Nonlinear model of the DNA molecule

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We study a simple nonlinear model that mimics many features of the DNA molecule, where the source of the nonlinearity is the hydrogen bonds between nucleotides. We find an asymptotic solution of the equations of motion in the limit of small amplitudes. For an arbitrary initial condition, however, the equations of motion have to be integrated numerically. In this case we find essentially two different regimes, one in which an initial pulselike disturbance is pinned, and another one in which it propagates along the chain. In this latter case, propagation is a linear effect, in which the nonlinearity plays little role.

I. INTRODUCTION

Energy tranport along the DNA molcule has lately been the topic of intensive research. Many authors have considered modeling this molecule in such a way that the energy transport is achieved by means of solitons. Muto *et al.*[1] have studied longitudinal propagation in a nonlinear elastic rod model of DNA. Yomosa[2] considered rotating bases about an axis parallel to the helical axis. Takeno[3] studied vibrating excitons that are nonlinearly coupled to lattice phonons. There are several others.[4]

Here we present a model of the DNA molecule consisting of two harmonic chains coupled by a nonlinear potential representing the hydrogen bonds (HB) between bases. This model was analyzed both theoretically and numerically with the aim of discovering possible quasisolitonic properties arising from the nonlinearity which would then provide a possible energy transport mechanism in the molecule.

In Sec. II, we describe the simplified geometry used for the calculations and we derive the corresponding equations of motion. After a brief description of the integration algorithm, we proceed in Sec. III to a detailed study of several dynamical phenomena pertaining to this model. First, we show that in the small amplitude limit, the equations of motion reduce to the nonlinear Schrödinger (NLS) equation and verify numerically that its solutions propagate in our system. Second, we show that an initial pulse of arbitrary shape can either propagate or be pinned depending on the relative importance of the linear and nonlinear forces acting on it. Finally, the "degeneration" of a small-amplitude vibrational mode of the system is studied numerically. We state our conclusions in Sec. IV.

II. MODEL

We consider the following simplified geometry for the DNA chain; the molecule is first untwisted and each strand is then represented by a set of point masses (nucleotides) connected by shearing linear springs while the interstrand interaction (i.e., the hydrogen bonds between base pairs) are modeled by a nonlinear spacing [see Fig. 1(a)]. The displacement from equilibrium of the nth mass point is denoted by u_n and v_n in the top and bottom chain, respectively. Only transverse motions are considered. The equations of motion for u_n and v_n are

$$m\ddot{u}_n = k(u_{n+1}+u_{n-1}-2u_n) - \frac{\partial\phi}{\partial(u_n-v_n)} , \tag{1}$$

$$m\ddot{v}_n = k(v_{n+1}+v_{n-1}-2v_n) + \frac{\partial\phi}{\partial(u_n-v_n)} , \tag{2}$$

where ϕ is the nonlinear potential describing the hydrogen-bond interaction. At this point, we want to emphasize again that the source of the nonlinearity in the model lies in the coupling between the strands, not between adjacent particles on the same strand. For the sake of simplicity, we have assumed a homogeneous chain, i.e., latice points have identical masses m, and similarly the shearing force constants k are the same throughout the chain. In center-of-mass coordinates

$$x_n = \frac{1}{\sqrt{2}}(u_n+v_n) , \tag{3}$$

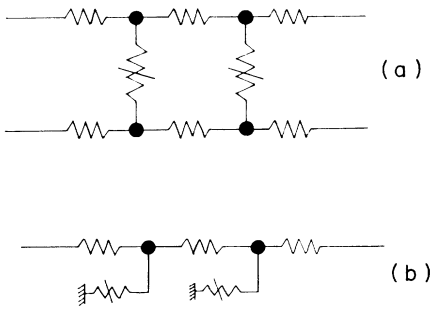

FIG. 1. (a) Simplified model for the DNA chain. Each base pair is represented by a point mass. Along a strand, the masses are connected by shearing linear springs. The hydrogen bonds are modeled by nonlinear springs. Motions are constrained to be transverse. (b) The equivalent one-dimensional chain with longitudinal displacements.

$$y_n=\frac{1}{\sqrt{2}}(u_n-v_n)\ , \tag{4}$$

Eqs. (1) and (2) become

$$m\ddot{x}_n=k(x_{n+1}+x_{n-1}-2x_n)\ , \tag{5}$$

$$m\ddot{y}_n=k(y_{n+1}+y_{n-1}-2y_n)-\frac{\partial\phi}{\partial y_n}\ . \tag{6}$$

x_n is the motion of the center of mass and y_n describes the motion about the center of mass. (As positive y_n represents a stretch.) The equations of motion are now uncoupled. Equation (5) represents a pure harmonic lattice with plane-wave solutions. In what follows, we shall focus our attention on the motion about the center of mass Eq. (6). This equation can be viewed as describing longitudinal displacements in the one-dimensional chain shown in Fig. 1(b).

