

Two-dimensional discrete model for DNA dynamics: Longitudinal wave propagation and denaturation

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In this paper, a simple, two-dimensional model of the deoxyribonucleic acid (DNA) is presented. In the model the two polynucleotide strands are linked together through the hydrogen bonds. The phosphodiester bridges in the backbone are described by the anharmonic potential of Toda kind, while the hydrogen bonds are described by the Lennard-Jones potential. Longitudinal wave propagation on *ring-shaped* DNA molecules is investigated. The model predicts a significant increase in the lifetime of the open states of the hydrogen bonds at physiological temperatures. Thus anharmonicity may play a role in DNA denaturation.

I. INTRODUCTION

In the recent years the possibility that anharmonic excitations could play a role in the dynamics of DNA has been considered by several authors.¹⁻¹⁶ The possibility that nonlinear effects might concentrate vibrational energy in DNA into localized *solitonlike* objects, was first developed by Krumhansl and his co-workers,¹⁻³ who suggested a theory of soliton excitations as an explanation of the open states of DNA. Related studies of solitons in DNA have also been presented by Yomosa,⁴ who proposed a soliton theory using a plane base-rotor model. This model was further refined by Takeno and Homma,⁵ who allowed discreteness effects to be taken into account, and by Zhang,⁶ who improved the model for base coupling.

Solutions of the above-mentioned models were always obtained in the continuum approximation, which is a questionable approximation for DNA. Moreover, the models did not treat thermal effects on DNA.

A first attempt to incorporate thermal effects in the soliton models for DNA has been presented by Muto *et al.*,¹¹⁻¹³ who investigated the possibility of solitons being generated thermally at physiological temperatures. To model longitudinal wave propagation on homogeneous DNA at different temperatures, their approach was based on a one-dimensional model using a nonlinear spring and mass system. In the model each mass represents a single base pair, and the nonlinear spring represents the van der Waals potential between adjacent base pairs. In particular, modeling DNA as a Toda lattice¹⁷ with parameters chosen to match experimentally measured properties of DNA, the number of solitons thermally generated in DNA as a function of absolute temperature and number of base pairs was calculated. In Refs. 11-13 a $T^{1/3}$ law for the dependence of the number of solitons on the temperature was found.

The first approach in investigating the statistical mechanics of a simple lattice model for denaturation of the DNA double helix has been presented by Peyrard and Bishop.¹⁵ They employ a transfer integral technique to

analyze the statistical mechanics of the model and determine the interstrand separation in the double helix as a function of temperature. In their model the potential for the hydrogen bonds is approximated by a Morse potential, and for each base pair there are two degrees of freedom which correspond to the displacements of the bases from their equilibrium position along the direction of the hydrogen bonds that connect the two bases in a pair. Finally, they assume a linear coupling due to the stacking between neighboring bases. Dynamical studies of a similar model of the DNA double helix are performed by Techera, Daemen, and Prohofsky.¹⁶

In series of papers¹⁸⁻²² Prohofsky and co-workers introduce the modified self-consistent phonon theory as a method for calculating hydrogen bond melting. The order of the melting temperatures for double helical DNA polymers is predicted close to actual melting temperatures for different DNA polymers.

In order to improve the description of the DNA dynamics, we will consider a model where the two polynucleotide strands are linked together through the hydrogen bonds described by a Lennard-Jones potential. The phosphodiester bridges in the backbone are described by an anharmonic Toda potential. In addition, both longitudinal vibration along the backbone direction and transverse vibration along the hydrogen bond direction are included. To describe the interaction of the system with a thermal reservoir at a finite temperature, a damping force and a noise force which simulate a thermal bath are added to the equation of motion for the molecular displacements. Performing dynamical simulations of a *ring-shaped* DNA molecule immersed in a thermal bath, from one hand the problem of longitudinal wave propagation and concentration of energy in localized packets is considered. On the other hand, the temperature dependence of the open states (the precursors to full denaturation) in the molecule is analyzed. It is found that at physiological temperature a significant number of solitons is present in the DNA. Results from inverse scattering transform theory are used to count the solitons. Moreover, a transition from double-stranded to single-stranded DNA

occurs locally around physiological temperature. Note that Toda solitons are not topological solitons. Thus their amplitude and energy can assume any positive values.¹⁷ In contrast, a minimum energy is required for breaking the hydrogen bond described by the Lennard-Jones potential.

