ISSN 0206-3166

ФИЗИКА МНОГОЧАСТИЧНЫХ СИСТЕМ

• J C Eilbeck, *Nonlinear vibrational modes in a hexagonal molecule*, in *Physics of Many-Particle Systems* **12**, ed. A Davydov, 41-51 (1987).

12
1987

UDC 536.1; 539.2

J. C. Eilbeck

NONLINEAR VIBRATIONAL MODES IN A HEXAGONAL MOLECULE

1. Introduction

The analysis of the dynamics of Davydov solitons on the protein α-helix or on acetanilide (Eilbeck et al. 1984, 1985a, 1985b) leads to a large set of nonlinear differential equations, a discrete generalization of the Nonlinear Schrödinger (NLS) equation (c. f. Dodd et al., 1982). This set of equations was named the Discrete Self-Trapping (DST) equation by the authors, and takes the form

$$i\mathbf{A} + \gamma \mathbf{D}(|\mathbf{A}|^2)\mathbf{A} + \epsilon M\mathbf{A} = 0, \tag{1.1}$$

where $\mathbf{A}$ is an n-component vector with complex coefficients, representing the probability amplitude of finding some conserved quantity on the n lattice sites, M is a $n \times n$ symmetric real matrix, normalized so that the largest coefficient is unity, which represents the (linear) coupling between the different lattice sites, and $\mathbf{D}(|\mathbf{A}|^2)$ is a diagonal $n \times n$ matrix with diagonal elements $|A_1|^2$, $|A_2|^2$, ..., $|A_n|^2$. The parameters γ and ϵ measure the strength of the nonlinear self-trapping term and the interaction, term respectively.

Equation (1) has the two conserved quantities

$$N = \sum_{i=1}^{n} |A_i|^2, \tag{1.2a}$$

$$H = -\frac{1}{2}\gamma \sum_{i=1}^{n} |A_i|^4 - \sum_{i,j} m_{ij} A_i^* A_j. \tag{1.2b}$$

Often N is chosen to be unity, although in quantum applications it may be more appropriate to allow it to take integer values. The value of N can always be adjusted by rescaling the value of γ.

Following a study of the DST equation, it was found that for small values of n, it also served as a model for the anharmonic vibrations of polyatomic molecules (Scott et al., 1985). Other applications have been made to a preliminary study of self-trapping in a simple model for globular proteins (Eilbeck, 1985), and to a model for thermodynamic processes in mesoscale systems (Wheatley et al., 1985). Some properties of the DST equations, or special cases of this equation, have also been studied by Kuprievich (1985), Scott and MacNeil (1983), Nussbaum and Fischer (1986), and Jensen et al. (1985).

In this paper we limit ourselves to one special case of the DST equations: the case when $n = 6$ and the interaction matrix has the simple circulant structure (Biggs, 1974).

$$M = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 0 & 1 & 0 \end{bmatrix}. \tag{1.3}$$

This is a simple model for the study of anharmonic vibrational modes in a benzene-like molecule, with hexagonal symmetry and nearest neighbour interactions. To apply this model to benzene, we assume the only nonlinear vibrational modes involve the CH stretch modes. In this paper we concentrate merely on the structure of the solutions of the DST equation (1.1) with an interaction matrix given by (1.3) and avoid a detailed discussion of applica-

tions to the spectra of benzene, since this topic is discussed elsewhere (Scott and Eilbeck, 1986a). We note also that a detailed study of chemical applications requires an investigation of the quantized version of the DST equations (Scott and Eilbeck, 1986b).

In Section 2 we discuss the so-called stationary solutions of the DST equation, where the time dependence of the solution takes a particularly simple form. In Section 3 more general time dependent solutions are studied, and a variety of interesting solutions involving temporal chaos with soliton-like spatial structures are displayed. Finally some conclusions are discussed in Section 4 We refer the reader to the references for a more detailed introduction to the DST equation and to the general properties of its solutions.