The potential energy ϕ is chosen to model the nonlinear HB interaction between base pairs. This is done by using the Morse potential[5]

$$\phi_M(y_n)=V_\infty(1-e^{-\sqrt{2}ay_n})^2\ , \tag{7}$$

which, with suitably chosen parameters, can provide a good description of a HB. It should be stressed, however, that the use of a Morse potential is by no means crucial in what follows. In fact, virtually any potential having similar characteristics will do, and indeed we reproduced our results with several other potentials.

III. RESULTS

A. Integration method and parametrization

The problem considered here implies the existence of two well-distinct time scales, one corresponding with the vibration of a single particle about some equilibrium position and a second one corresponding to the propagation and/or relaxation of a pulse in the chain. The existence of different time scales is a well-known problem; it causes the eigenvalues of the Jacobian matrix of the system of differential equations to vary greatly in magnitude. This renders the numerical integration extremely difficult, and one has to make use of special techniques in order to deal with these so-called stiff problems. The equation of motion for y_n [Eq. (6)] was integrated by using Gear's method,[6] which we believe is the best method currently available to solve stiff differential equations.

We take special care to maintain energy conservation (kinetic+harmonic+nonlinear) throughout the numerical integration procedure. In the following calculations, we were always careful to maintain energy conservation to a maximum discrepancy of 0.1%. This point has been stressed by several authors[7] since energy nonconservation leads to observation of phenomena that are not representative of the actual physical system. Maintaining energy conservation is, however, only a necessary condition, but it is not enough to guarantee that the results are correct. A more severe test of the integration procedure consists in starting with a completely symmetric configuration and checking that symmetry is conserved at any subsequent time. We used this test several times in order to check the correctness of our integration procedure.

The distance between base pairs was taken to be $d=3$ Å. The ratio k/m equals 22.2 rad^2/ps^2 corresponds to a frequency of 25 cm^{-1}. The potential used was the Morse potential Eq. (7) with the following parameters: $a=2.5$ Å^{-1} leading to a well width of approximately 0.2 Å and the depth V_∞ was taken to be 0.4 eV, unless otherwise specified, in order to simulate two to three HB. We studied a chain of 125 particles and used periodic boundary conditions.

B. Asymptotic solution

To the best of our knowledge, Eq. (6) with a Morse potential (or a potential of this type) has never been solved analytically. In the solitary-wave analysis by Davydov[8] of the one-dimensional α helix, the equation describing the system is the NLS equation. Prohofsky[9] has suggested that the nonlinearity of the HB's stretching modes might be important enough to support the same type of solitary-wave behavior. Here we show how the equations of motion for our model can be reduced to the NLS equation via the multiple-scale expansion method.[10]

First, the nonlinear term in Eq. (6) with the Morse potential is expanded up to third-order terms in y_n:

$$m\ddot{y}_n=k(y_{n+1}+y_{n-1}-2y_n)-4V_\infty a^2y_n+6\sqrt{2}V_\infty a^3y_n^2-\tfrac{28}{3}V_\infty a^4y_n^3\ . \tag{8}$$

This expansion is valid only for small displacements and therefore we have to restrict ourselves to small-amplitude pulses (the polynomial expansion in Eq. (8) is valid for displacements smaller than the inflexion point). A solution of this equation can be obtained via the multiple-scale expansion method

$$y_n=F_1(\epsilon nd,\epsilon t)e^{i(qnd-\omega t)}+F_1^*(\epsilon nd,\epsilon t)e^{-i(qnd-\omega t)}+\epsilon[F_0(\epsilon nd,\epsilon t)+F_2(\epsilon nd,\epsilon t)e^{2i(qnd-\omega t)}+F_2^*e^{-2i(qnd-\omega t)}]\ , \tag{9}$$

where d is the separation between successive base pairs, and ω and q are related by the lattice dispersion relation. In the limit of long wavelengths ($\lambda\gg d$), it is legitimate to use a continuum approximation leading to the nonlinear Schrödinger equation