The paper is organized as follows. In Sec. II the physical model for DNA dynamics is described, and in Sec. III its Hamiltonian and the equations of motion are given, and our approach to thermalization is described. In Sec. IV the corresponding numerical results of the dynamical study are presented. Finally conclusions are given in Sec. V. In the Appendix we display the normalized version of the perturbed system which describes the DNA molecule immersed in a thermal bath.

II. MODEL

To improve the description of the DNA dynamics presented in Refs. 11–13, we propose here another model consisting of two chains transversally coupled. Each chain models one of the two polynucleotide strands of the DNA molecule. To simplify the calculations, we will neglect the helical structure of the DNA. So, instead of the double helix we will consider two parallel strands, each having the form of a straight line. Each of the two chains is a spring and mass system. Each mass of the model represents a single base of the base pair. The longitudinal springs connecting masses of the same strand represent the van der Waals potential between adjacent base pairs. The transverse springs connecting corresponding masses of the two strands represent the hydrogen bonds that connect the two bases in a pair. We assume a homogeneous DNA molecule, therefore each particle has mass M .

For each base pair, the model includes four degrees of freedom, u_n, x_n , and v_n, y_n , for the two strands, respectively. The $u_n = u_n(t)$ and $v_n = v_n(t)$, $n = 1, 2, \dots, N$ denote the *transverse displacements*, i.e., the displacements of the bases from their equilibrium positions along the direction of the hydrogen bonds that connect the two bases of the base pair. The $x_n = x_n(t)$ and $y_n = y_n(t)$, $n = 1, 2, \dots, N$ denote the *longitudinal displacements*, i.e., the displacements of the bases from their equilibrium positions along the direction of the phosphodiester bridge that connect the two bases of the same stand. Our model is schematically shown in Fig. 1. Being interested in *ring-shaped* DNA molecules, we assume periodicity of the displacements, namely $x_{N+n} = x_n$, $y_{N+n} = y_n$, $u_{N+n} = u_n$, and $v_{N+n} = v_n$, where N is the number of base pairs in the DNA.

We model the phosphodiester bridge by the following Toda potential¹⁷:

$$V(r_n) = a/b \exp(-br_n) + ar_n, \quad (2.1)$$

where r_n denotes the relative displacements, and a and b are positive parameters. The reason for this is twofold. First, (2.1) makes a reasonable approximation to the more commonly used van der Waals potential. Second, the Toda lattice has mathematical properties convenient for analysis.^{11–13}

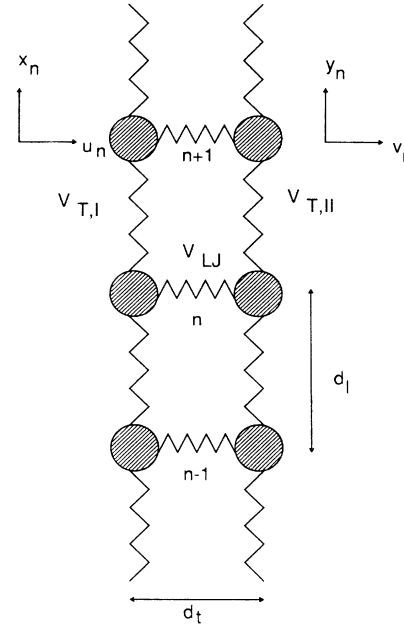


FIG. 1. Schematic plot of the two-dimensional model for DNA double helix. The two identical anharmonic Toda chains are connected by a Lennard-Jones potential representing the H bonds between the two strands.

Denoting the first strand by I , the anharmonic potential is given by

$$V_{T,I}(\lambda'_n - d_l) = a/b \exp[-b(\lambda'_n - d_l)] + a(\lambda'_n - d_l). \quad (2.2)$$

A similar expression is valid for the potential $V_{T,II}(\lambda''_n - d_l)$ of the second strand. In the Toda potential (2.2) a and b are parameters which will be given later, and are computed to correspond to experimentally measured properties of DNA. In expression (2.2) λ'_n denotes the distance between the n th and the $(n+1)$ th base in strand I , and its expression is given by

$$\lambda'_n = [(d_l + x_{n+1} - x_n)^2 + (u_{n+1} - u_n)^2]^{1/2}. \quad (2.3)$$

Here d_l is the equilibrium distance between adjacent bases in the same strand measured along the helix axis ($d_l = 3.4 \text{ \AA}$).²³ An expression analogous to (2.3) is valid for λ''_n denoting the distance between adjacent bases in strand II .

