Journal of Biological Physics **18**: 19–29, 1991.

Nonlinearly Coupled Double Chain Systems

KYLE FORINASH and JOHN KEENEY
Natural Science Division, Indiana University Southeast, New Albany, IN 47150, U.S.A.

(Received: 23 May 1990; revised: 31 October 1990)

Abstract. We report here on numerical studies of a pair of linearly coupled mass chains with nonlinear ϕ^4 coupling between the two chains. General implications for double chain systems known to exist in nature such as DNA and RNA are discussed.

Key words. Double chain system, ϕ^4 coupling.

1. Introduction

In this paper, we study the dynamics of a double chain system with linear coupling along the chains and nonlinear coupling between the chains. The motivation for studying such a system, apart from the intrinsic interest of expanding the well-studied singlechain model for crystal structure to two dimensions, is a possible connection with DNA and RNA which are known to be double chain systems. That a biological system should include nonlinear forces comes from the observation that in order for living organisms to grow and reproduce, normal dissipative processes must be overcome. One of the interesting phenomena seen in nonlinear dynamical systems is the self-focussing of energy with the existence of long-lived coherent structures. It is this property that has led to various attempts to apply nonlinear dynamics to biological systems [1–5]. Recent attempts by Peyrard and Bishop to model DNA molecules have focussed on the inter-chain hydrogen bond and the melting process in which the two chains become separated [6]. That paper proposed a Morse potential as the inter-chain coupling. Although a Morse potential is known to accurately represent the hydrogen bond, the present paper takes the view that because of the complicated environment surrounding the DNA molecule, it is appropriate to examine a more general inter-chain potential such as the ϕ^4 potential. For example, it is known that large proteins attach to the DNA and RNA molecule during transcription and replication processes and it seems evident that this must affect the inter-chain bonding. The ϕ^4 potential was chosen because it has two stable states and can thus model the observed open and closed states of DNA and RNA.

The outline of the paper is as follows: Section 2 describes the details of the model and approximate analytical solutions. Part 3 discusses results of a numerical simulation of the discrete model. The final part recapitulates the results found in the previous sections and notes possible implications for biological systems.

2. The Model

Two important processes occurring in DNA (transcription and replication) involve changes in the hydrogen bond link between chains. In the transition from closed to open states, changes occur primarily in the hydrogen bond length rather than in the phosphate backbone spacing. For this reason, only transverse motion is considered in the following discussion. Other mechanical changes, for example longitudinal motion, unfolding and uncoiling, are not taken into account.

Let u_n stand for the displacement from equilibrium of the nth base in the top chain and w_n correspond to the displacement from equilibrium of bases in the bottom chain. Assuming a linear coupling along the lengths of each chain (but with vertical motion only) and a nonlinear ϕ^4 potential of

$$V(u_n - w_n) = -g(u_n - w_n)^2 + (1/4)\lambda(u_n - w_n)^4$$

between the upper and lower chain gives an equation of motion for each chain of

$$m\ddot{u}_n = k(2u_n - u_{n-1} - u_{n+1}) - g(u_n - w_n) + \lambda(u_n - w_n)^3,$$
$$m\ddot{w}_n = k(2w_n - w_{n-1} - w_{n+1}) + g(u_n - w_n) - \lambda(u_n - w_n)^3.$$

The figures below were generated by calculating velocities and accelerations and subsequent new positions directly from these force equations for each mass, thus representing a truly discrete model. Free end boundary conditions were chosen to reflect more realistically the conditions found in an actual DNA molecule. Energies were calculated directly from the model and were conserved within 1%. The position calculations were checked in two ways. The two equations were reduced to four first-order equations and a fourth-order Runga–Kutta algorithm was used to time step to the new positions [7]. A second test program was written using a packaged subroutine (using Gear's method) which simultaneously time stepped the $4n$ equations of motion to new values for u and w. All three methods agreed in their results.

In order to arrive at approximate but analytic solutions, the continuous case is obtained with the following standard substitutions

$$u_{n-1} = u_n - Du'_n + D^2u''_n/2 + \cdots,$$
$$u_{n+1} = u_n + Du'_n + D^2u''_n/2 + \cdots,$$

where D is the distance between molecules on the chain. Identical expansions can be used for the lower chain so that the following continuous equations result:

$$mu_{tt} = k_0u_{xx} + g(u - w) - \lambda(u - w)^3,$$
$$mw_{tt} = k_0w_{xx} - g(u - w) + \lambda(u - w)^3,$$

where u and w are now continuous functions of x and t and subscripts refer to derivatives. Also $k_0 = D^2k$.