$$i\frac{\partial F_1}{\partial(\epsilon^2t)}+P\frac{\partial^2F_1}{\partial\xi^2}+Q|F_1|^2F_1=0\ , \tag{10}$$

where $\xi=z-v_gt$ and z denotes position in the (continuous) chain. v_g is the group velocity and the constants P and Q are given by

$$Q=16\frac{V_\infty a^4}{m\omega}\ , \tag{11}$$

$$P=\frac{2kd^2V_\infty a^2}{m^2\omega^3}\ . \tag{12}$$

The solution of the nonlinear Schrödinger equation is well known and can be found in Ref. 11 for instance. For

our purpose here, it is sufficient to know that it consists of a cosine wave modulated by a hyperbolic secant. We used this solution as an initial condition in our model and integrated the equations of motion numerically. In Fig. 2 we show that such solutions indeed propagate easily along the chain. In addition, a collision between two such pulses is shown to be nonlinear, with the pulses surviving the collision. In order to test the robustness of the solution, we replaced the hyperbolic secant by a Lorentzian, and see that the pulse still propagates.

C. Purely harmonic limit

For future reference, we first consider the trivial case where the nonlinear potential is completely omitted

$$m\ddot{y}_n = k(y_{n+1}+y_{n-1}-2y_n) \ . \tag{13}$$

In this case, we find that pulses of virtually any shape propagate without dispersing much over biologically significant distances (hundreds of base pairs). An initial condition that relates to solitary-wave solutions is, for example,

$$y_n = A \ \mathrm{sech}(qnd-\omega t)|_{t=0} \ , \tag{14}$$

with $A=8$ Å and $q=0.2$ Å^{-1} corresponding to a width at half-maximum of approximately six base pairs. We gave to each particle in the pulse an initial velocity corresponding to the time derivative of Eq. (14) with $v \equiv \omega/\alpha = 15$ Å/ps. This behavior is shown in Fig. 3. If the pulse is given no initial velocity, it breaks up into two smaller pulses propagating without dispersing in opposite directions. This case is interesting for two reasons, first because whatever the biochemical process which creates an initial stretch is, it is questionable that it will give the particles in the pulse a velocity corresponding precisely to the derivative of Eq. (14); second, it allowed us to check that our computer program was indeed working properly. When propagation occurs and no nonlinear forces are present, the pulse is a simple superposition or wave packet which degrades in shape only at a rate determined by the dispersion among the various wave components.

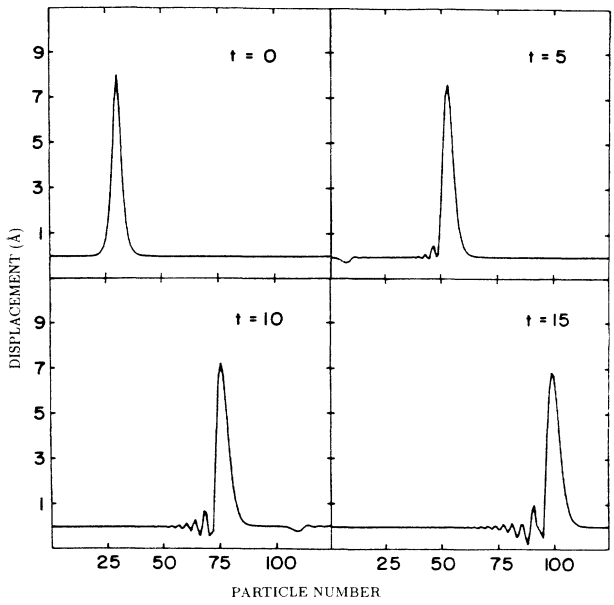

FIG. 3. Propagation of a pulse [$A=8$ Å, $q=0.2$ Å^{-1}, see Eq. (14)] with an initial velocity of 15 Å/ps in the purely harmonic case. Time is indicated in picoseconds.