The two bases in a pair are connected through hydrogen bonds which we model by a Lennard-Jones potential. This type of potential is generally accepted to model the effect of hydrogen bonds.^{24–27} Thus the anharmonic potential for the transverse springs modeling the hydrogen bonds is given by

$$V_{LJ}(\tau_n - d_l + d_h) = 4\epsilon \left[\left(\frac{\sigma}{\tau_n - d_l + d_h} \right)^{12} - \left(\frac{\sigma}{\tau_n - d_l + d_h} \right)^6 \right]. \quad (2.4)$$

In the Lennard-Jones potential (2.4) ϵ and σ are parameters which will be given later, and are computed to correspond to experimentally measured properties of the hydrogen bonds in DNA. $\tau_n - d_t + d_h$ is the length of the hydrogen bond between the two bases in the n th pair, and τ_n denotes the distance between two bases of the two strands and is given by

$$\tau_n = [(d_t + v_n - u_n)^2 + (y_n - x_n)^2]^{1/2}. \quad (2.5)$$

Moreover, d_t is the equilibrium distance between the bases in a pair, namely the diameter of the helix ($d_t = 20 \text{ \AA}$),²³ and $d_h = 2^{1/6}\sigma$ (Ref. 27) is the equilibrium length of the hydrogen bond.

An important point is the determination of the parameters a and b appearing in the Toda potentials $V_{T,I}(\lambda'_n - d_t)$ and $V_{T,II}(\lambda''_n - d_t)$ [cf. Eq. (2.2)], and of the parameters ϵ and σ appearing in the Lennard-Jones potential $V_{LJ}(\tau_n - d_t + d_h)$ [cf. Eq. (2.4)].

From previous studies,¹¹⁻¹³ the mass of a base pair has been determined as 1.282×10^{-24} kg. Therefore the mass of each base is $M = 6.41 \times 10^{-25}$ kg. Moreover, the values for the parameters a and b appearing in the Toda potential were obtained by fitting the exponential function to the 6-12 potential function and using experimental properties of DNA.¹¹⁻¹³ Since here the model consists of two parallel chains, the nonlinear parameter b will be the same, while the parameter a will be half the previously computed value. Therefore the values used in the present model are $a = 2.5635 \times 10^{-10}$ N and $b = 6.176 \times 10^{10} \text{ m}^{-1}$, respectively.

For the Lennard-Jones's parameters, it is known that for hydrogen bonds^{26,27} their values are approximately $\epsilon = \epsilon_{LJ} = 0.22 \text{ eV} = 0.35244 \times 10^{-10} \text{ N m}$ and $\sigma = 4.01 \times 10^{-10} \text{ m}$ (corresponding to $d_h = 4.5 \text{ \AA}$). In following sections different values of ϵ will be considered in order to see how the strength of the hydrogen bond influences the longitudinal wave propagation as well as the local breaking of hydrogen bonds. Choosing $d_h = 3 \text{ \AA}$ we get $\sigma = 2.7 \times 10^{-10} \text{ m}$. However, we have checked that the dynamical results are insensitive to changes within this range of σ values.

III. HAMILTONIAN AND THERMALIZATION OF THE PROBLEM

The equations of motion for the system described above are obtained from the Hamiltonian of the system

$$\begin{aligned} H = & \sum_{n=1}^N \frac{1}{2} M (\dot{x}_n^2 + \dot{u}_n^2) + \frac{1}{2} M (\dot{y}_n^2 + \dot{v}_n^2) \\ & + V_{LJ}(\tau_n - d_t + d_h) \\ & + V_{T,I}(\lambda'_n - d_t) + V_{T,II}(\lambda''_n - d_t), \end{aligned} \quad (3.1)$$

where the anharmonic potentials $V_{T,I}(\lambda'_n - d_t)$, $V_{T,II}(\lambda''_n - d_t)$, and $V_{LJ}(\tau_n - d_t + d_h)$ are given in Sec. II.

Denoting the displacement variables by $\Delta_n^{(i)}$, such that $\Delta_n^{(1)} = x_n$, $\Delta_n^{(2)} = u_n$, $\Delta_n^{(3)} = y_n$, $\Delta_n^{(4)} = v_n$, the equations of motion derived from the Hamiltonian (3.1), can be briefly written as

$$M \ddot{\Delta}_n^{(i)} = -\partial H / \partial \Delta_n^{(i)}, \quad (3.2)$$

where $i = 1-4$, and $n = 1, 2, \dots, N$.

