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Coupled Multi-Component Systems: A Simple Membrane Model

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Abstract. We present initial results regarding the existence, stability and interaction of linear and nonlinear vibrational modes in a system of two coupled, one dimensional lattices with unequal numbers of masses. The effects on these nonlinear modes of coupling a near continuum system to a discrete system using a nonlinear coupling are examined. This numerical model is a first step towards investigating the dynamical behavior of a flexible sheet coupled nonlinearly to a semi-rigid support, a system which could conceivably represent a biological cell membrane with a supporting protein network. General implications for the dynamical behavior of continuum systems coupled nonlinearly to discrete systems are introduced.

Key words: Breather modes, discrete systems, intrinsic localized modes, membrane dynamics, nonlinear systems

1. Introduction

A real membrane-cytoskeleton interface is extremely complex with large molecules floating in what is basically a two dimensional fluid analogous to a liquid crystal. Some of these imbedded molecules extend outward from only one side of the membrane while others span the membrane forming channels for ion flow through the membrane [1, 2]. In most cells the external membrane shape is determined internally by an elastic system of proteins (the cytoskeleton) which is coupled to other proteins embedded in the cell membrane. This combined system is responsible for the shape and locomotion of some cells and the distinctive shape of erythrocytes (the most studied, experimentally, of cells).

Earlier attempts to numerically model a biological membrane have for the most part focused on the membrane bi-layer (see [3] and references therein) and static quantities such as the shear modulus, although at least a few recent authors have alluded to the dynamics of the attached protein structure which acts as a flexible support or framework for the membrane [4–7]. It is clear from experimental data that the protein cytoskeleton plays an important role in membrane structure and function and several authors have remarked on the dynamical aspects of the membrane system, including the effects of coupling between the membrane and supporting skeleton [8–12]. As an initial step towards modeling the dynamical be-

havior of this complicated structure we have created a computer model of a double chain system of unequal numbers of masses. The chain with the larger number of masses in this model represents a flexible sheet (a continuum) whereas the chain with fewer masses represents the protein substructure (a discrete system). As the ratio of the number of masses between the two chains increases the model more accurately represents a continuum system attached to a discrete but flexible support system.

This model is an extension of a well studied double chain model (with equal numbers of masses) thought to be representative of the dynamical behavior of DNA and similar two component systems [13–15]. The interesting dynamics found in that earlier work forms part of the motivation for studying the present model. The view that biological systems incorporate nonlinear forces arises 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 both biological systems and nonlinear dynamical systems is self focussing of energy with the existence of long lived coherent dynamical structures (see for example [16]). The present work extends these observations to a system where near continuum and discreteness are coupled.

The outline of the paper is as follows; section two describes the details of the model and the numerical scheme used to solve the dynamical equations. Part three discusses results of numerical simulations of the model for several parameter ranges. The final part recapitulates the results found in the previous sections and speculates on the implications for systems where discreteness interacts with a continuum through nonlinear coupling.

2. The Model

In any attempt at modeling complex systems choices must be made as to the relevant features to try to include in the model. Real cell membranes typically consist of a bi-layer of phospholipid molecules which exhibit complex interactions with each other and the immediate environment, including Van der Waals forces between the phospholipid tails, hydrophobic and hydrophilic interactions with the surrounding medium and packing forces between phospholipid heads. The attached cytoskeleton further complicates the system to be modeled.

The bi-layer is essentially a two dimensional liquid with the result that lateral positional order of the molecules is expected to change over short distances and times. As a result, lateral motion is expected to be damped. This also indicates that average properties such as tension, elasticity and bending are the more appropriate characteristics to include in a model of the bi-layer [2].