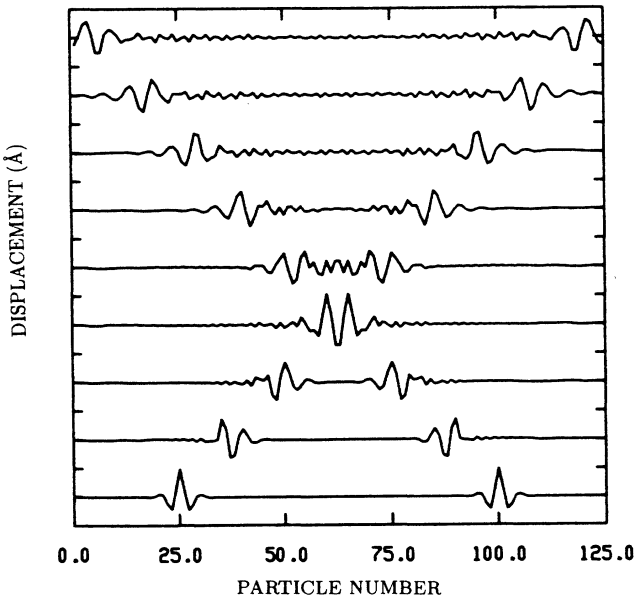

FIG. 2. Collision between two solutions of the NLS equation in our model. The amplitude of the initial pulse is 0.05 Å and the pulse width is approximately 30 Å. The chain is shown every 8 ps, starting at $t=0$. The vertical scale has been shifted up by 0.1 Å for each time. $V_\infty = 0.24$ eV corresponding to two hydrogen bonds.

D. General (nonlinear) case

Before proceeding to a detailed analysis of our work, we want to mention here one of the conclusions of our study, namely the existence of two distinct dynamical regimes in the system (excluding the special case of the exact asymptotic solution of Sec. III B). The first regime corresponds to the propagation of an initial pulse along the chain while the second one is a regime where an initial pulse is pinned and does not propagate. As will be shown in more detail below, the occurrence of one regime or the other depends crucially on the relative values of a few parameters describing the system.

The fact that the chain is described by a set of nonlinear differential equations makes it difficult to find a criterion for propagation. More precisely, one can ask the question: When, given all the characteristics of the chain, does an initial pulse of arbitrary shape propagate? We resort to more heuristic arguments in order to find a

propagation criterion. When the nonlinear force is present in the equation of motion for y_n, propagation depends crucially on the balance between the shearing forces (acting between nearest neighbors) and the nonlinear force [acting wholly within a base pair, or in the case of the equivalent model of Fig. 1(b), on each particle individually]. If the forces acting on the particles in the pulse are essentially shearing forces, then the pulse propagates over long distances, but this case is merely the one mentioned in Sec. III C where the nonlinear force was omitted. On the other hand, if the nonlinear forces dominate over, or at least are comparable to the shearing forces, our numerical calculations indicate that the pulse is pinned. This observation provides a basis for the derivation of a simple propagation criterion. If the net shearing force acting on most particles in the pulse is greater than the nonlinear force, the pulse will propagate since the harmonic terms dominate in the equations of motion. We can illustrate this point in a more quantitative way by calculating the net shearing force

$$F_s = k(y_{n+1}+y_{n-1}-2y_n) \tag{15}$$

for each particle in the pulse and comparing it to the nonlinear force acting on the corresponding particle

$$F_{\rm nl} = -\frac{\partial \phi_M}{\partial y_n} \ . \tag{16}$$

[Here and henceforth, for the sake of definiteness, we use the Morse potential Eq. (7).] At this point, in order to make definite predictions, the shape of the the initial pulse has to be selected; we took a hyperbolic secant

$$y_n(x) = A\ \mathrm{sech}(qx) \ . \tag{17}$$

Several examples of the distribution of these forces along the chain will be given later. For the time being, we can obtain a rough idea of how the various parameters, for example, the pulse width and height or the nonlinear potential, affect the propagation by comparing the maximum shearing force to the maximum nonlinear force. The calculations are somewhat tedious but straightforward and will not be reproduced here. One finds for the maximum shearing force

$$F_s^{\max} = kA\left[\frac{1}{\cosh[\mathrm{arccosh}(1+\cosh qd)+qd]}\right. \tag{18}$$

$$\left. + \frac{1}{\cosh[\mathrm{arccosh}(1+\cosh qd)-qd]} - \frac{2}{1+\cosh qd}\right] , \tag{19}$$

and for the maximum non-linear force

$$F_{nl}^{\max} = \frac{\ln 2}{2}\frac{V_\infty}{p} \ , \tag{20}$$

where d is the separation between base pairs, p is the inflexion point of the Morse potential, and V_∞ is the asymptotic value of the nonlinear potential.