2. Stationary States

Stationary states of the DST equations are defined to be those with time behaviour

$$\mathbf{A}(t) = \mathbf{\Phi} \exp\{i\omega t\}, \tag{2.1}$$

where $\mathbf{\Phi}$ is a constant complex n-vector, and ω is a parameter. Clearly $|\mathbf{A}(t)|^2$ is constant in time for this type of solution. If we insert (2.1) in the DST equation (1.1) we get a nonlinear eigenvalue problem for $\mathbf{\Phi}$ and ω.

$$-\omega\mathbf{\Phi} + \gamma \begin{bmatrix} |\Phi_1|^2 & & & \\ & |\Phi_2|^2 & & \\ & & \ddots & \\ & & & |\Phi_n|^2 \end{bmatrix} \mathbf{\Phi} + \epsilon M\mathbf{\Phi} = 0. \tag{2.2}$$

Because of the simple form of the nonlinearity in the DST equation (1.1), we can often find equations for stationary solutions in closed form for all values of γ. In two limiting cases, it is possible to find all the solutions of (2.2). In the linear limit $\gamma = 0$, the values of ω and $\mathbf{\Phi}$ are simply the eigenvalues and eigenvectors of the linear eigenvalue problem

$$M\mathbf{\Phi} = (\omega/\epsilon)\mathbf{\Phi}. \tag{2.3}$$

In the strong nonlinear limit $\gamma \to \infty$, we can set $\epsilon = 0$ and (2.2) become a set of n decoupled equations.

$$-\omega\Phi_j + \gamma|\Phi_j|^2\Phi_j = 0, \quad j = 1, \ldots, n. \tag{2.4}$$

The solution to these equations are

$$\begin{aligned} \Phi_j &= \exp\{i\sigma_j\}\sqrt{(\omega/\gamma)}, \quad j \in s_1, \\ \Phi_j &= 0, \qquad\qquad\quad j \in s_2, \end{aligned} \tag{2.5}$$

where s_1 and s_2 are two mutually disjoint subsets of $\{1, \ldots, n\}$ and $s_1 \cup s_2 = \{1, \ldots, n\}$. The phase constants σ_j are arbitrary angles. If we seek real solutions of the equations, then clearly $\sigma_j = 0$ or π and the nonzero Φ_j satisfy $\Phi_j = \pm\sqrt{(\omega/\gamma)}$.

If m is the number of nonzero Φ_j and if N is normalized to unity we have $\omega = \gamma/m$. Although for the $\epsilon = 0$ problem the σ_j are arbitrary, as soon as any linear coupling, however small, is switched on, these phase constants must satisfy the full equation (2.2) and only a limited number of solutions will be present.

We consider only real solutions only in the $\epsilon \to 0$ limit, then the Φ_j behave like a spin 1 system, taking on values $\pm\sqrt{(\omega/\gamma)}$, 0. If we restrict ourselves to solutions with at least one nonzero component, and treat solutions as equivalent up to group transformations of the system ($\Phi_j \to -\Phi_j$, $j = 1, \ldots, n$; $\Phi_j \to \Phi_{j+1}$, $j = 1, \ldots, n-1$, $\Phi_n \to \Phi_1$), then the number of physically distinct solutions for $n = 6$ can easily be calculated: there are a total of 51, excluding the zero solution. These are listed in Table. This table uses the following notation: 1 (—1) represents $\Phi_i \to +$ (—) $\sqrt{(\omega/\gamma)}$ in the $\epsilon \to 0$

