomenon occurs; the larger the value of $\langle u^2\rangle$, the stronger the melting. We can find the functional relation of $\langle u^2\rangle$ with respect to the temperature from equation (44). It can be approximately denoted by

$$\langle u^2\rangle = \frac{r_0}{m\beta v_1\sqrt{8C_2}}\left\{1 - \frac{(1-2\beta q_3)}{4}\mathrm{e}^{-\beta q_3}\tanh[q_4\exp(-\beta q_3)]\right\}. \tag{46}$$

Utilizing the above values of the physical parameters in the systems, we can find the dependence of $\langle u^2\rangle$ on the temperature, T. This result is shown in figure 9(a). We see clearly from this figure that the melting effect increases with increasing temperature. This is basically consistent with Chen *et al*'s numerical results [65]. We know that the size of $\langle u^2\rangle$ is related to the self-consistent 'softening' of frequency of hydrogen atoms and 'thermal expansion' of the hydrogen bond or that it designates the degree of melting of base-pairs in DNA. Therefore the melting effects are different at different temperatures and positions on the DNA strands. We know from equations (26) and (27) that the width of the soliton, equation (27), corresponding to equation (26) is $1/\mu$. Utilizing the above values for the parameters, we can find the width of one soliton to be 80–10 base-pairs. Thus, the melting of DNA is localized and extended gradually. Meanwhile, from this figure we see that $\langle u^2\rangle = 0.0398$ Å^2 at the biological temperature $T = 300$ K, and $\langle u^2\rangle = 0.0409$ Å^2 at $T = 310$ K. This shows that in normal physiological

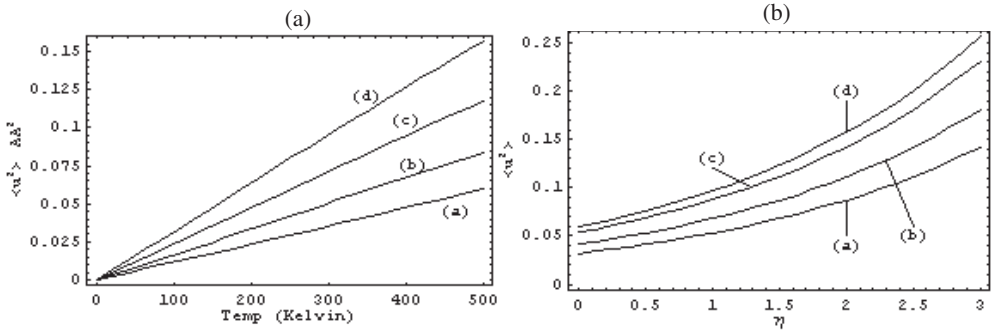

Figure 9. The dependence of average square-displacement of hydrogen atom, $\langle u^2 \rangle$, on the temperature and salt concentration. (a) shows the changes with varying of temperature, T, where a, b, c and d are $\eta = 0$, 0.7, 1.4, and 2, respectively. (b) shows the changes with varying of η, where a, b, c and d are $T = 273$, 350, 450 and 500 K respectively.

conditions DNA can melt and undergo normal transcription. This is consistent with Prohofsky *et al*'s prediction [17–19]; they thought that if $\langle u^2 \rangle_{\rm cr} = 0.04$ Å^2, the hydrogen bonds between these base-pairs are destroyed, the ordered duplex DNA separates into two single strands, the melting of base-pairs in poly(dG)–poly(dC)s and the transcription process all occur.

We now determine the critical temperatures of the melting by using the theory of first-order phase transition and relations of changes of thermodynamic functions. If we assume $S = 0$ in the ordered B-DNA state, then the state $S \neq 0$ should correspond to the beginning of the melting of DNA. The temperature of transformation of entropy between the two phases should represent the subcritical temperature, $T_{\rm subcr}$, of the first-order phase transition or melting, at which the ordered state of B-DNA begins to transform into the melting state through a first-order phase transition. Thus we can find $T_{\rm subcr}$ from the above representation of entropy. From equation (45) we approximately get

$$\mathrm{D_3X^3 + C_3X^2 + B_3X + A_3 = 0} \tag{47}$$

where

$$D_3 = \mathrm{Ln}\left(\frac{2\pi}{v_1}\right) + \frac{5}{2} + \frac{(1-q_4)}{q_1}, \qquad C_3 = 1 - \frac{q_3 q_4^2}{2} - \frac{q_3 q_4}{q_1},$$
$$B_3 = q_4^2 q_3, \qquad A_3 = -\tfrac{1}{2} q_3^3 q_4^2, \qquad X = K_{\rm B} T.$$