In order to describe the interaction of the system with a thermal reservoir at a finite temperature, a damping force and a noise force are added to the equations of motion for the displacements (3.2), leading to Langevin equations,^{28,29}

$$M \ddot{\Delta}_n^{(i)} = -\partial H / \partial \Delta_n^{(i)} = -M \Gamma \dot{\Delta}_n^{(i)} + \eta_n^{(i)}(t). \quad (3.3)$$

Here Γ is the damping coefficient and $\eta_n^{(i)}(t)$, $i = 1-4$, are the random forces acting on the bases. The noises $\eta_n^{(i)}(t)$ are assumed to be Gaussian processes with zero mean and correlation functions of the form

$$\langle \eta_n^{(i)}(t) \eta_{n'}^{(j)}(t') \rangle = 2M \Gamma k_B T \delta_{nn'} \delta_{ij} \delta(t - t'). \quad (3.4)$$

Here k_B is the Boltzmann constant and T is the absolute temperature; $\delta_{nn'}$ and δ_{ij} are the Kronecker deltas and $\delta(t - t')$ is the Dirac delta function.

During the numerical simulations reported in the next section, it has been verified that over sufficiently long time intervals the thermal equilibrium has been reached. This means that the mean kinetic energy is

$$\left\langle \sum_{n=1}^N \frac{1}{2} M (\dot{x}_n^2 + \dot{u}_n^2) \right\rangle = N k_B T = \left\langle \sum_{n=1}^N \frac{1}{2} M (\dot{y}_n^2 + \dot{v}_n^2) \right\rangle, \quad (3.5)$$

for each particle on the first or second strand. Here, $\langle \rangle$ denotes time average.

IV. NUMERICAL RESULTS

In this section the numerical results are presented. The perturbed system, derived in the appendix, has been integrated numerically using a Runge-Kutta method. The calculations have been initialized choosing initial conditions corresponding to a double chain of N masses initially at rest in their equilibrium position. The calculations have been run until thermal equilibrium has been reached and then continued for several hundred time units. Figure 2 shows a typical example of how kinetic and potential energies settle at thermal equilibrium. The energies shown in Fig. 2 are per base pair, and given in units of $\frac{1}{2} k_B T$ (for each base pair there are four degrees of freedom).

The spectral analyzer of the Toda lattice, described elsewhere in detail,¹¹⁻¹³ is used to compute the number of solitons on each of the two chains. The average of these two numbers is denoted by N_S . Our typical results are shown in Fig. 3, where the ratio N_S/N is plotted versus the temperature T in a logarithmic scale, for different choices of the Lennard-Jones parameter ϵ . The perturbed system modeling the double chain immersed in a thermal bath has been integrated for 64 masses, $N = 32$ on each of the identical chains, and with a damping coefficient $\gamma = 1.0$. The values are computed for $\epsilon = \epsilon_{LJ}$, and for $\epsilon = \epsilon_{LJ}/10$ (octagons and diamonds) and compared with results for the one-dimensional model (corresponding to $\epsilon = \infty$) obtained in Refs. 11 and 12. In par-