Summary of $n = 6$ asymptotic solutions

							Analytic form?	Period
1	1	1	1	1	1	unstable	Yes	1
1	1	1	1	1	0	unstable		
1	1	1	1	1	−1	unstable		
1	1	1	1	0	0	unstable		
1	1	1	1	0	−1	unstable		
1	1	1	1	−1	−1	unstable		
1	1	1	0	1	0	unstable		
1	1	1	0	1	−1	unstable		
1	1	1	0	0	0	unstable		
1	1	1	0	0	−1	unstable		
1	1	1	0	−1	0	unstable		
1	1	1	0	−1	−1	unstable		
1	1	1	−1	1	−1	unstable		
1	1	1	−1	0	−1	unstable		
1	1	1	−1	−1	−1	unstable	Yes	6
1	1	0	1	1	0	unstable	Yes	3
1	1	0	1	1	−1	unstable		
1	1	0	1	0	0	unstable		
1	1	0	1	0	−1	unstable		
1	1	0	1	−1	0	unstable		
1	1	0	1	−1	−1	unstable		
1	1	0	0	1	−1	unstable		
1	1	0	0	0	0	unstable		
1	1	0	0	0	−1	unstable		
1	1	0	0	−1	0	unstable		
1	1	0	0	−1	−1	unstable		
1	1	0	−1	1	−1	unstable		
1	1	0	−1	0	−1	unstable		
1	1	0	−1	−1	0	unstable	Yes	6
1	1	−1	1	1	−1	unstable	Yes	3
1	1	−1	1	0	−1	unstable		
1	1	−1	1	−1	−1	unstable		
1	1	−1	0	0	−1	unstable		
1	0	1	0	1	0	unstable	Yes	2
1	0	1	0	1	−1	unstable		
1	0	1	0	0	0	unstable		
1	0	1	0	0	−1	unstable		
1	0	1	0	−1	0	unstable		
1	0	1	−1	1	−1	stable		
1	0	1	−1	0	−1	unstable	Yes	6
1	0	0	1	0	0	unstable	Yes	3
1	0	0	1	0	−1	stable		
1	0	0	0	1	−1	stable		
1	0	0	0	0	0	stable		
1	0	0	0	0	−1	stable		
1	0	0	0	−1	0	stable	Yes	6
1	0	0	−1	1	−1	stable		
1	0	0	−1	0	0	stable	Yes	6
1	0	−1	1	0	−1	stable	Yes	3
1	0	−1	1	−1	0	stable		
1	−1	1	−1	1	−1	stable	Yes	2

Total 51 independent states. 11 stable at $\omega = 20$.

limit, whereas 0 represents a component Φ_i that is zero or tending to zero in this limit.

Table contains other information about these solutions. The linear stability of a given stationary state can be investigated numerically by a straightforward eigenvalue calculation (Carr and Eilbeck, 1985). This calculation was carried out for a «large» value of ω ($\omega = 20$) for each of the 51 distinct solutions and recorded in the table: at this value of ω only 11 states are stable. Those solutions for which simple analytic forms are known are recorded, and are described below and the periodicity of these solutions on the 6-lattice are noted. In addition to these known real solutions, there are two known complex solutions, one of period 6 and one of period 3.

Those solution curves that are known in simple analytic form in the $n = 6$ case are given below. (For simplicity we set $\epsilon = 1$: solutions for different values of $\epsilon > 0$ can easily be calculated by scaling. For $\epsilon < 0$, which corresponds to the physical case of benzene, we would need also to scale all the solutions by Φ_2, Φ_4, $\Phi_6 \to -\Phi_2$, $-\Phi_4$, $-\Phi_6$).

In the listing below and in Fig. 1 we use a rather more sophisticated notation than in Table 1: here ↑ (↓) represents $\Phi_i \to +(-)\sqrt{(\omega/\gamma)}$ in the $\epsilon \to 0$ limit, whereas · represents a component $\Phi_i \to 0$ in this limit and 0 represents a component that is precisely 0 for all ϵ. Complex components are denoted by $_*$.

↑↑↑↑↑↑

$$\Phi_i = 1/\sqrt{6}, \quad \omega = \gamma/6 + 2. \tag{2.6}$$

This branch is stable for $(0 \leqslant \gamma \leqslant 3)$ and unstable for $\gamma > 3$. There are bifurcation points at $\gamma = 3, 9, 12$, the first two being double points. The «soliton» solution ↑..... bifurcates from this solution at $\gamma = 3$ and appears to be stable for all γ.

↑↓↑↓↑↓

$$\Phi_i = (-1)^{i+1}/\sqrt{6}, \quad \omega = \gamma/6 - 2. \tag{2.7}$$

This solution is stable for all $\gamma > 0$ and has no bifurcation points.

↑.↑.↑.

$$\Phi_1 = \Phi_3 = \Phi_5 = [(1+s)/6]^{1/2}, \quad \Phi_2 = \Phi_4 = \Phi_6 = [(1-s)/6]^{1/2}, \tag{2.8}$$
$$s = (1 - 144/\gamma^2)^{1/2}, \quad \omega = \gamma/3.$$

This solution bifurcates from the ↑↑↑↑↑↑ branch at $\gamma = 12$. It is probably unstable for all γ.