The subcritical temperature of melting can be represented by

$$X = K_{\rm B} T_{\rm subcr} = g_1\{-Q/2 + [(Q/2)^2 + (G/3)^3]\}^{1/3} + g_2[-Q/2 - [(Q/2)^2 + (G/3)^3]]\}^{1/3} - C_3/3D_3 \tag{48}$$

where

$$G = [3D_3B_3 - C_3^2]/3D_3^2, \qquad Q = [27A_3D_3^2 + 3C_3^2D_3 - C_3^3 - 9C_3B_3]/27D_3^3$$
$$g_1, g_2 = 1, [-1 + \mathrm{i}\sqrt{3}]/2, [-1 - \mathrm{i}\sqrt{3}]/2.$$

By substituting the above values of the parameters into equation (48) we finally find that $T_{\rm subcr} = 275$–286 K.

The entire melting of DNA is a biomolecular dissociation process, wherein the initial state is a duplex DNA and the final state is the separated single strands. According to the above study and Prohofsky *et al*'s result we know that $\langle u^2 \rangle_{\rm cr} = 0.04$ Å^2 shows just that

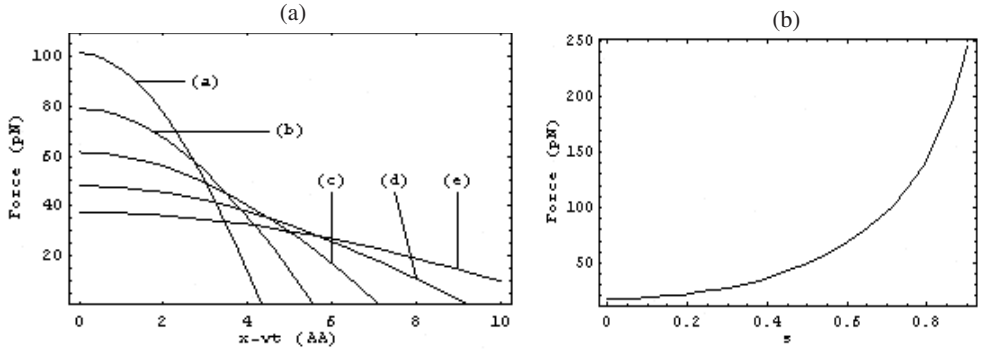

Figure 10. The force of the phase transition of DNA and its relation with salt concentrations. (a) shows the distance dependences; here a, b, c, d and e are $\eta = 0$, 0.5, 1, 1.5 and 2, respectively. (b) shows the dependence of force versus the velocity of the hydrogen atom.

the hydrogen bonds between these base-pairs are destroyed, and the ordered duplex B-DNA transforms completely into the two separated single strands. Thus we can utilize the relation of $\langle u^2\rangle = \langle u^2\rangle_{\rm cr} = 0.04$ Å^2 to determine the critical temperature of complete transformation of DNA, $T_{\rm com}$, in the melting. From equation (46) and the above relation we approximately get

$$(P_1 - A)X^4 + (R_1 + 0.04)X^3 - S_1X^2 - T_1X - U_1 = 0 \tag{49}$$

where $P_1 = (1-q_4^2/3)Aq_4/4$, $R_1 = (q_4^2-2)Aq_3q_4/4$, $S_1 = 5Aq_4q_3^2[q_3-q_4(1+q_3)/3+1/2]$, $T_1 = (3+11q_4^2/3)Aq_4q_3^3/4$, $U_1 = (1+29q_4^2/24)Aq_4q_3^4$, $A = q_4^2q_3^2/2$, $X = K_{\rm B}T$. Utilizing the previous values of the parameters and equation (49), we can approximately obtain $T_{\rm com} =$ 299–306 K. The above values of the critical temperatures for the beginning and complete transformation of DNA in the melting or transcription process are reasonable and appropriate to the practical cases of DNA. Therefore the new model is available and credible.