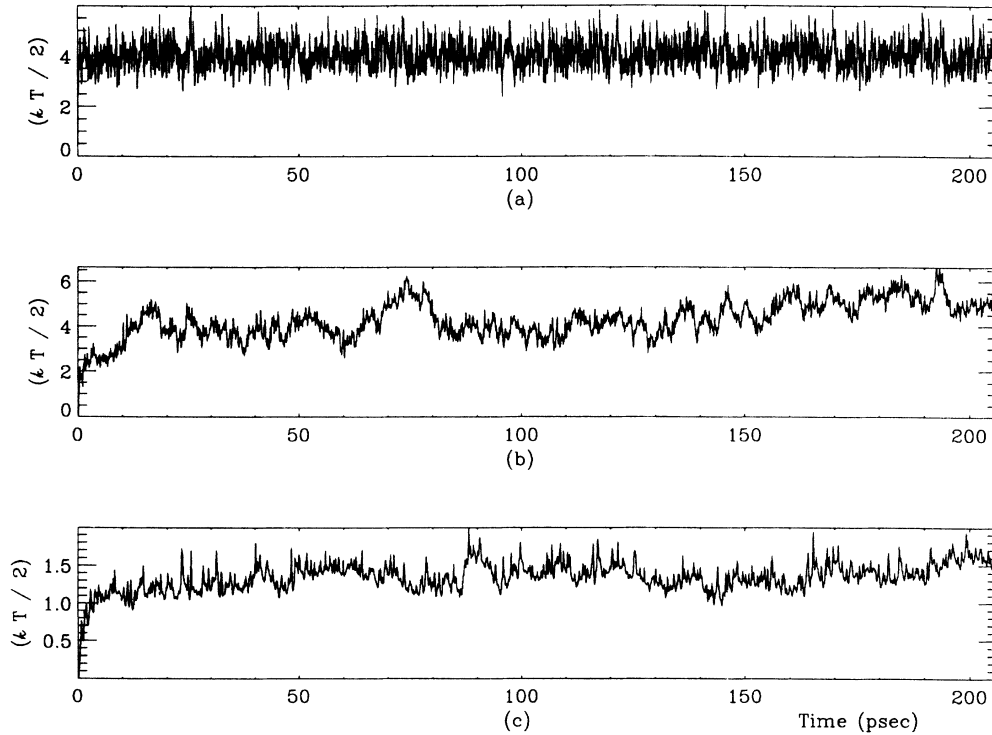


FIG. 2. (a) Averaged kinetic energy, (b) Toda potential energy, (c) Lennard-Jones potential energy as function of time. $T=310$ K, $\varepsilon=\varepsilon_{LJ}/5$.

ticular, the dotted line describes the results for the single unperturbed Toda lattice thermalized through initial conditions.¹¹ The values, denoted by crosses, are obtained by perturbing the single Toda lattice by damping and noise terms ($\gamma=1.0$).¹² As seen from Fig. 3 increasing the strength of the hydrogen bond gives closer agreement to the results for the one-dimensional perturbed model. For increasing temperatures the transverse oscillations

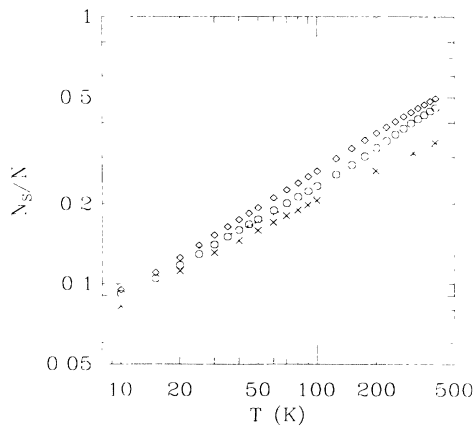


FIG. 3. Logarithmic plot to base 10 of ratio N_S/N vs temperature T . The dotted line and the values denoted by the crosses are the ones obtained in Refs. 11 and 12. The values denoted by the octagon and the diamond are calculated for the perturbed system with DNA parameters, and Lennard-Jones parameters ε equal to $\varepsilon=\varepsilon_{LJ}$ and $\varepsilon_{LJ}/10$, respectively. Damping coefficient $\Gamma=ab/M$, and number of masses in the system $N=32$.

augment the anharmonicity of the two-dimensional model. This feature is absent in the one-dimensional model. Thus the soliton counter predicts a higher value of N_S in the two-dimensional model than in the one-dimensional model.

Next we consider the local denaturation of the DNA molecule. From a biochemical point of view, the denaturation happens when the two strands of the DNA helix readily come apart, because the hydrogen bonds between its paired bases are disrupted. This can be accomplished by heating a solution of DNA or by adding acid or alkali to ionize its bases. The denaturation temperature depends markedly on its base composition. In the present work we consider a homogeneous DNA molecule, and we compute the hydrogen bond stretching in the molecule for different values of the Lennard-Jones parameter ε , which gives the strength of the hydrogen bond between its paired bases. The results are shown in Fig. 4 where the time average of the transversal distances between bases has been plotted as a function of temperature T , for different values of ε . When the transversal distance between the bases in a pair is bigger than 4 \AA the hydrogen bond is broken. Note that for $\varepsilon=\varepsilon_{LJ}/5$ this *open state* occurs for $T \approx 310$ K. A few test runs for $N=64$ (instead of $N=32$) indicate a slightly increased density of open states as well as an increase of the average hydrogen bond stretching. While this work primarily deals with the denaturation precursors, a study of the denaturation requires longer systems.