↑0↓↑0↓

$$\Phi_1 = -\Phi_3 = \Phi_4 = -\Phi_6 = \frac{1}{2}, \quad \Phi_2 = \Phi_5 = 0, \quad \omega = \gamma/4 - 1. \tag{2.9}$$

This branch is stable for $7 \leqslant \omega \leqslant 20$, $-1 \leqslant \omega \leqslant 0$, unstable for $0 \leqslant \omega \leqslant 7$ (it is likely that these inequalities are exact, but this has not been proved). Nothing is known concerning bifurcation points.

↑↑↓↑↑↓, ↑↑.↑↑., ↑..↑..

These three (period three) solutions can be obtained from Heggie's solution for the $n = 3$ case (Eilbeck et al., 1985) by a change of normalization. The second two bifurcate from ↑↑↑↑↑↑ at $\gamma = 9$. All are thought to be unstable for all γ.

↑↑0↓↓0

$$\Phi_1 = \Phi_2 = -\Phi_4 = -\Phi_5 = \frac{1}{2}, \quad \Phi_3 = \Phi_6 = 0, \quad \omega = \gamma/4 + 1. \tag{2.10}$$

This solution is probably unstable for all γ. The branch ↑0↓.0. bifurcates from this branch at $\omega = 2$, $\gamma = 4$. No other bifurcations on this branch are known.

↑0↓.0.

$$\Phi_1 = -\Phi_3 = a, \quad \Phi_4 = \Phi_6 = b, \quad \Phi_2 = \Phi_5 = 0, \quad \omega = \gamma/2, \quad \omega \geqslant 2, \tag{2.11}$$

where

$$a = \frac{1 + (1 - 4/\omega^2)^{1/2}}{4}, \quad b = -\left(\frac{1}{2} - a^2\right)^{1/2}.$$

This solution bifurcates from ↑↑0↓↓0 branch at $(\omega, \gamma) = (2, 4)$ and appears to be stable for large γ.

↑..↓.., ↑↑↑↓↓↓, ↑.↑↓.↓

All these three branches are parametrised by the solution

$$\Phi_1 = -\Phi_4 = a, \quad \Phi_2 = -\Phi_3 = -\Phi_5 = \Phi_6 = b, \tag{2.12}$$

where

$$a = \frac{2}{\sqrt{3}}\left(\frac{\omega - 1}{\gamma}\right)^{1/2} \sin\left(\theta - \frac{\pi}{3}\right), \quad b = \frac{2}{\sqrt{3}}\left(\frac{\omega - 1}{\gamma}\right)^{3/2} \sin\theta,$$
$$\frac{\omega - 1}{\gamma} = 3\sqrt{3}\sin\left(\theta - \frac{\pi}{6}\right)/\sin 3\theta. \tag{2.13}$$

Since this type of solution appears frequently in studies of the DST equation, it may be useful to sketch the derivation of this form. Assuming a solution of