These two equations can be combined in two ways, representing the motion of the upper and lower chains which is in-phase or out-of-phase with each other. The in-phase motion does not stretch the nonlinear bond, thus representing a single linear chain and will not be considered here. The single equation representing out-of-phase motion of the top and bottom chain is represented by

$$m(u_{tt} - w_{tt}) = k_0(u_{xx} - w_{xx}) + 2g(u - w) - 2\lambda(u - w)^3.$$

Introducing the variable $y = u - w$ as the relative interchain displacement, we arrive at the kink equation

$$my_{tt} = k_0 y_{xx} + 2gy - 2\lambda y^3.$$

This equation has the following solitary wave solutions [8]

$$y(x, t) = \pm y_0 \tanh((x - vt)/L)$$

with

$$y_0 = (g/\lambda)^{1/2} \quad \text{and} \quad L = (m(c_0^2 - v^2)/g)^{1/2}.$$

Here, $c_0^2 = k_0/m$ is the linear speed of sound on the chain and L is the length of the soliton.

3. Numerical Results

In the following figures, we used the hyperbolic tangent solution for the continuous approximation as the initial conditions in the discrete computer model with one-half of the total displacement on the top and bottom chain. The parameters m and λ were chosen to be equal to one. The linear coupling k was chosen in most cases to be 50 and g was equal to 1.4. Other values were also examined, but the present values seemed to be the most convenient for graphing purposes. Most of the simulations were with 93 pairs of mass points. Other chain lengths were examined but the length did not seem to affect the results.

Our computer model shows stable stationary (Figure 1) and stable translating forms of this solution for values of L larger than several D. It is expected that discreteness effects such as trapping will appear for small values of L [9]. Cases of small L are not examined in this paper.

We tested the stability of the our solitary wave in the following ways: The hyperbolic tangent shape was perturbed; kink anti-kink pairs were collided at various speeds; small amplitude linear wave packets were collided with a single kink; random noise representing a thermal bath was included on some runs.

When the shape of a solitary solution was perturbed, the shape oscillates around the hyperbolic tangent shape with some radiative loss (Figure 2). This gives a moving solution the appearance of speeding up and slowing down. This is of some