In Fig. 5 the transversal distances between bases are shown in grey-scale plots, for T equal to 310 K and (a)

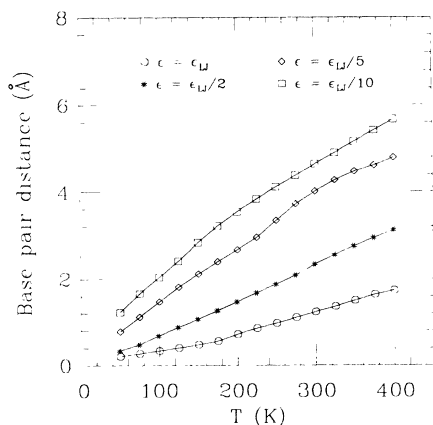


FIG. 4. Time average of transversal distance between bases vs temperature T for different values of the Lennard-Jones parameter ϵ : ϵ_{LJ} (octagon), $\epsilon_{LJ}/2$ (star), $\epsilon_{LJ}/5$ (diamond), $\epsilon_{LJ}/10$ (square).

$\epsilon = \epsilon_{LJ}$, and (b) $\epsilon = \epsilon_{LJ}/5$. The system has been integrated up to a normalized time of 1024 units, corresponding to 206.0 ps. In the grey-scale plots the white areas denote the maximum values of the distance between bases, while the black ones correspond to minimum values of the hydrogen bond stretching. As seen in Fig. 5(b), the fact that the average stretching of the hydrogen bonds is above 4 Å does not imply that all bonds are permanently broken. Such a state of full denaturation requires higher temperatures than investigated here.

Information about the averaged lifetime of the open states as a function of the temperature (for $\epsilon = \epsilon_{LJ}/10$) is given in Fig. 6. The open states are divided into three bins. The first bin contains open states with a life time shorter than 3 ps. We have not considered these states in the calculations of the averaged lifetimes. The second bin contains open states with lifetime between 3 and 17 ps. The averaged values of this group are plotted as open symbols in Fig. 6. Finally, the third bin contains the open states with a lifetime longer than 18 ps. These averaged values are plotted by stars. It is clear from Fig. 6 that for temperatures above 250 K, the presence of open states which last for more than 20 ps is significant.

V. CONCLUSIONS

In this paper, a simple two-dimensional model of DNA has been presented. Particular attention has been devoted to longitudinal wave propagation from an anharmonic perspective and to temperature dependence of local denaturation of *ring-shaped* DNA molecules.

The approximations made in the present work are the following: (i) It is assumed that DNA dynamics can be modeled with a mass-spring system made of two longitudinal chains which are coupled transversally. The longitudinal springs are described by a Toda potential, and the transversal springs by a Lennard-Jones potential. (ii) The system is thermalized by perturbing the equations of motion with a damping force and a noise force to model the interaction between the DNA and a thermal reservoir