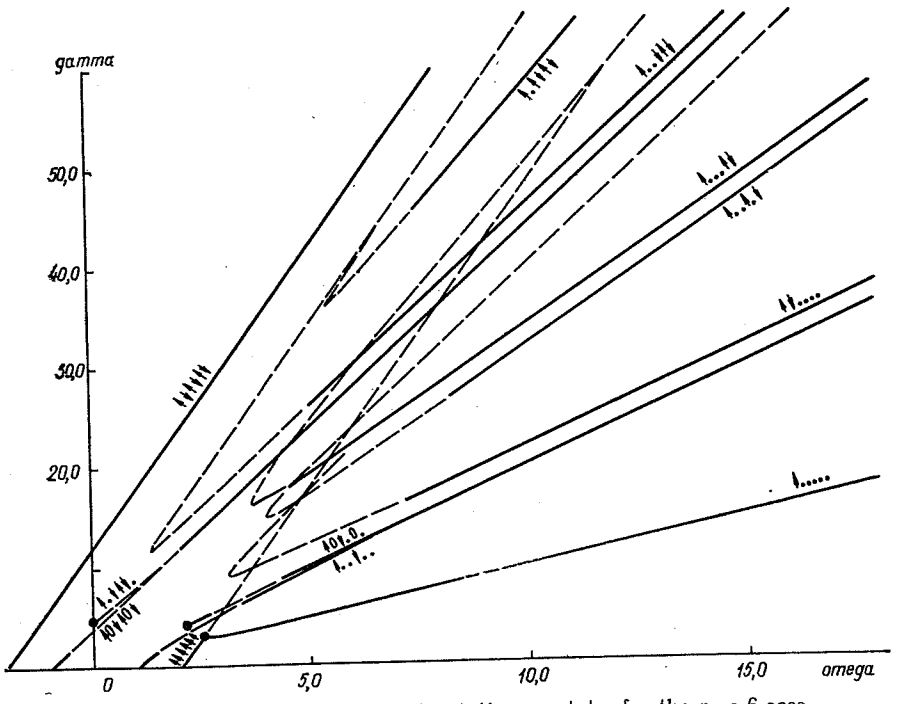

Fig. 1. Bifurcation diagram for the stationary states for the $n = 6$ case.

the type (2.12), then from (2.1) we have only two independent equations

$$-\omega a + \gamma a^3 + 2b = 0, \qquad (2.14)$$
$$-\omega b + \gamma b^3 + (a - b) = 0.$$

Adding these two equations gives

$$-\omega(a+b) + \gamma(a+b)(a^2 - ab + b^2) + (a+b) = 0. \qquad (2.15)$$

Assuming $a \neq -b$ we have

$$a^2 - ab + b^2 = (\omega - 1)/\gamma. \qquad (2.16)$$

Completing the square

$$\left(a - \frac{1}{2}b\right)^2 + 3b^2/4 = (\omega - 1)/\gamma. \qquad (2.17)$$

Parametrizing $3b^2/4 = \sin^2\theta\,(\omega - 1)/\gamma$ gives, after some trigometric manipulation, $a^2 = 4\sin^2(\theta + \pi/3)(\omega - 1)/3\gamma$. Inserting these formulae into the first of (2.14) gives the required relation for $\omega - 1$ in terms of θ and γ. Other similar solutions of the DST equations are derived in the same way, except that sometimes it is necessary to take the difference of the two equations corresponding to (2.14) instead of the sum.

In (2.13), the branch $\uparrow..\downarrow..$ corresponds to $\theta \in (0, \pi/6]$, tne other two branches by $\theta \in (\pi/3, 2\pi/3)$. The branch $\uparrow..\downarrow..$ is a «soliton-antisoliton» pair and seems stable for large γ.

The two known complex solutions are given by

$\uparrow{*}{*}\downarrow{*}{*}$

$$\Phi_j = \frac{1}{\sqrt{6}}\exp\{i2\pi j/6\}, \quad j = 1, \ldots, n, \quad \omega = \gamma + 1. \qquad (2.18)$$

$\uparrow{*}{*}\uparrow{*}{*}$

$$\Phi_j = \frac{1}{\sqrt{6}}\exp\{i2\pi j/3\}, \quad j = 1, \ldots, n, \quad \omega = \gamma - 1. \qquad (2.19)$$

This completes the list of known analytic solutions in the $n = 6$ case with M given by (1.3).

In Fig. 1 some of the real solution branches are plotted in the (ω, γ) plane — each point on the curves corresponds to a given solution for Φ. Most of these solutions are obtained numerically using the pathfinding techniques