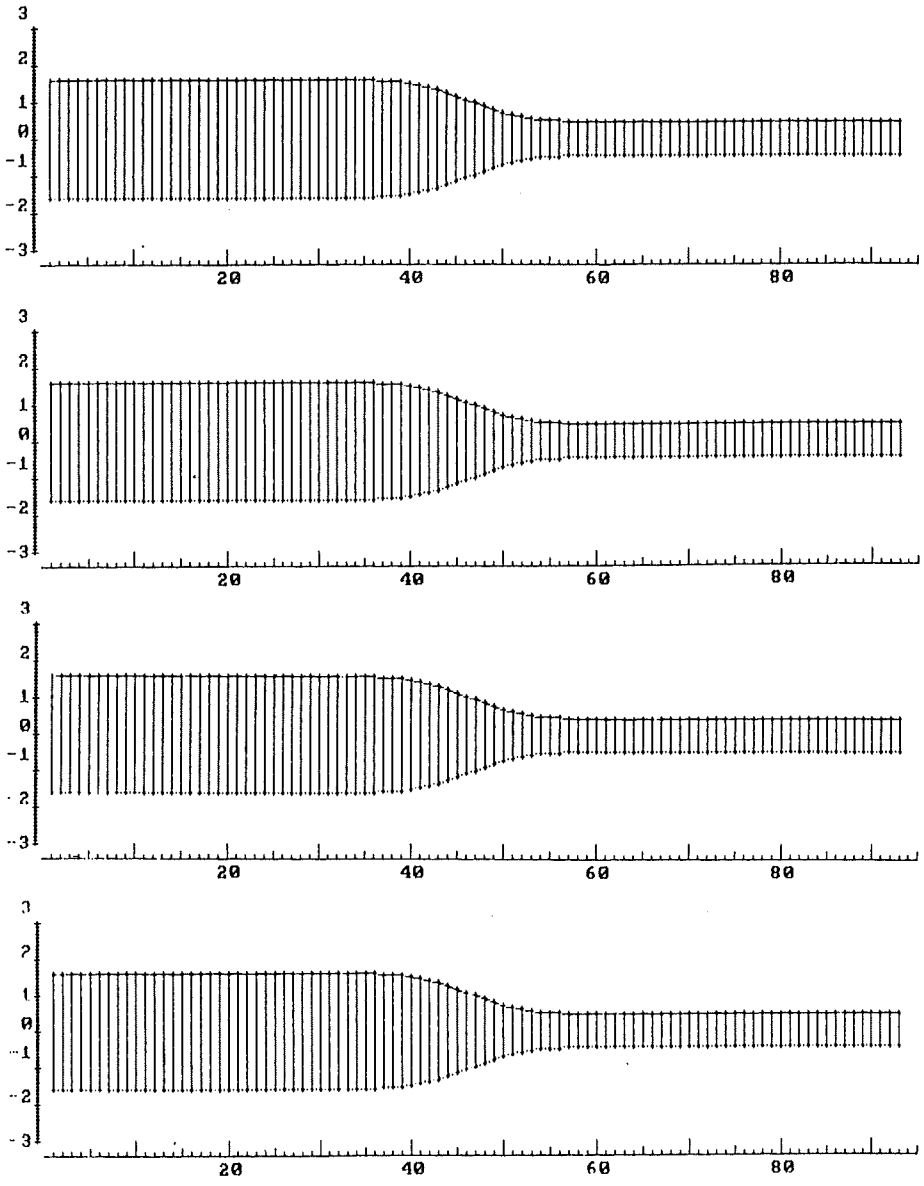

Fig. 1. Time sequence of a stable soliton at $t = 0$, $t = 10$, $t = 20$, and $t = 30$ time units. The initial condition is the analytic hyperbolic tangent solution. Here $\lambda = 1$, $g = 1.4$, and $k = 50$.