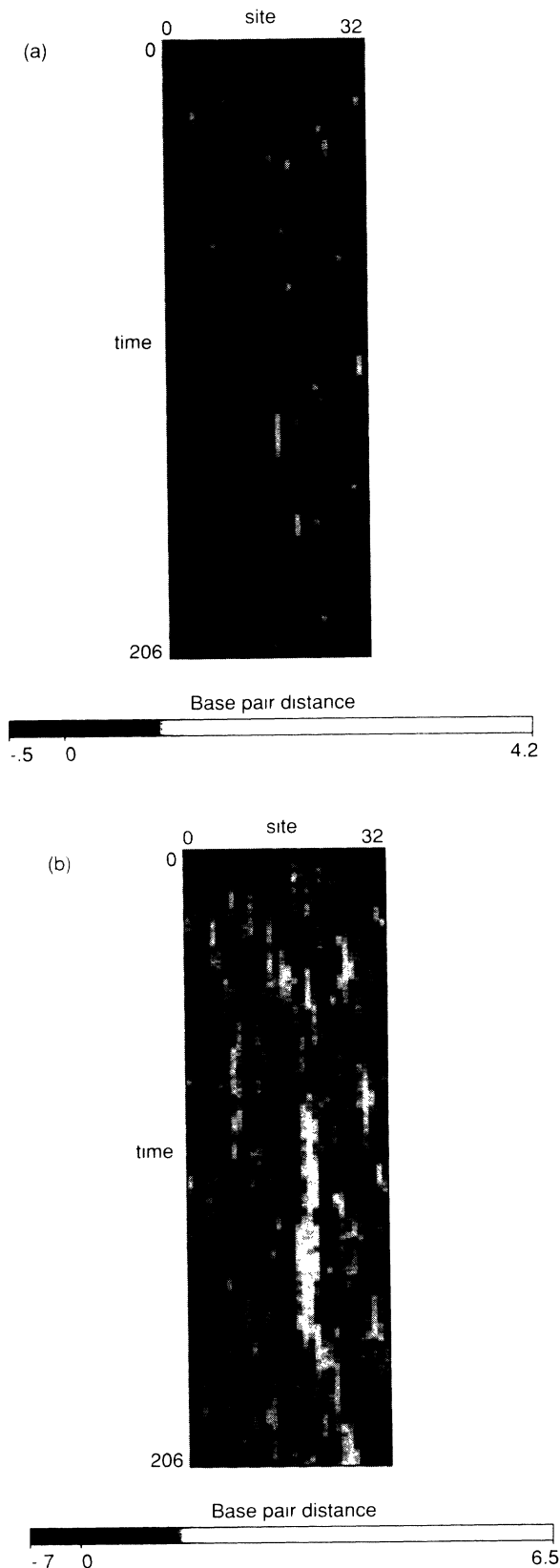


FIG. 5. Grey-scale plots of transversal distance between bases vs site number n and time t . $T = 310$ K, and ϵ equal to (a) ϵ_{LJ} , (b) $\epsilon_{LJ}/5$.

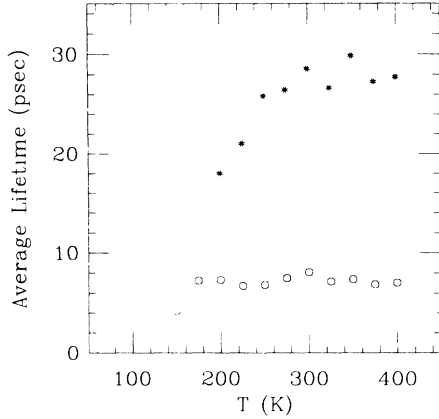


FIG. 6. Averaged lifetime of open states vs temperature T , for $\epsilon_{LJ}/10$.

at temperature T . (iii) The procedure to count the number of solitons, which is exact for the unperturbed Toda lattice, is approximately valid for the perturbed double-strand system.

The number of thermally generated solitons (N_S) is found to be proportional to the number of base pairs (N) in the DNA molecule. Furthermore, there is a $T^{1/3}$ dependence on the number of solitons, at least at low temperatures. This law was also found in the single-strand model.

For reasonable choices of the parameters in the system there is a remarkable dependence of the transversal distance between bases on the temperature. In fact, the lifetime of the open states increases significantly at 310 K.

Thus anharmonicity may play a role in the DNA denaturation.

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APPENDIX

Introducing dimensionless time, $\sqrt{ab/M}t \rightarrow t^*$, and distances, $bx_n \rightarrow x_n^*$ e.g., we get the dimensionless Hamiltonian, $H/(a/b) \rightarrow H^*$.

$$\begin{aligned}
 H^* = & \sum_{n=1}^N \frac{1}{2} (\dot{x}_n^{*2} + \dot{u}_n^{*2} + \dot{y}_n^{*2} + \dot{v}_n^{*2}) \\
 & + 4\bar{\epsilon} \left[\left(\frac{\sigma}{\tau_n - d_t + d_h} \right)^{12} - \left(\frac{\sigma}{\tau_n - d_t + d_h} \right)^6 \right] \\
 & + \exp[-(\lambda'_n - d_l)] + \exp[-(\lambda''_n - d_l)] \\
 & + (\lambda'_n + \lambda''_n - 2d_l), \tag{A1}
 \end{aligned}$$

where $\bar{\epsilon} = 8.49$ for $\epsilon = \epsilon_{LJ}$, and $\sigma = 24.8$, $d_t = 123.5$, $d_h = 27.8$, and $d_l = 21.0$. After adding the damping force and the noise force, the normalized dynamical equations for strand I become

$$\begin{aligned}
 \ddot{x}_n^* = & -\gamma \dot{x}_n^* + \xi_n^{(1)}(t^*) - \{1 - \exp[-(\lambda'_{n-1} - d_l)]\} \left[\frac{d_l + x_n^* - x_{n-1}^*}{\lambda'_{n-1}} \right] + \{1 - \exp[-(\lambda'_n - d_l)]\} \\
 & \times \left[\frac{d_l + x_{n+1}^* - x_n^*}{\lambda'_n} \right] + 24\bar{\epsilon} \left[\frac{1}{\tau_n - d_t + d_h} \right] \left[\frac{\sigma}{\tau_n - d_t + d_h} \right]^6 \left[1 - 2 \left[\frac{\sigma}{\tau_n - d_t + d_h} \right]^6 \right] \left[\frac{y_n^* - x_n^*}{\tau_n} \right], \tag{A2a}
 \end{aligned}$$