A simple criterion for propagation would thus be

$$F_s^{\max} \gtrsim F_{nl}^{\max} \ . \tag{21}$$

This condition allows us to discuss, at least qualitatively, the influence of various parameters on the propagation.

For example, increasing the nonlinear potential V_∞ or moving the inflexion point of the potential towards 0; i.e., decreasing p sufficiently, pins the initial pulse; a small value for V_∞ favors propagation, but in this case, as already mentioned before, we are essentially in a situation where the harmonic forces dominate the nonlinear forces and the propagation is mostly harmonic having little to do with the nonlinearity. Even more interesting is the influence of the pulse shape, namely its height A and width $\sim q^{-1}$. The harmonic forces being proportional to A, the higher the pulse, the better for propagating along the chain. The influence of the pulse width is not as obvious, but a careful examination of Eq. (18) leads to the conclusion that sufficiently narrow pulses (q large) propagate whereas broad pulse do not. All these conclusions, although obtained from a very rough analysis, have been checked by numerous computer simulations. Some of the results are presented below. Finally, one could argue that this analysis depends strongly on the shape chosen for the initial pulse, but if the pulse propagates, it does so without dispersing to much and hence the previous analysis can be repeated at any subsequent time. If the pulse does not propagate initially, it rapidly becomes jagged and it is very unlikely that for $t>0$ the shearing forces will ever be able to dominate over the nonlinear forces for most of the particles in the pulse. Let us now examine several examples in more detail.

Pinning. Since we fixed V_∞ and p at realistic values for the DNA chain, let us pin the pulse by making it broad ($q=0.0615$ Å^{-1}), corresponding to a width at half-maximum of ~ 40 Å). The initial harmonic and nonlinear force distributions Eqs. (18)–(20) are shown in Fig. 4. It is clear from this figure that the harmonic forces and the nonlinear forces have comparable magnitudes for a large number of particles in the pulse, hence we do not expect propagation to take place. Indeed, the peak displacement fluctuates in the close vicinity of the initial position while the amplitude of the pulse oscillates wildly between a maximum of 4.0 Å, the initial amplitude, and small amplitudes corresonding to a dispersed pulse. This behavior is shown Fig. 5.

The form in which the energy is stored is the system is plotted as a function of time in Fig. 6. It can be seen that the system relaxes from its initial perturbed state to a dynamically stable one in which its total kinetic energy, shearing potential, and Morse potential energy fluctuate about some constant value. In fact, we can approximately calculate these values by assuming that for large times the amplitude of motion for the particles are fairly small and thus expand the Morse potential in a harmonic approximation leading to

$$m\ddot{y}_n = k(y_{n+1}+y_{n-1}-2y_n) - 4V_\infty a^2 y_n \ , \tag{22}$$

which has plane-wave solutions of amplitude y_0. These can now be substituted into

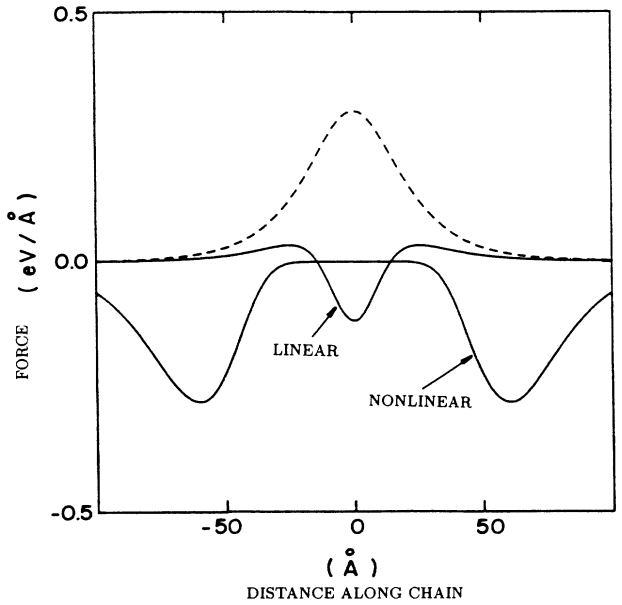

FIG. 4. Force distribution functions for a pinned pulse. The nonlinear force is the dominant term in the equation of motion [Eq. (6)]. The dashed line indicates the initial pulse, Eq. (14) (not to scale).