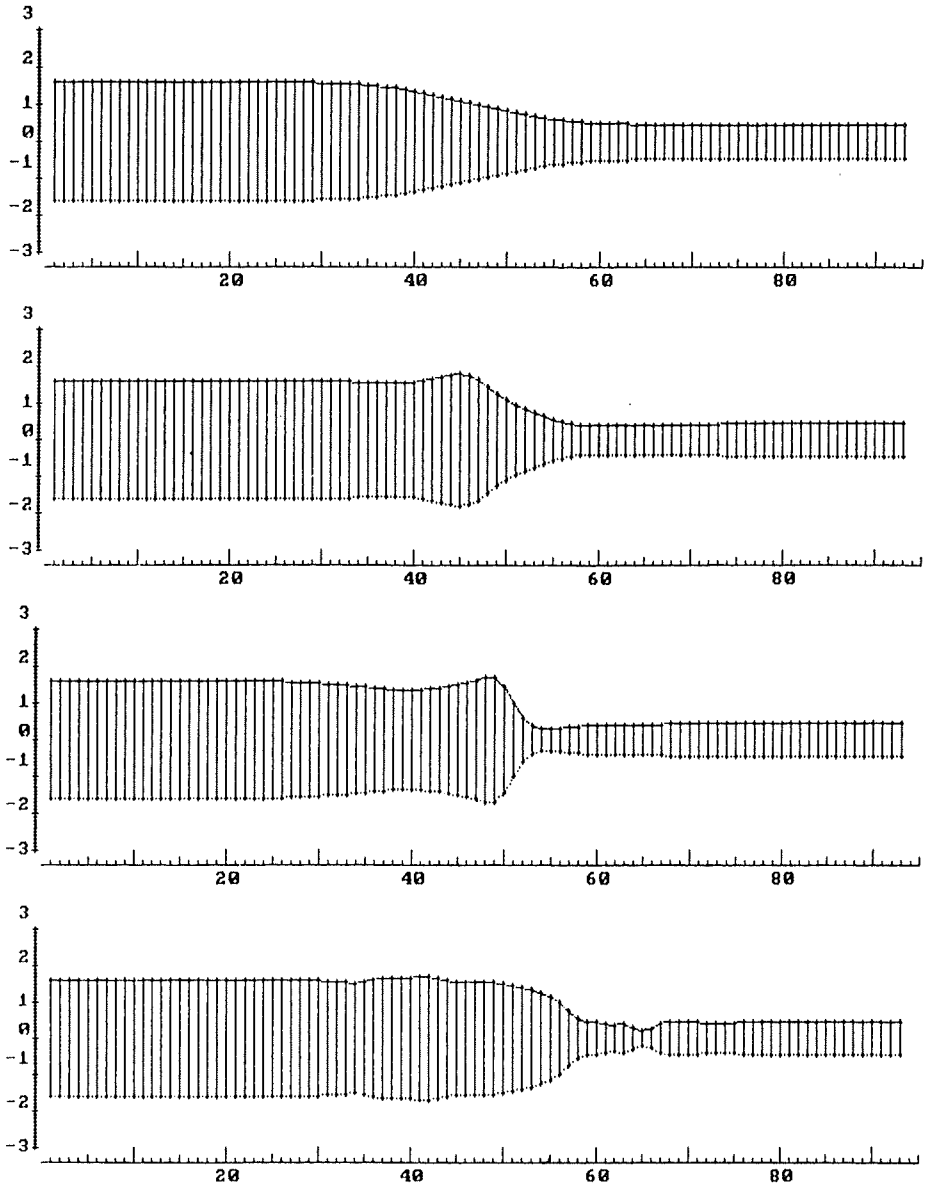

Fig. 2. Time sequence of a perturbed hyperbolic tangent solution as initial condition at $t = 0$, $t = 1.6$, $t = 2.4$, and $t = 10$ time units. Here $\lambda = 1$, $g = 1.4$, and $k = 10$.