We now analyse the mechanical features of the phase transition in the melting process. From above results in equation (27) and figure 4 we see that the displacements of these hydrogen atoms in DNA have different values in different positions, and the distribution forms a kink shape. This show that the forces accepted by these hydrogen atoms in the phase transition process are also different in different positions in this distortion or melting domain. Therefore, the melting or transcription of DNA is an asymptotic extension process. In the light of mechanical laws we can find the force of the phase transition determined by the energy, equation (35), arising from this phase transition. It is of the form

$$F = \frac{mC_2v_1(1-s_1^2)^{1/2}}{2r_0\sqrt{2D_2}}\left\{\frac{2}{(1-s^2)}\,\mathrm{sech}^4[\mu(z-vt)] - 1\right\}\cosh^2[\mu(z-vt)]. \tag{50}$$

In figure 10(a) we show the distribution of the force in the phase transition process in the time–space domain, and its changes with increasing velocity v. From this figure we see that the force decreases with increasing of distances from the equilibrium positions.

According to the thermodynamic theory we can find the internal energy $e = f - T\frac{\partial f}{\partial T}$ and specific heat $C_v = -\frac{\partial e}{\partial T}$ at constant volume from the above free energy in equation (44) in such a case. Using $C_v = -T\frac{\partial^2 f}{\partial T^2}$, we finally find the specific heat of DNA to be of the form

$$C_v/K_{\rm B} = 1 + q_3q_4[2 + \tfrac{1}{2}\beta q_3]\mathrm{e}^{-\beta q_3}\tanh g_0 + \tfrac{1}{2}\beta^2 g_0^2 q_3^2\,\mathrm{sech}^2\, g_0. \tag{51}$$

Using the above values of these parameters we give the temperature dependence of specific heat of DNA, which is shown in figure 11. From this figure we see that the specific heat increases

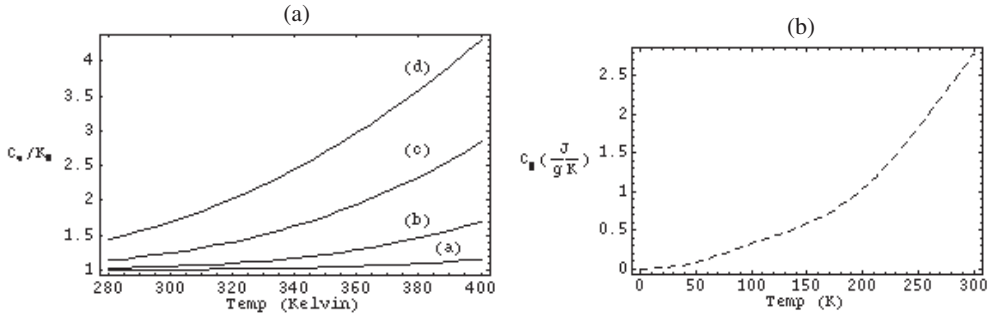

Figure 11. The temperature dependence of specific heat; in (a), a, b, c and d, are the values at $\eta = 0, 0.5, 1$, and 2, respectively. (b) shows the experimental data by Mrevlishvilii *et al*.

with increasing of temperature, specially in the region of the biological temperature. This concords with Mrevlishvilii *et al*'s experimental results [66] as is shown in figure 11(b). From figure 11 we see that the theoretical result is basically the same as the experimental datum. This shows that our model is correct and available.