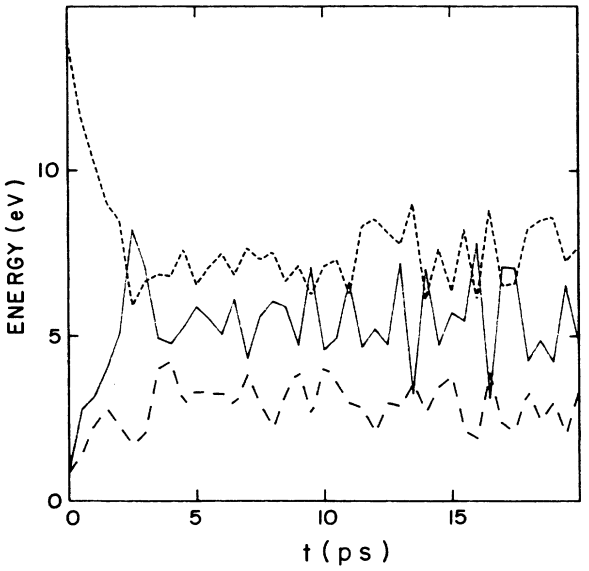

FIG. 6. Total kinetic, (shearing) harmonic, and nonlinear energy (in eV) in the pulse vs time (in picoseconds). The solid line is the kinetic energy. The dashed line is the harmonic potential energy and the dotted line is the nonlinear potential energy stored in the hydrogen bonds.

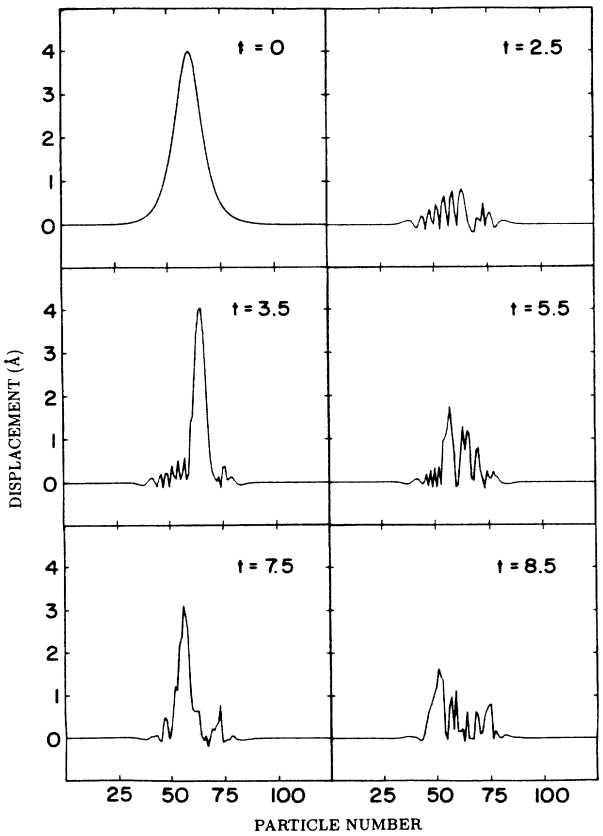

FIG. 5. Solution of the equation of motion for a pinned disturbance. The stretch y_n (in angstroms) is shown vs the position of a particle in the chain. Time is in picoseconds.

$$\bar{\phi}_{\text{Morse}} = \frac{\omega}{2\pi}\int_0^{2\pi/\omega} dt\, 2V_\infty a^2 y_n^2(t) = V_\infty a^2 y_0^2 , \tag{23}$$

$$\bar{\phi}_{\text{shearing}} = \frac{\omega}{2\pi}\int_0^{2\pi/\omega} dt \frac{k}{2}[y_n(t)-y_{n-1}(t)]^2 , = k y_0^2 \sin^2(qd/2) . \tag{24}$$

The ratio of these quantities is

$$\frac{\bar{\phi}_{\text{Morse}}}{\bar{\phi}_{\text{shearing}}} = \frac{V_\infty a^2}{k}\frac{1}{\sin^2(qd/2)} , \tag{25}$$

where $q=2\pi/\lambda$ is the wave number. When the above linearization is valid, i.e., for large t, the chain has become jagged (Fig. 5). The corresponding wavelength of the spatial oscillations, however, cannot become smaller than the separation $2d$ between base pairs because of the discrete nature of the lattice. Hence, taking $\lambda=2d$ (i.e., $q=\pi/d$) in Eq. (24), the ratio becomes 2.8 for the numerical values used previously, which is in good agreement with the computed values (Fig. 6). As expected, the harmonic energy fluctuates in phase with the nonlinear potential energy since any stretching of the lattice will increase both of them simultaneously. Both of these energies are, in turn, out of phase with the kinetic energy, which is at a minimum when the stretches are at a maximum. Perhaps the most important feature of this system is the fact that even though the system relaxes relatively rapidly, the energy of an initial disturbance remains fairly

localized for biologically significant durations.