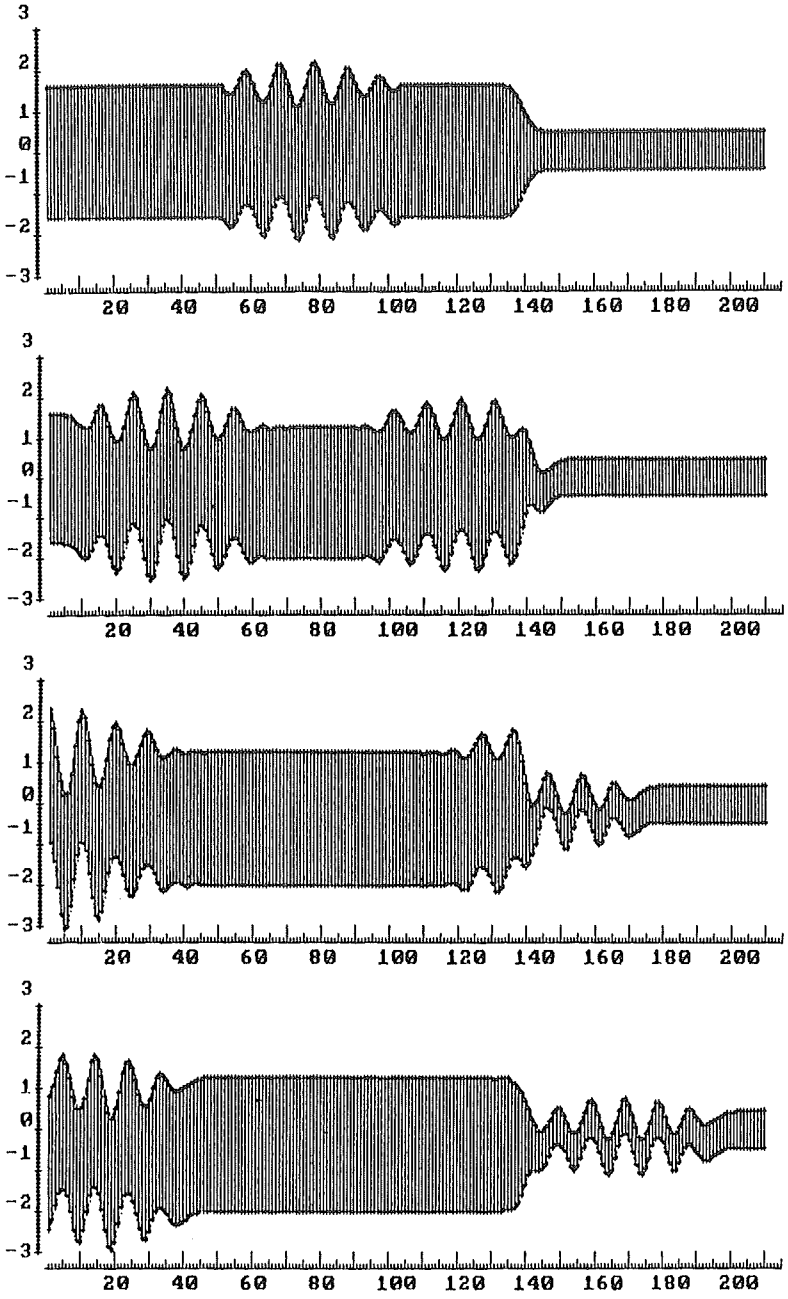

Fig. 3. Time sequence of a stationary kink hit with a small amplitude wave packet at $t = 0.2$, $t = 14.6$, $t = 22.8$, and $t = 30$ time units. Here $\lambda = 1$, $g = 1.4$, and $k = 50$. (The wave packet has no initial velocity and therefore splits into two wave packets traveling in opposite directions.)

interest in the biological problem, since the process of opening and closing along a DNA chain and the transcription process is observed to change speeds, accelerating and then slowing down (Freifelder [11], p. 329). For larger perturbations, the hyperbolic shape was not stable but broke up into phonons.

Theodorakopoulous *et al.* [10] have examined the stability of the ϕ^4 discrete single chain under collisions with small amplitude (linear) wavepackets. They found that the kink remains stable under such collisions but wavepackets of shorter wavelength cause the kink to broaden and to gain a velocity. Identical results were obtained in our model (Figure 3). (This figure has more mass pairs than the other figures.) The implications for a real DNA chain are several. It is known that transcription is controlled by the attachment of proteins at promoter and inhibitor locations [11]. It is reasonable to suppose that protein attachment could have several mechanical effects, including the creation of linear wavepackets on the chain, thus prompting motion of existing bubbles (i.e. kinks).

The ϕ^4 equation is known not to have true breather modes (analytic solutions consisting of stable paired kink anti-kink solutions). However, it has been shown that breather-like modes can exist over short periods of time [8]. With faster initial velocities, kink and anti-kink appear to quickly bounce off each other like true solitons but with linear radiative loss, possibly as a consequence of discreteness (Figure 4). Our model also shows temporary breather modes (Figure 5). The initial conditions which give rise to such modes require a kink anti-kink collision of low velocity. The incoming pair interact for a much longer time than would be expected for a simple collision and appear to form a breathing mode. The motion of the incoming pair appears to slowly stop and then start up again as the kinks reverse direction. For the parameters chosen for Figure 5, the kinks remained trapped in a breather mode for times equal to our longest time run of 50 time units.

The effect of random perturbations of the individual displacements away from the hyperbolic tangent solution was examined. This noise was introduced periodically (every 20 time steps) and represents interaction with a thermal bath. Solutions were found to be very stable for the time durations examined and for perturbations in displacements up to an amount large enough to carry the mass into the other stable state.

We have also examined the consequences of allowing the kinks to interact with the free ends of the chain. In these cases, the kink or anti-kink reflects off the end with unchanged velocity. One result of reflection is the possibility that the temporary breather modes mentioned previously will reappear periodically as the kinks return to the same position on the chain after reflection from an end. In other words, once launched, these breather modes would reoccur periodically at the same location on the chain. Of interest is the observation that bubbles form in DNA chains as (apparently) random fluctuations which molecular biologists also refer to as breathers [11].