The absences of long term or long range lateral correlation in the bi-layer of a real biological membrane coupled with the fact that real membranes exist in their normal state with thermally induced out of plane 'roughness' or undulations indicates that transverse motion of the membrane is a significant feature to be included

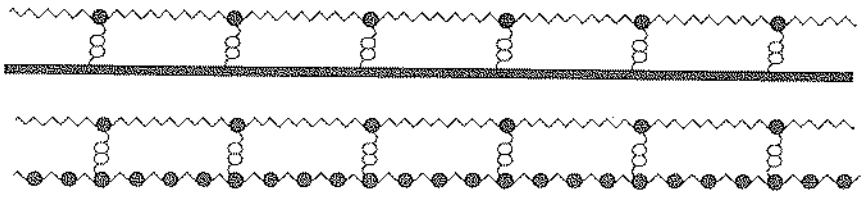

Figure 1. A one dimensional cross section of a flexible sheet attached periodically and nonlinearly to a linear mass chain (1a). The actual system modeled, a double chain system with different numbers of masses on each chain, is shown in 1b.

in the model. For this reason and a desire to keep the computer model tractable, motion is restricted to out of plane (transverse) motion only. Other mechanical changes, for example longitudinal motion, in-plane rotation of molecules, separation of the protein sub structure (bottom chain) from the membrane (top chain), and extension to a three dimensional model have not been considered here.

Although the membrane bi-layer shows no long term or long scale order (being essentially a fluid) the cytoskeleton, in contrast has a very regular structure with periodic features which show clearly in electron micrographs of erythrocyte structure [1]. For this reason and to establish a basis of known results for future work the present paper examines interactions between periodic arrays with fixed periodicity rather than a random or disordered pattern.

The model envisioned here is a one dimensional cross section of a linear, flexible sheet attached periodically and nonlinearly to a linear mass chain (Figure 1a). The actual computer model is of a chain of many masses coupled periodically to a chain of fewer masses (Figure 1b). Let u_m stand for the displacement from equilibrium in the top layer (imagined to be continuous but actually discrete locations labeled by m) and v_n correspond to the displacement from equilibrium of masses in the bottom chain. Assuming a linear coupling along the lengths of each chain (but with vertical motion only) and a nonlinear Morse potential between the chain gives an equation of motion for the top chain of

$$\frac{d^2u_m}{dt^2} =$$

$$k(u_{m+1} + u_{m-1} - 2u_m) + 2D\delta_{m,bn}\exp\{-(u_m - v_n)\}[\exp\{-(u_m - v_n)\} - 1]$$

and

$$\frac{d^2v_n}{dt^2} =$$

$$k'(v_{n+1} + v_{n-1} - 2v_n) - 2D\exp\{-(u_{bn} - v_n)\}[\exp\{-(u_{bn} - v_n)\} - 1]$$

for the bottom chain.

The bottom chain is assumed to have fewer masses than the top determined by the parameter b. In the model b determines how often a mass on the top chain is

connected to a mass on the bottom so that location n on the bottom is connected to location bn on the top or $m = bn$. A value of $b = 1$ is the case of the same number of masses on the top as on the bottom. The model approaches a true continuum system attached to a discrete system as b increases. The parameters k and k' are the linear coupling along the top and bottom chains respectively and$D$ sets the strength of the nonlinear coupling (a generic Morse potential) between the chains.

The figures shown in this paper below were generated by calculating velocities and accelerations and subsequent new positions directly from the force equations for each mass. The two coupled equations were reduced to four first order equations and a fourth order Runga-Kutta algorithm was used to time step to the new positions [17]. Periodic boundary conditions were chosen to reflect more realistically the conditions found in an actual membranes. Energies were calculated directly from the model and were conserved within 0.01% except in cases where damping was included.

Although some measurements of the force constant for the coupling between the membrane and the cytoskeleton have been made it is not clear how those results relate to in-vivo parameters since the techniques used are generally destructive [11]. Simplifications made in the model also make a direct comparison of parameter choices with a real biological system problematic. For this paper the linear coupling constants k' and k were chosen to be in the range 0.2 to 25 with the constraint $k' = kb^2$ except where noted. For the nonlinear coupling, D, values between 0.001 and 1 were used. Values of b from 1 up to 10 were examined in the simulations discussed below. These parameter choices represent a wide spectrum of values ranging from a discrete model to the case approaching a near continuum chain coupled nonlinearly to a discrete chain.

It should be noted that the $b = 1$ case has been investigated in detail as a model for DNA in [14] and [15]. Approximate analytic solutions are known in the continuum limit which lead to soliton wave behavior. For the $b = 1$ case in the discrete limit intrinsically localized modes or ILMs (also know as discrete breather modes) exist, showing a rich variety of interesting nonlinear behavior. Part of the intent of this paper is to demonstrate the existence of similar types of nonlinear effects for systems which combine discreetness with near continuum components.