Propagation. According to our simple propagation criterion, for a given V_∞ and a given p, a sufficiently narrow pulse should propagate if its amplitude is not too small. We took $q=0.2$ Å^{-1} and $A=8$ Å. The results are shown in Fig. 7. The force distributions functions are shown in Fig. 8 and it can be seen that the harmonic (shearing) force largely overcomes the nonlinear force so that propagation occurs. A rather high pulse had to be used because of the rather large value of V_∞; this might be a problem because the shearing forces in the pulse are now quite large. Hence it suggests that if a V_∞ should be large in a model representing the DNA molecule, pulses are unlikely to propagate along the DNA chain.

Propagation in this case is similar to propagation in a completely harmonic chain; the nonlinear forces are negligible compared to the shearing harmonic forces and play no role in the propagation. The pulses that propagate are narrow and large-amplitude ones, i.e., those the Fourier transform of which contains many short-wavelength components, hence, as they propagate, they will also disperse greatly. This appears clearly in Fig. 7. One should compare Fig. 7 with Fig. 3; they correspond to the propagation of the same initial pulse in the presence and in the absence of the nonlinear potential, respectively. It can be seen that the addition of the nonlinear forces does not cause any narrowing of the propagating pulse. The nonlinear pulse is broadened compared to the harmonic case. That propagation is primarily a linear phenomenon is further supported by the fact that during a collision of two pulses, the total displacement is the sum of the two pulses.

At this point, it is useful to summarize the results we have obtained as far as propagation is concerned. When the initial pulse is of arbitrary shape, we have seen that it propagates only if it is such that the linear forces dominate in the equation of motion. This is the essence of the propagation criterion described before. In particular, it means that a small-amplitude pulse is unlikely to propagate because in that case, the linear forces are too small. This is true *except* when the initial (small-amplitude) pulse is a solution of the NLS equation. Then, the pulse propagators (Fig. 2), and the forces responsible for the propagation are the nonlinear forces (Fig. 4).

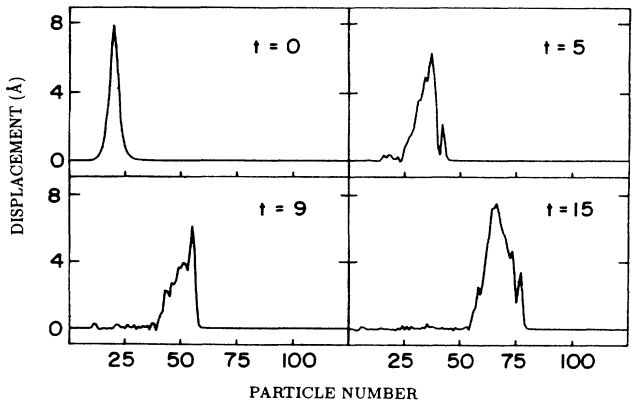

FIG. 7. Propagation of a narrow, high pulse in a nonlinear chain [$A=8$ Å, $q=0.2$ Å^{-1}, see Eq. (14)]. Notice that the pulse disperses rather quickly. Time is indicated in picoseconds.

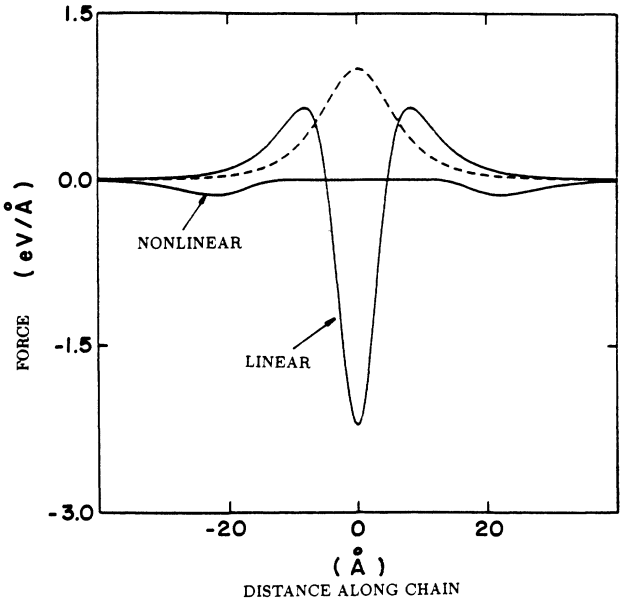

FIG. 8. Force distribution function for the pulse of Fig. 7. The linear (shearing) force largely dominates over the nonlinear force. The dashed line indicates the initial pulse (not to scale).