The above analytic kink solutions do not specify how much of the displacement is initially in the upper chain and how much in the lower chain. Thus, displacements

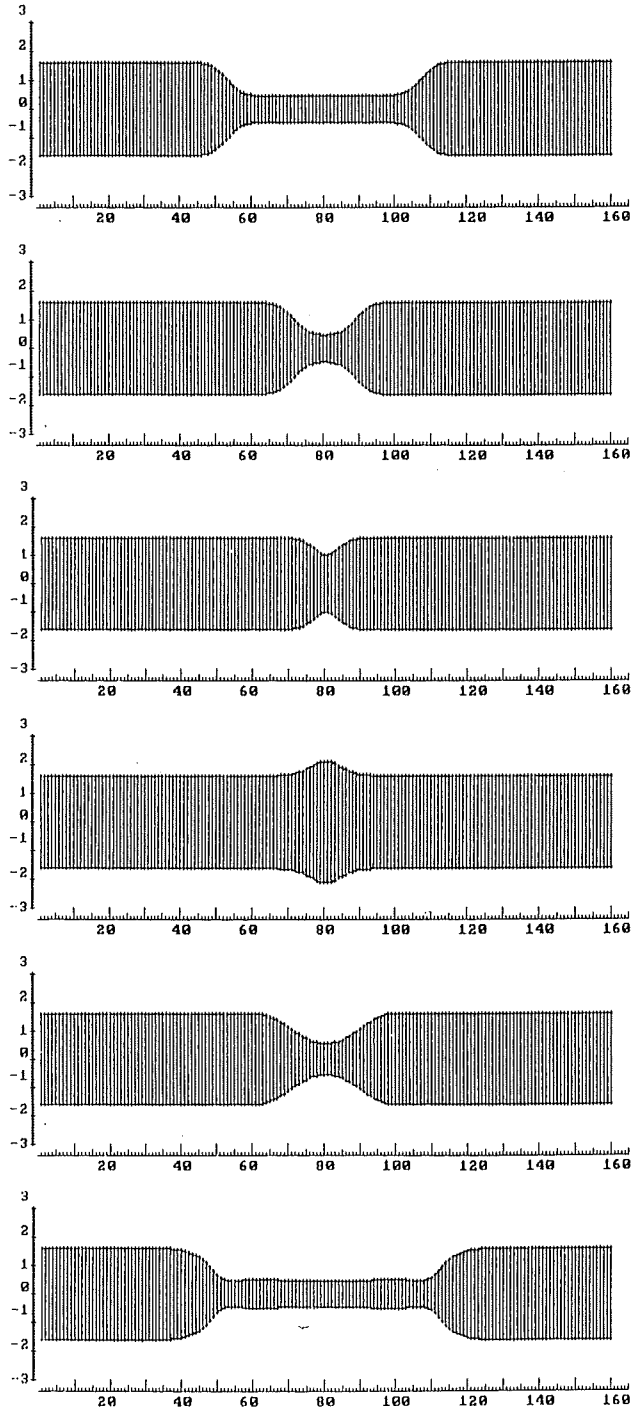

Fig. 4. Time sequence of colliding anti-kinks at $t = 0$, $t = 3.7$, $t = 4.9$, $t = 5.7$, $t = 7.6$, and $t = 13.1$ time units. Here $\lambda = 1$, $g = 1.4$, and $k = 50$ and initial speeds are set at 5 (in arbitrary units).