3. Numerical Results

3.1. PHASE LOCKING AND ENERGY SHARING BETWEEN CHAINS

Linear traveling waves were placed on the upper and lower chains in various configurations and with a variety parameter choices to investigate general features of nonlinear energy transfer between two linear waves. In these simulations the waves were launched initially in-phase with each other. Traveling waves with the same speed on both chains and also with slightly different initial speeds were used as initial conditions. The speed on each chain is determined by the linear coupling constant along the chain but in order to have the same speed on two chains of the

same length but with different numbers of masses (and therefore different mass spacing) the coupling constants must be different. The condition for having the same speed on the top and bottom chain is $k' = kb^2$. A general feature of these simulations is that phase locking between the top and bottom chains occurred for cases where the nonlinear coupling was strong ($D = 1$) and did not occur for weak nonlinear coupling ($D < 0.01$) for waves initially near the same initial speed (linear speeds within 15% of each other).

In cases of low to moderate nonlinear coupling ($0.01 < D < 0.1$) between waves of slightly different initial linear speed a gradual shift on energy back and forth between the two chains was seen. The frequency of this shifting was proportional to the nonlinear coupling and the phase diagrams did not exactly close after a cycle. Figure 2 shows a series of snapshots showing the relative amplitudes of waves on the top and bottom chain at different times for a case of low coupling ($D = 0.04$, $b = 2$). A surface plot of the top chain (Figure 3a) shows the changes in amplitude of the sine wave on the top chain as the energy moves to the bottom chain and back. Figure 3b is a plot of the energy flow between the two chains and figure 3c shows a phase plot between times $t = 150$ and $t = 175$. Complex phase patterns arise for cases of moderate nonlinear coupling.

Mechanical stress of biological membranes appears to have some effect on the opening of protein channels through the membrane surface [18]. If this turns out to indeed be the case, a mechanical mechanism involving energy transfer from the cytoskeleton inside the cell to the cell membrane (and back) could possibly have biological ramifications.

3.2. THE MEMBRANE/SUPPORT SYSTEM AS A FREQUENCY FILTER

Because the number of masses on the top and bottom chain can be adjusted to be different, the range of possible frequencies found in each portion of the system is different. For this reason the system can act as a filter for certain frequencies. Figure 4a shows a combined long and short wavelength wave on the top chain as an initial condition. In this simulation damping was placed on the bottom chain only and $b = 10$. Figure 4b shows a snapshot of the resulting motion after several time iterations. The larger wavelength part of the combined wave moved to the bottom chain and was damped out but the shorter wavelength did not. The energy diagram in Figure 4c shows the energy localized and stable on the upper chain in spite of considerable damping in the system.

Whether frequency filtering is a feature of real biological systems with important biological implications remains to be seen but it is known that cell membranes have a natural undulatory surface motion sometimes referred to as 'flicker' or 'roughness'. In particular it has been speculated that the flicker of erythrocyte membranes may help the erythrocyte move through tiny capillaries without sticking in cases where the capillary diameter is actually smaller than that of the erythrocyte.