5. Influence of the salt concentration on the transcription of DNA

As is known, a lot of functions of DNA including the transcription are performed in a water solution. The so-called physiological condition, in which DNA is placed in a natural condition, corresponds simply to a 0.1 M solution of NaCl. In this condition DNA is an acid: there are some hydrogen ions (protons) in this solution (one proton per phosphate group), which results in a negative charge of the molecule. The hydrogen ions with positive charges in the hydrogen bond and the base with negative charge then have interactions with the counterions Na^+ and Cl^- in the solution, respectively [49, 50]. Meanwhile, the charges in the phosphate groups in DNA could interact with these counterions in the surrounding solvent [56, 58]. In the normal case the centre of DNA, where the base dipoles and hydrogen atoms are located, are protected from the ionic continuum of the solvent. However, the phosphate groups on the framework or strand of DNA have negative charges, and the cation in the solvent can partially neutralize the phosphate groups charges; thus the interaction and corresponding distance between the double helix chains in DNA are changed, and the interactions between the hydrogen bonds or the potential of hydrogen atoms and the conformations of DNA are also changed. If the salt concentration increases in the solution, then these effects are more obvious. Experiments show that the conformation changes from B-DNA to A-DNA and Z-DNA are considerably related to the amount of salt concentration in the solvent. Certainly, the transcription or melting of DNA also is not exceptional [67], although this effect is indirect. Therefore we should believe the influence of salt concentration on the melting of DNA. From the above study we know that the salt concentration affects mainly the interaction potential of hydrogen atoms in the base-pairs in our model. If we use the factor η to denote the salt concentration, then this influence can be approximately represented by $e^{-\eta}$ in accordance with common rules. Thus, the effective potential of the system in equation (32) is changed, which can be approximately represented by

$$U'_{\text{eff}}[u(z,t)] = -\tfrac{1}{2}C_2 e^{-\eta}u^2 + \tfrac{1}{4}D_2 e^{-\eta}u^4. \tag{52}$$

In such a approximation the influence of salt concentration amounts to the interaction coefficients, C_2 and D_2 in the above formulae, being replaced by $C_2 e^{-\eta}$ and $D_2 e^{-\eta}$, respectively.

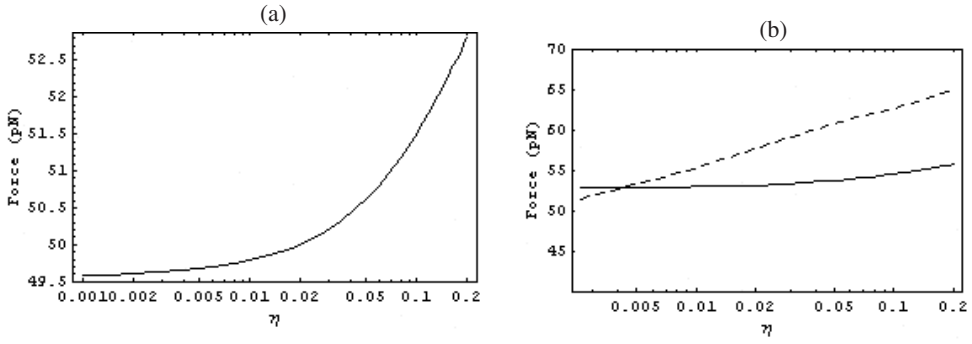

Figure 12. (a) The dependence of the force on the salt concentration, η and (b) comparison with experimental data which is denoted by the dashed line.

Then the influence of salt concentration on the effective potential in such a case can be found, which is shown in figure 5. From this figure we see that the depth of the double-well potential decreases with increasing salt concentration. Thus the energy, equation (33), exciting the solitary wave, equations (19) or (27), which causes the melting of DNA, decreases with increasing salt concentration, as shown in figure 6. The changes, arising from the salt concentration, result in the variations of free energy, equation (44), and entropy, equation (45), and specific heat, equation (51), of the DNA system, and of the mean square displacement of hydrogen atoms, equation (46) which are shown in figures 7, 8, 11(a) and 9, respectively. From these figures we clearly see that the entropy, specific heat and $\langle u^2 \rangle$ increase, but the free energy decreases with increasing salt concentration: especially at $\eta = 1$, the temperature dependence of specific heat closely approaches the experimental curve in figure 11(b). This shows the correctness of the above theoretical model. At the same time, the changes of force of the phase transition with increasing salt concentration is also obtained, which are shown in figure 10. From this figure we see that the force increases as the salt concentration increases. In the region $0.001 < \eta < 0.2$, the changed tendency of force of the phase transition agrees basically with Wenner *et al*'s experimental results [68], which are shown in figure 12. This also shows that our model is correct. These results obtained show that the transcription of DNA depends not only on its structure and the energy absorbed but also on the temperature and salt concentration of the solution around it.