E. Degeneration of a small-amplitude vibrational mode

If one performs an expansion of the Morse potential and only the linear terms are kept in the equations of motion, the solutions are pure plane waves

$$y_n = y_{n0}\exp[-i(qnd-\omega t)] \,. \tag{26}$$

ω and q are related by the dispersion relation

$$\omega^2 = \frac{4}{m}\left[k\sin^2\left[\frac{qd}{2}\right]+V_\infty a^2\right] \,. \tag{27}$$

This is an optical dispersion branch. The simplification is valid only for small amplitudes. It is easy to check that with the values adopted in Sec. III D for the various parameters appearing in Eq. (27), ω depends on q only very weakly.

The nonlinearity has a dramatic effect on such vibrational mode. In order to study this situation, we excited the chain in one of its vibrational modes, Eqs. (26) and (27) (the amplitude was taken to be 0.05 Å, the wavelength was 75 Å) and we integrated the equations of motions [Eq. (6)] numerically. The results are shown in Fig. 9. In time, the initial cosine wave becomes peaked, i.e., large stretches appear and propagate in the chain. This degeneration of a vibrational mode becomes even

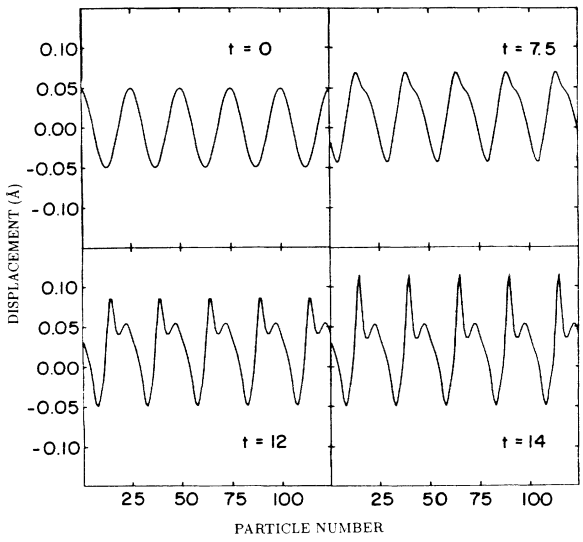

FIG. 9. Propagation of a small-amplitude vibrational mode along the chain. Time is given in picoseconds.

more pronounced for longer times. It is, in fact, the asymmetry of the Morse potential for positive and negative values of y_n which favors stretches over compressions and causes this interesting phenomenon to appear.

IV. CONCLUSIONS

Perhaps the most important conclusion of our study is the existence of two different dynamical regimes, one in which the linear shearing forces dominate over the nonlinear forces and propagation of an initial pulselike disturbance takes place. This propagation is harmonic; nonlinearity does not play any role in this case. We find a second regime in which the nonlinear forces are of magnitude comparable to or larger than that of the linear forces, in which case an initial disturbance is pinned. This seems to indicate that the nonlinearity of the HB between base pairs plays little role in cases where propagation occurs, its principal effect is to pin sufficiently small and/or sufficiently broad pulses. Physically, this is caused by the fact that the nonlinear springs in the one-dimensional equivalent chain [Fig. 1(b)] do not participate directly in the energy transfer between adjacent particles. But, if the initial pulse is a small-amplitude solution of the NLS equation, it can propagate even though the nonlinear forces are now the most important ones in the equations of motion. This is, however, a very special case and it is questionable whether a biochemical process could generate such a pulse.

This dynamical property that the model prevents the spreading of an initial energy pulse is not necessarily a drawback since it provides us with a mean of localizing small amounts of energy in the DNA chain over possibly significant periods of time. The nonlinear springs store a large fraction of the total energy and prevent its spreading in the lattice. This can be easily understood if we realize that as soon as the stretch is large enough, a constant amount of energy is stored in the nonlinear springs while their role in the dynamics is now unimportant since the potential is then almost flat (i.e., zero force).

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