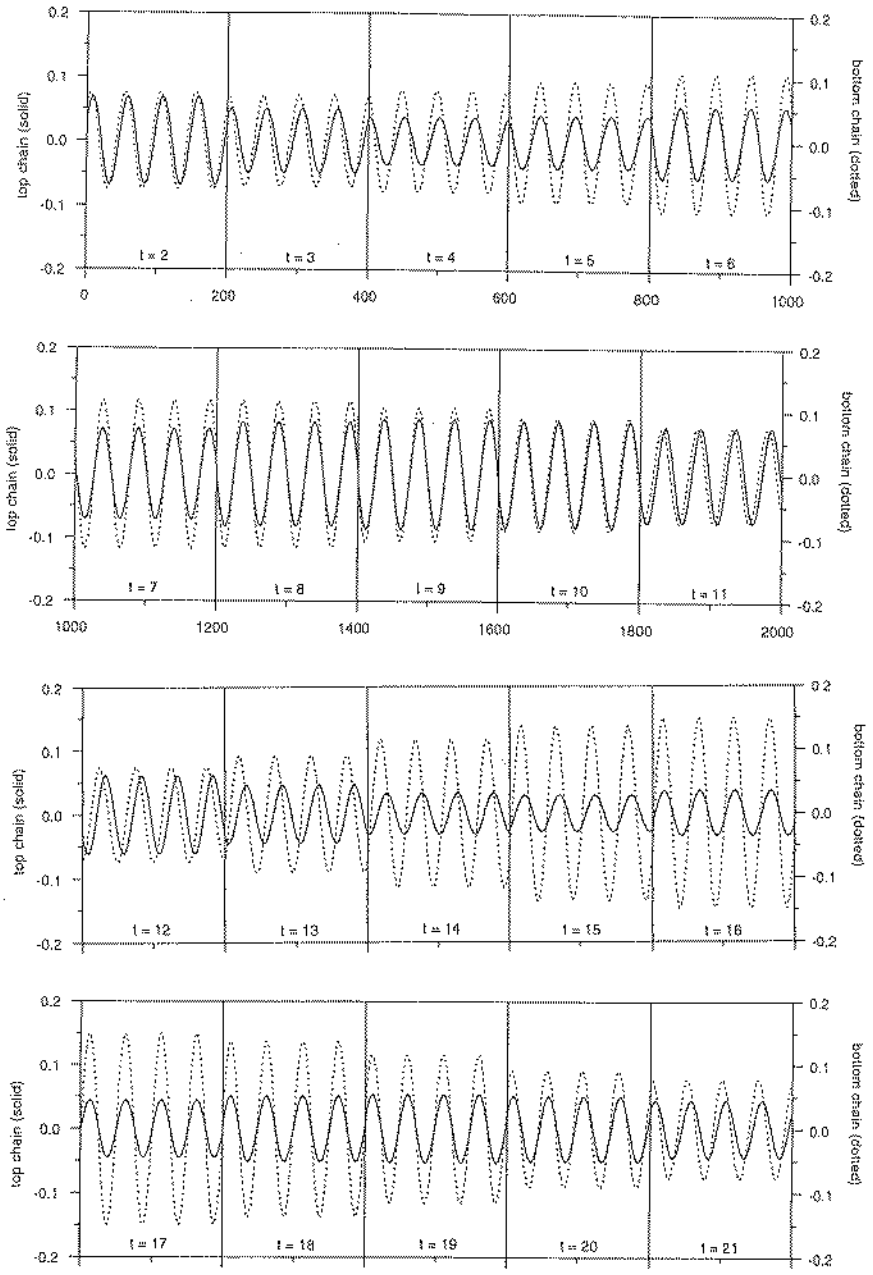

Figure 2. A series of snapshots showing the relative amplitudes of waves on the top and bottom chain at different times for a case of low coupling ($D = 0.04$, $b = 2$, $k = 3.5$, $k' = 1.0$). The parameters in this case bring the two linear waves close to phase locking.