$$\begin{aligned}
 \ddot{u}_n^* = & -\gamma \dot{u}_n^* + \xi_n^{(2)}(t^*) - \{1 - \exp[-(\lambda'_{n-1} - d_l)]\} \left[\frac{u_n^* - u_{n-1}^*}{\lambda'_{n-1}} \right] + \{1 - \exp[-(\lambda'_n - d_l)]\} \left[\frac{u_{n+1}^* - u_n^*}{\lambda'_n} \right] \\
 & + 24\bar{\epsilon} \left[\frac{1}{\tau_n - d_t + d_h} \right] \left[\frac{\sigma}{\tau_n - d_t + d_h} \right]^6 \left[1 - 2 \left[\frac{\sigma}{\tau_n - d_t + d_h} \right]^6 \right] \left[\frac{d_t + v_n^* - u_n^*}{\tau_n} \right], \tag{A2b}
 \end{aligned}$$

and similar expressions for strand II. Here $\gamma = \Gamma \sqrt{M/ab}$ with $\sqrt{M/ab} = 0.201$ ps and $\xi_n^{(i)} = \eta_n^{(i)}/a$. The index n runs from 1 to N .

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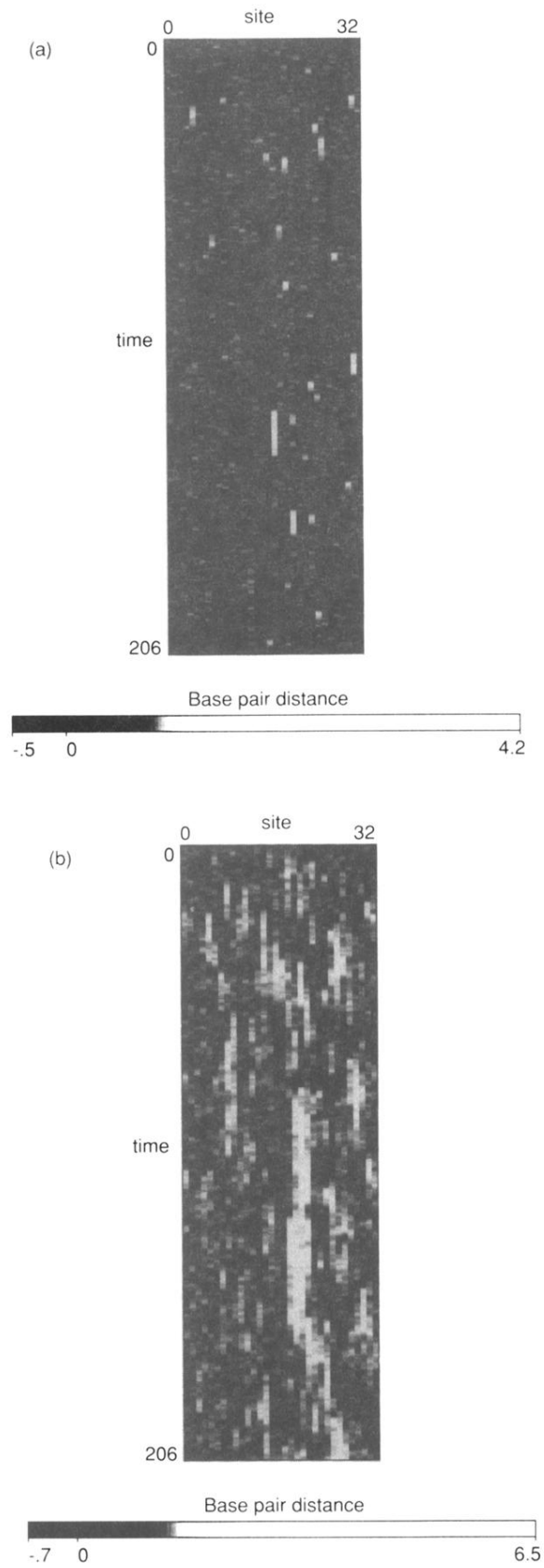


FIG. 5. Grey-scale plots of transversal distance between bases vs site number n and time t . $T=310$ K, and ϵ equal to (a) ϵ_{LJ} , (b) $\epsilon_{LJ}/5$.