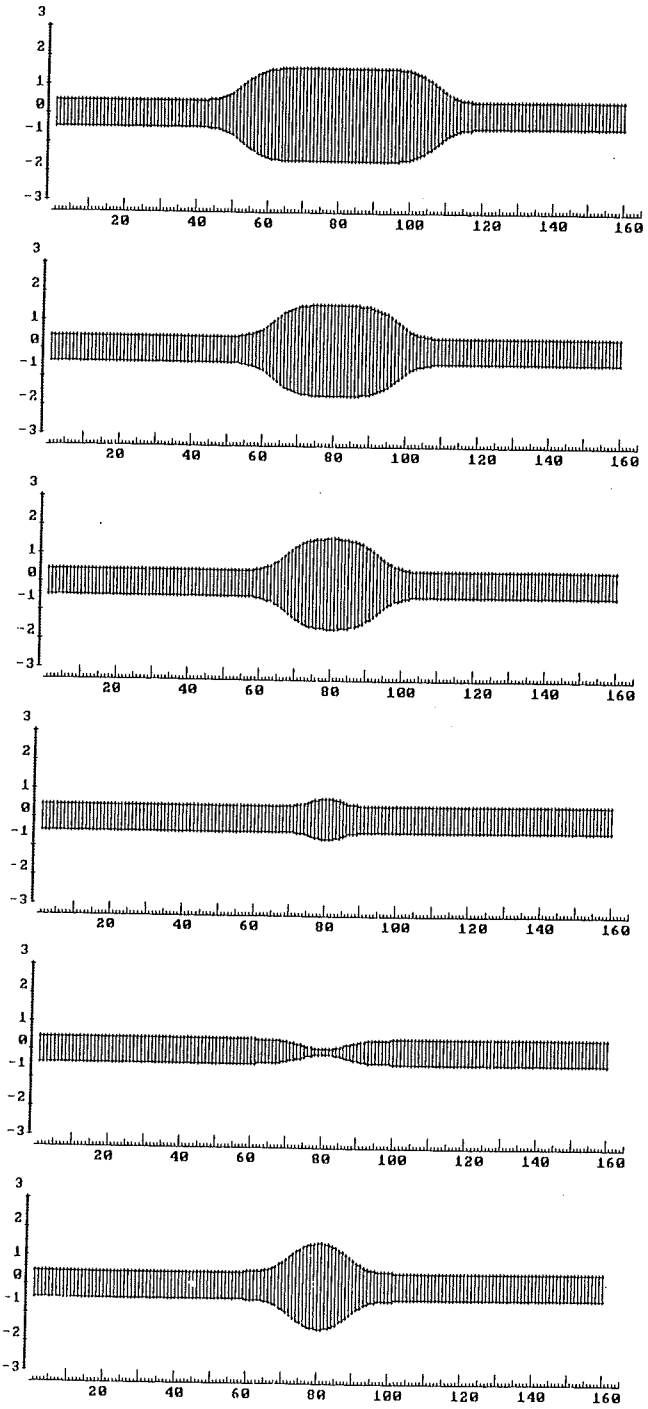

Fig. 5. Time sequence of slowly colliding kinks forming a long-lasting breather mode at $t = 0$, $t = 10.0$, $t = 14.5$, $t = 20.0$, $t = 21.2$, and $t = 24.5$ time units. Here $\lambda = 1$, $g = 1.4$, and $k = 50$ and initial speeds are set at 1 (in arbitrary units).