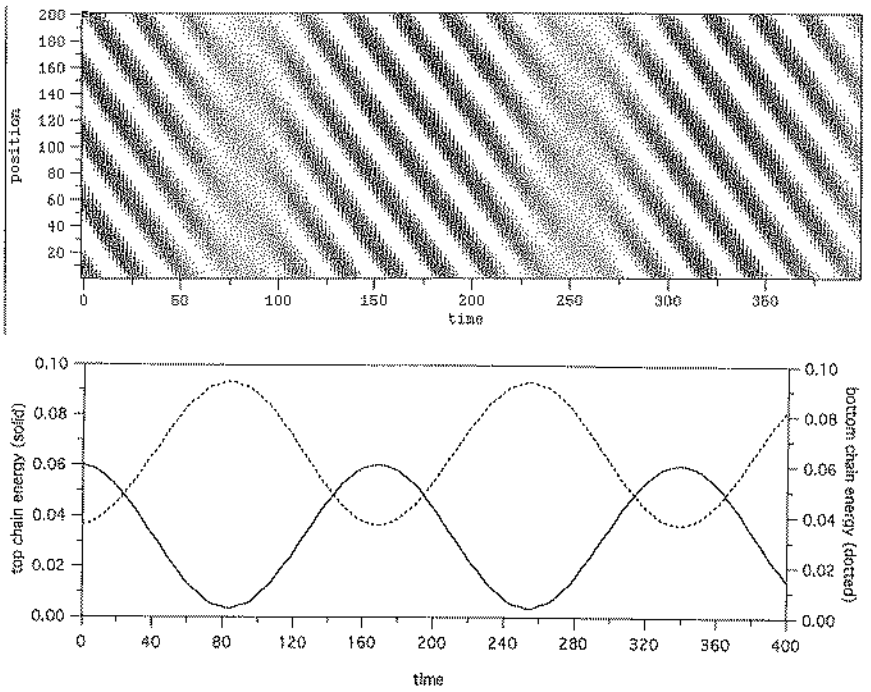

Figure 3. A surface density plot of the top chain (3a) showing the changes in amplitude of the top linear wave as the energy moves to the bottom chain and back for the case $D = 0.04$, $b = 2$, $k = 3.5$, $k' = 1.0$ (not quite strong enough for phase locking). The energy flow between the two chains is shown in 3b and a phase plot between times $t = 150$ and $t = 175$ is shown in 3c.

3.3. EXISTENCE OF ILMS AND LOCALIZATION OF ENERGY

It is now well known that intrinsically localized modes (ILMs) or breather modes exist in discrete systems with nonlinearity and may have extremely long lifetimes (see [19] and references therein). These can be very discrete (three mass sites wide) large amplitude vibrational modes which may remain centered on one location or in some systems be able to propagate. They are stable with large energies in some systems because the frequency of the nonlinear mode lies outside the the linear phonon band, thus removing the possibility of energy loss by phonon emission. A feature of ILMs of interest for possible application in the biological realm is their ability to localize energy. For some systems it has been shown that an ILM will grow in amplitude and energy at the expense of smaller ILMs in the vicinity, thus localizing large amounts of energy [20].

The existence of ILMs in a two component system has been established previously [15]. It is not clear however, given additional channels of energy flow, whether ILMs can exist in more complex systems. Part of the purpose of the present work is to establish the existence of energy localization in more complex systems. This is of particular interest in biological systems where discrete components are coupled to elements which are effectively continuous.