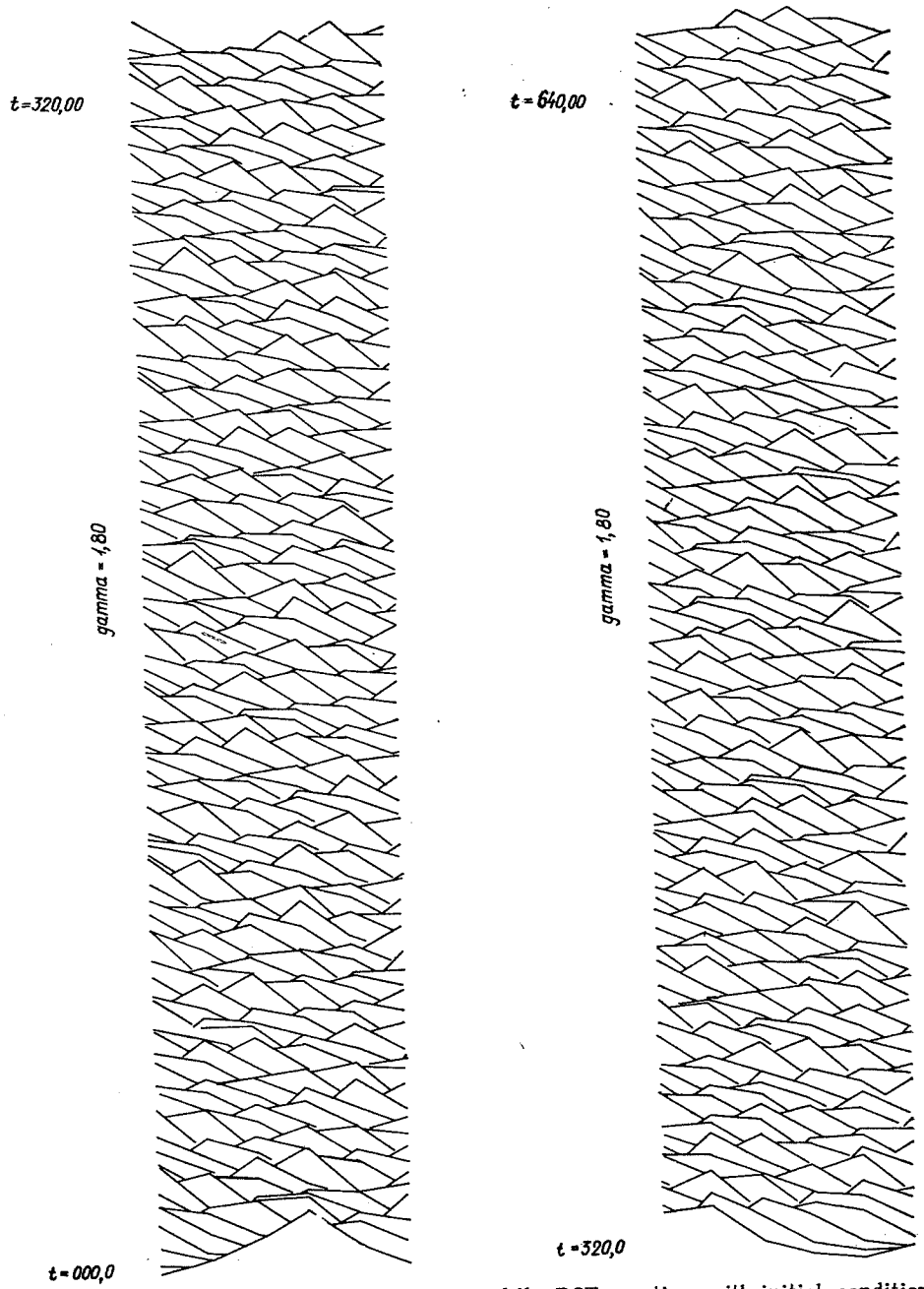

Fig. 2. Time dependent calculation of solutions of the DST equations with initial conditions as given in the text and $\gamma = 1.8$.

described in Eilbeck et al. (1984). Only a small number of the 51 known branches are plotted — mainly those which are known to be stable at $\omega = 20$. Fig. 1 shows the richness of the solution structure in the stationary solution case. It is worth noting that the introduction of extra sub and supra diagonal terms in (1.3) gives additional perturbations to this structure — in many cases the bifurcation points marked on the diagram as dots will be «unfolded» by these perturbations to give distinct non-intersecting curves. In Figure 1 those solutions which are stable are drawn as continuous curves, whereas the unstable branches or parts of branches are shown as broken lines.