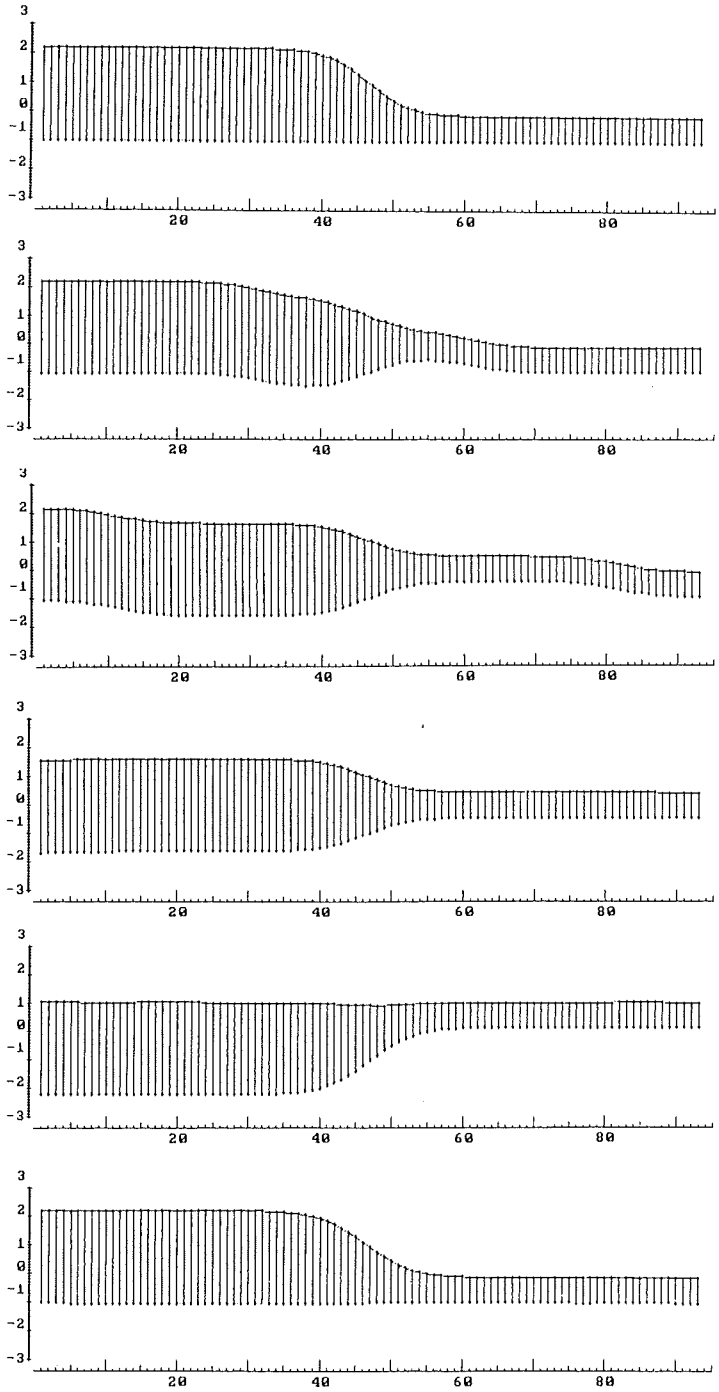

Fig. 6. Time sequence with an initial condition of all displacement on one side at $t = 0$, $t = 2.0$, $t = 5.0$, $t = 6.6$, $t = 13.0$, and $t = 26.7$. Here $\lambda = 1$, $g = 1.4$ and $k = 50$.

of the shape shown in Figure 6 with all of the displacement on one chain should also be a solution. Although there is some radiative loss, these initial conditions give rise to stable configurations on the double chain. These initial conditions reappear after reflection from the ends with only small changes in shape. In fact, keeping the total displacement y constant but shifting the relative displacement of the top and bottom chains by any amount, always results in stable configurations.

4. Conclusion

It has been shown in this paper that the special case of a double chain with nonlinear coupling between chains where only vertical motion stretching the interchain bonding is allowed, reduces to a well-known soliton equation in the continuum limit. Numerical studies show the analytic solutions to the continuum approximation to be stable but not exact solutions of the discrete case. These solutions are also stable under perturbations of initial conditions and continued random perturbations representing thermal motion. Collision with wave packets also has no serious detrimental effects to the stable solutions.

A simple double chain model with only linear coupling cannot result in stable open and closed states but rather dissipates energy uniformly throughout its length. This indicates that, in order for the physical structures known to occur during replication and transcription process in DNA and RNA, nonlinear mechanisms must be active [12]. It is encouraging that open and closed states resulting from the double minimum of the ϕ^4 potential are stable under the various perturbations described here. That such a generic nonlinear potential results in stable configurations even in the discrete case indicates that nature does not have to be particularly devious to account for the observed events.

References

1. Englander, S. W., Kallenbach, N. R., Heeger, A. J., Krumhansl, J. A., and Kitwin, S.: *Proc. Natl. Acad. Sci. U.S.A.* **777** (1980), 7222.
2. Yomosa, S.: *Phys. Rev. A* **27** (1983), 2120; **30** (1984), 474.
3. Takeno, S. and Homma, S.: *Progr. Theoret. Phys.* **77** (1987), 548.
4. Zhang, Chun-Ting: *Phys. Rev. A* **35** (1987), 886.
5. Muto, V., Scott, A. C., and Christiansen, P. C.: *Phys. Lett.* **A136** (1989), 33.
6. Peyrard, M. and Bishop, A. R.: *Phys. Rev. Lett.* **62** (1989), 2755.
7. Press, W. H., Flannery, P. B., Teukolsky, S. A., and Vetterling, W. T.: *Numerical Recipes*, Cambridge University Press, Cambridge, 1989.
8. Dodd, R. K., Eilbeck, J. C., Gibbon, J. D., and Morris, H. C.: *Solitons and Nonlinear Wave Equations*, Academic Press, London, 1982.
9. Peyrard, M., Pnevmatikos, S., and Flytzanis, N.: *Physica* **19D** (1986), 268.
10. Theodorakopoulos, N., Wünderlich, W., and Klein, R.: *Solid State Comm.* **33** (1980), 213.
11. Freifelder, D.: *Molecular Biology*, Jones and Bartlett, Boston, 1987.
12. Prohofsky, E. W.: *Phys. Rev.* **A 38** (1988), 1538.