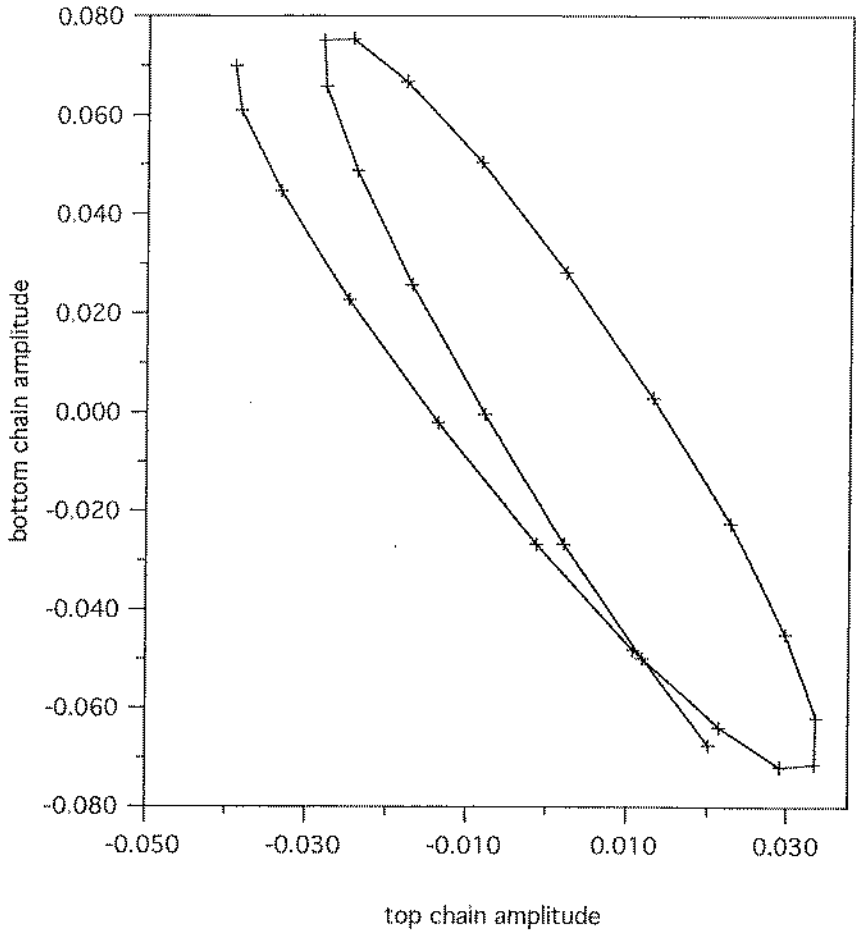

Figure 3. Continued.

Biological systems are clearly able to localize mechanical energy but the exact mechanisms are not always well understood. For example, the exact means by which a cell can localize enough mechanical energy at a particular point on the cell membrane to begin the process of endocytosis is not known although several models have been proposed (for example the 'thermal ratchet' mechanism [21] where the capture of small amplitude thermal motion is proposed as a localization mechanism).

In most systems solutions for an analytic shape of ILMs are not available although in some cases a means for finding exact shapes by numerical iteration have been devised [22]. As a first step in understanding energy localization in the present model solutions for the $b = 1$ case (determined in previous work) were used as initial conditions for other choices of b (where solutions are not yet known). The