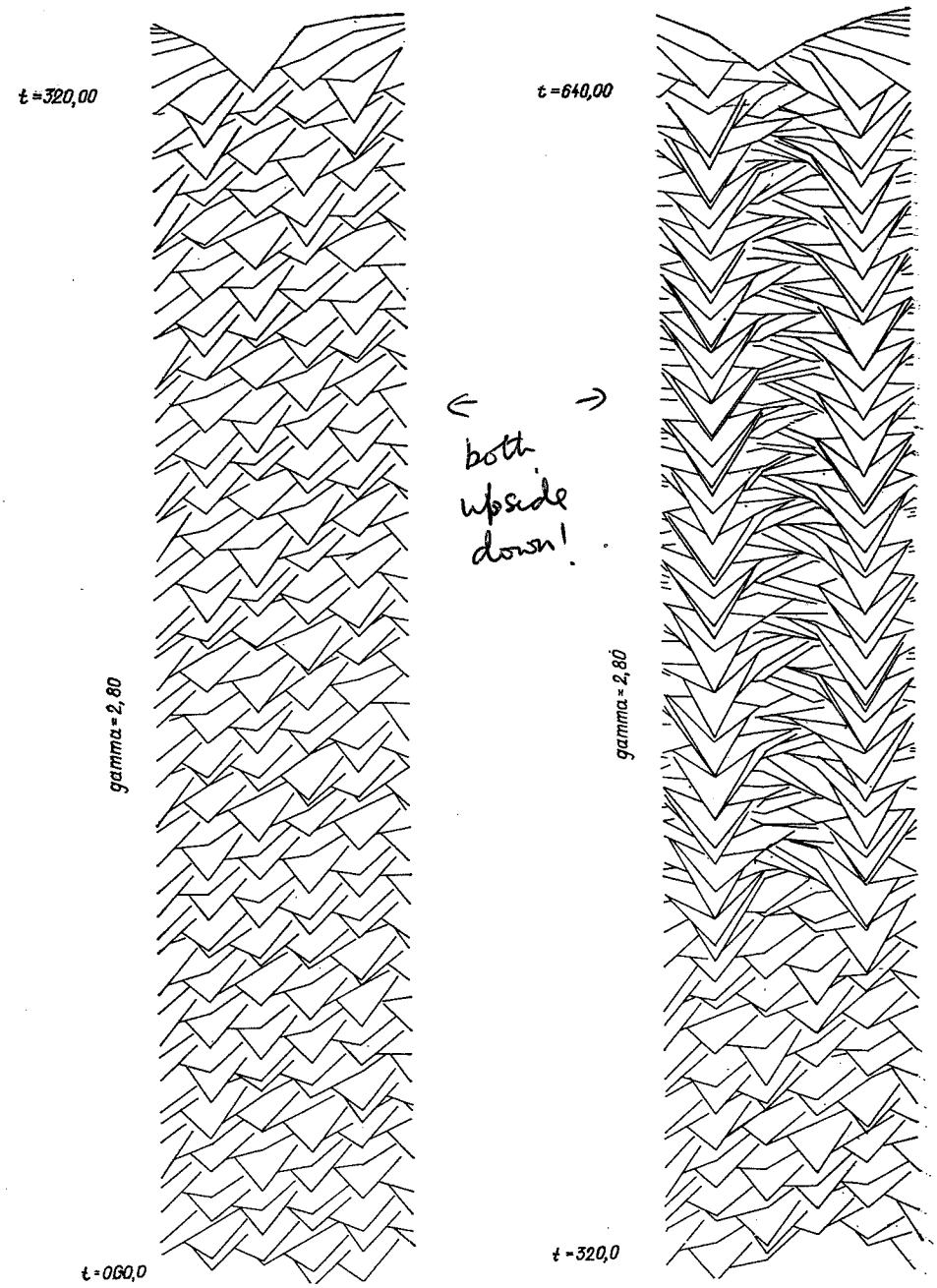

Fig. 3. As Fig. 2, with $\gamma = 2.8$.

3. Non-Stationary States

Once we drop the restriction that solutions of (1.1) should have the form (2.1), in general there will be no analytic solutions and numerical calculations are our only guide. Even then there is difficulty since we have to consider a range of possible values of γ, and the solutions we obtain will depend critically on the initial condition **A** (0) chosen. We have restricted our studies here to a small range of γ values ($2 \leqslant \gamma \leqslant 6$), and to a single set of initial conditions **A** (0) = (0,1370 + 0,0058i, 0,2643 — 0,0572i, 0,4043 — 0,0730i, 0,5520 + 0,0769i, 0,3260 + 0,1615i, 0,1277 + 0,1377i). This apparently arbitrary set of initial data was derived in the following way: a long chain ($n = 50$) with nearest-neighbour interactions and $\gamma = 3 \cdot 4$ was set up