6. Conclusions

Here we have studied the melting and transcription of DNA by a new model, which is proposed based on experimental results. In this model we have introduced three variables per base, the displacement of the hydrogen atom, u_n, the displacement of the base (nucleotide), R_n, and the rotation angle of the base, φ_n. These variables depict the vibrations of the hydrogen atom, the vibration of the base and its rotation in DNA, respectively. In this model we stress specially the important role of the hydrogen atom in the hydrogen bonds in the base-pairs which is very helpful in revealing the mechanism and properties of melting and transcription of DNA. According to their properties of motion we have given the Hamiltonian of the system and corresponding equations of motion, and found their soliton solutions. The solitons formed by the displacements of hydrogen atoms and bases and their rotations are the excitation states which can occur, only if the energy is absorbed by the DNA working at the biological temperature. Based on this model we give the thermodynamic properties, for example, the free energy, entropy and specific heat of the thermal excitation state in the melting of DNA

system with biological temperatures by means of the transfer integral and theory of first-order phase transitions. Utilizing the properties of these thermodynamic functions and their changes, we explain the mechanism and processes of the melting and transcription of DNA with the aid of the transforms of energy carried by the soliton in such a case. We further give the properties of transcription of DNA with the help of these features of average value of mean square of displacement of hydrogen atom and the values of critical temperatures of the beginning and complete transformations and the force of the phase transition, and their variations. Finally, we demonstrate the validity of the new model of dynamics of DNA through the comparisons between theoretical and experimental results of specific heat and force of the phase transition and critical temperatures of DNA. Therefore we conclude that the transcription of DNA not only depends directly on the properties of its structure and the energy absorbed, but is also influenced by the temperature and salt concentration of the solution of DNA; thus it demonstrates also that the new model is correct.

However, on checking and looking in detail at the new model we find that this model has the following defects.

(1) Since DNA is a biomacromolecule, its structure and dynamical processes are very complicated and variant; hence it is not sufficient to describe its dynamical processes by the above three microscopic coordinates per base-pair. In further studies we will introduce more dynamic variables containing some mesoscopic variables to involve various modes of motion of DNA and to describe its different dynamic states. At the same time, the introduction of additional degrees of freedom is also very necessary because of the low sensitivity of the vibrational behaviour of DNA to the number of bridging hydrogen bonds, which suggests that the melting of hydrogen-bond bridging is only part of the strand separation process. These studied results will be presented in another paper.

(2) It is well known that the dynamical processes of DNA are related not only to its own structure and the energy transformation in it, but also the states of solution or water around it. This means that DNA dynamics cannot even be approximately treated by a simple energy-conserving Hamiltonian that omits the water. The influences of water on its dynamics should be embodied by the overdamping effect and the thermal noise disorder effect, arising from the biological temperature. These effects will change the structure and states of the solitons. These problems have been not considered in this paper; this shows that our model is simple and has some limitations. We will eliminate these shortcomings in future studies. The results of these studies will be described in detail in another paper.

(3) The model for the influences of salt concentration on features and critical temperatures of melting of DNA is simple and crude. From the results of this study we can only know some elementary effects of salt concentration on features of DNA and states of the solitons. In fact, the effects of salt concentration on the dynamics of DNA are various: in particular, the dependence of melting or critical temperatures on salt concentration is a complicated problem, which needs serious study. Also, we have not treated the concrete effect of salt on the single strands, as well as the duplex. These problems are described in another paper.

(4) In our model, the changes of coupling constants, J, χ_1, χ_2, λ and C_2 give only a phenomenological description; it is necessary to do numerical calculations and to find their explicit representations. In the meantime, our model does not consider the inhomogeneities present in natural DNA. These effects will result in a complexity of calculation and could be performed in numerical simulation. These problems will be investigated in other papers.

Therefore, the results presented here are only the first step towards the understanding of the transcription of DNA, in which some detailed processes are not delineated. The above problems needs to be further studied completely in other work.

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