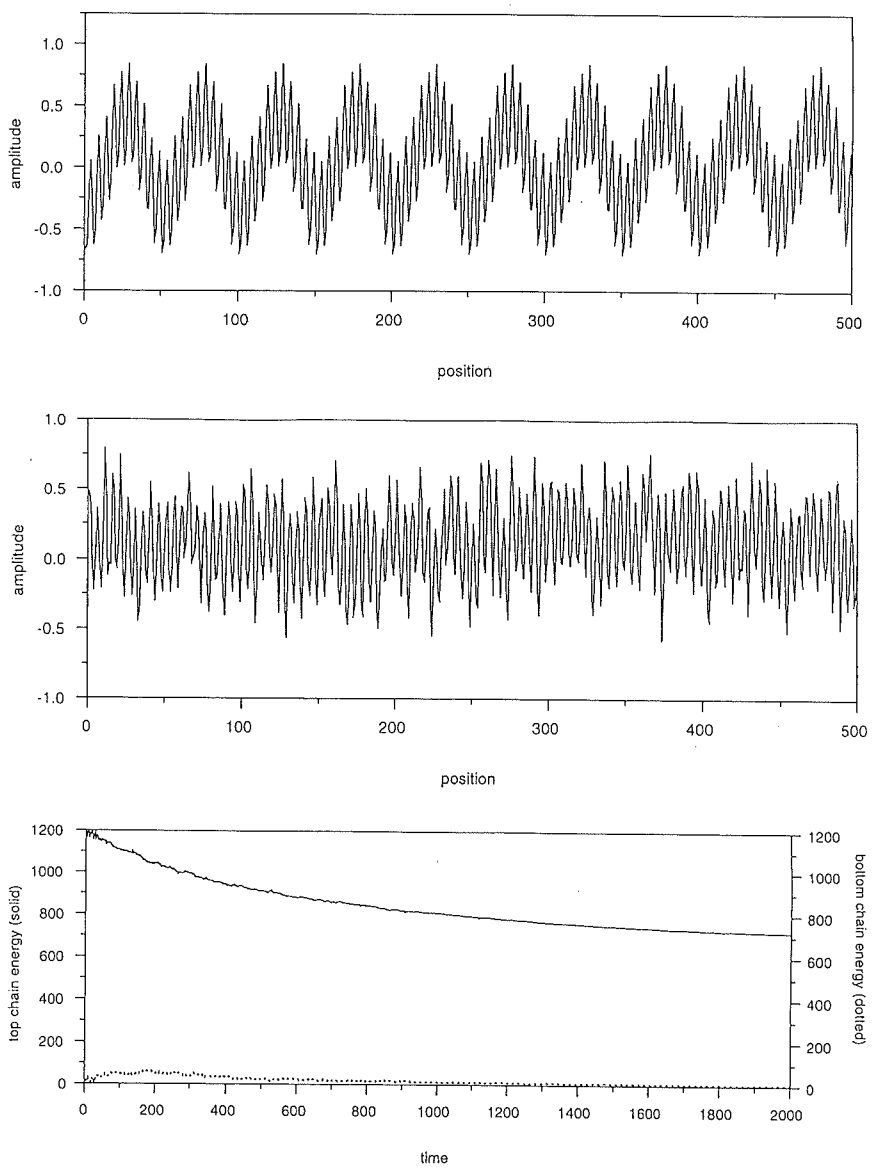

Figure 4. A combined long and short wavelength wave placed the top chain as an initial condition with damping on the bottom chain only. Here $D = 1$, $b = 10$, $k = 20$, $k' = 0.2$. Figure 4b shows a snapshot of the resulting top chain after 1800 time iterations. The energy on each chain is plotted against time in 4c.

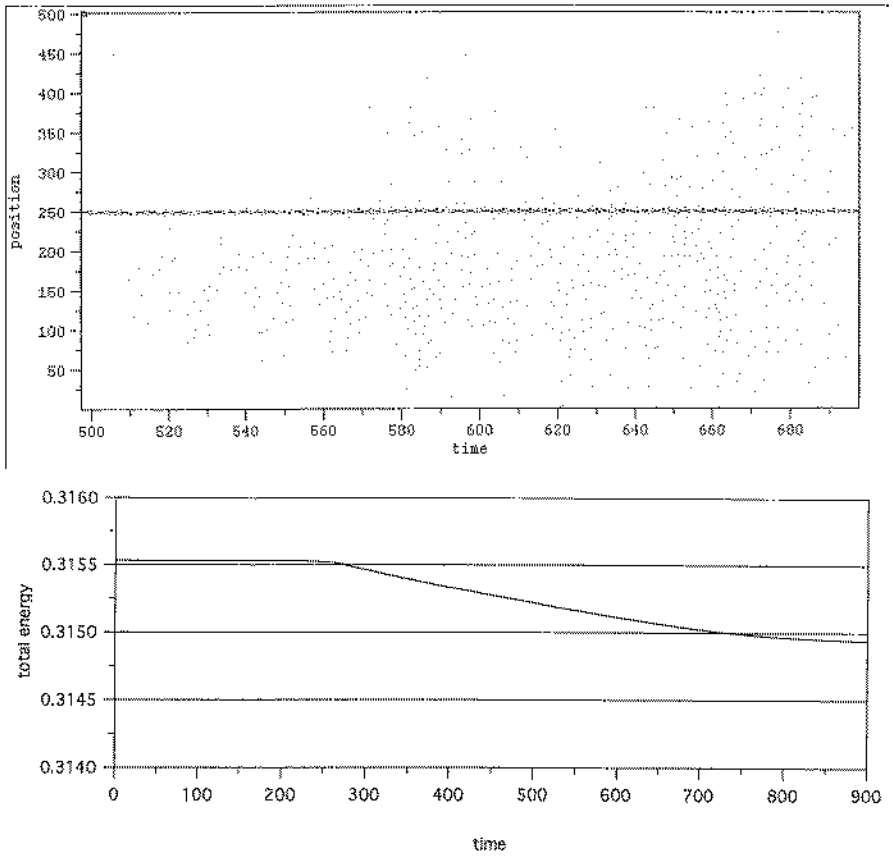

Figure 5. A surface density plot of the top chain amplitude for an initial condition which has relaxed into a stable ILM (5a) showing energy localization at position 250. The 'breathing' motion can clearly be seen from the alternating dark (into page motion) and light (out of page motion). Energy is given off at each oscillation initially (the chevron appearance out away from the breather). In this simulation $D = 1$, $b = 5$, $k = 0.2$, $k' = 0.2$ and there is damping on the chain ends to absorb the emitted energy. The total energy (5b) remains constant until the energy shed from the ILM reaches the damping on the ends of the chain and then stabilizes as the ILM relaxes into a stable state.

simulation was then run for long time periods to see if the initial condition would relax into a stable ILM. In order to determine if the mode was stable, damping was applied to the ends of the system, well away from the initial shape with the assumption that once a stable energy localization has occurred there will be no further energy loss. Figure 5a shows the case where an initial condition has relaxed into a stable ILM for $b = 10$. Figure 5b shows the energy loss of the chains due to damping which begins to stabilize after a sufficient time, indicating a stable localized configuration (an initial time delay before any damping occurs is required for the energy to reach the ends of the chain where the damping is applied).

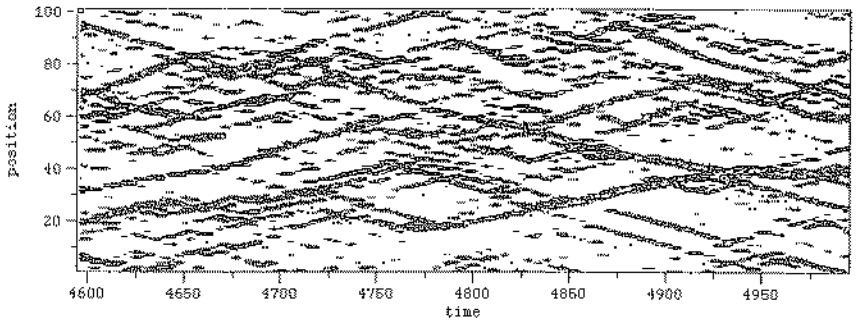

Figure 6. Energy contour plot for out-of-phase sine wave initial conditions. Strong coupling ($D = 1$, $b = 4$, $k = 0.6$, $k' = 0.6$) and out-of-phase initial linear wave conditions result in the formation of traveling ILM like behavior.

Similar results showing the existence of stable ILMs were found for many different ranges of coupling and several different values of mismatch parameter b. The significance for complex structures such as biological systems is that in the presence of nonlinearity, energy can remain localized in a discrete element even when coupled to a near continuous component.

3.4. MODULATIONAL INSTABILITY AND PATTERN FORMATION FROM SINE WAVE INITIAL CONDITIONS

Modulational instability in nonlinear systems is known to cause the breakup of sine waves into other wave forms including ILMs [23]. Prior to the present work it was not know if these familiar sorts of behaviors would be present in a muli-component system. Simulations of the present model were executed with sine wave initial conditions to see if modulational instability would result in energy localization. The sine waves were seeded with very slight imperfections in shape (less than 0.1% of the sine wave amplitude) to accelerate the onset of instability.

Cases of small and large nonlinear coupling starting with sine waves in phase between the top and bottom chains have been discussed above. Strong coupling ($D = 1$) and out-of-phase initial conditions resulted in the formation of ILM like behavior shown in Figure 6. According to the simulations, large scale localized modes can be brought into existence by a wide range of initial conditions such as thermal fluctuations represented here by traveling sine waves.

Again, it is not clear what the implications might be for real biological systems with larger degrees of complexity but it is of interest that energy localization and transfer is not limited to simple one or two component systems. The present work is important in that it shows that additional degrees of freedom do not destroy certain kinds of intrinsically nonlinear behavior.

4. Conclusion

In this work dynamical features of a pair of linear mass chains with unequal numbers of masses and nonlinear coupling between them were investigated using a numerical model. Phase locking and energy sharing between chains, filtering of frequencies between chains, existence and stability of intrinsically localized modes, and formation of localized energy from sine wave initial conditions in a system mixing near continuum and discrete features were examined. The simulation results show an extensive range of interesting nonlinear behavior making the model a useful tool for the investigation of a nonlinear interaction between linear systems. In particular interactions between a discrete system and a near continuum system have not previously been examined. It might have been thought that a (near) continuum component would allow frequency coupling so that some nonlinear features would not exist or be extremely short lived. The results of the simulations indicate this not to be the case.

The present system was intended to be a first step towards the development of a prototype representing a membrane-cytoskeleton interface. As such the current version is obviously too crude to be an accurate model of all the complexities found in a real biological cell membrane with a supporting protein network. Never the less the model has many significant features of intrinsic interest which may have important implications for biological systems. In particular the energy localization found in this multi-component system where discreteness and continuum are coupled is significant for living organisms.

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