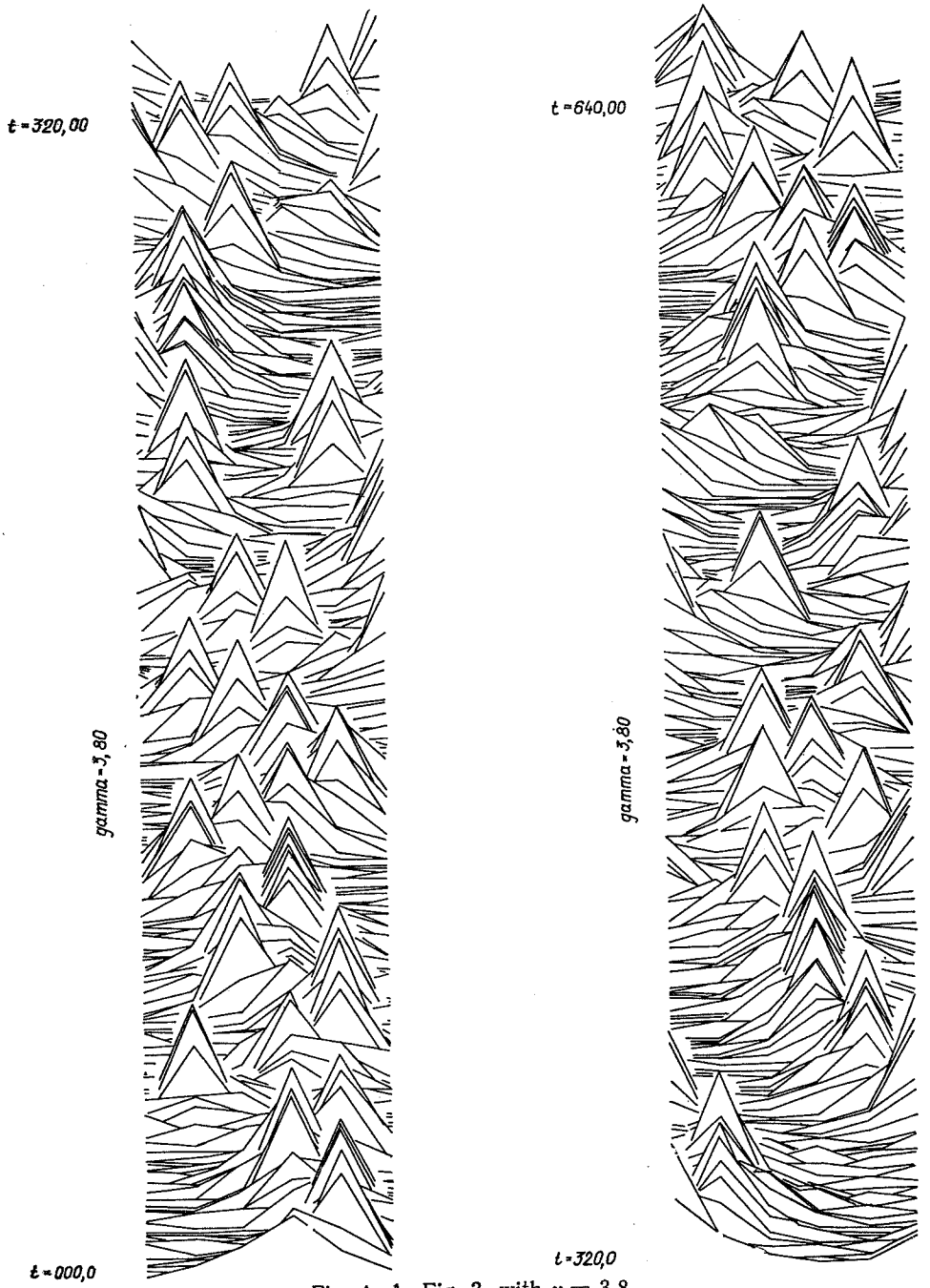

Fig. 4. As Fig. 3, with $\gamma = 3.8$.

as described in Eilbeck 1986. Down this chain was launched an exact soliton solution of the continuous approximation (the Nonlinear Schrödinger equation) to the DST equation. Once this had settled down to a steadily progressing soliton-like solution on the **discrete** chain, the six lattice point values closest to the maximum of the soliton were recorded as the values of **A** (0) given above. Hence these values should, in some sense, approximate a moving soliton-like pulse on the smaller ring of six lattice sites (albeit at $\gamma = 3{,}4$: no correction or alteration to these values were made for other γ values). With these initial conditions, and for various values of γ, the DST equation (1.1) was integrated numerically using an Adams — Bashforth — Moulton 4th order predictor-corrector method. The value of the invariant N was monito-

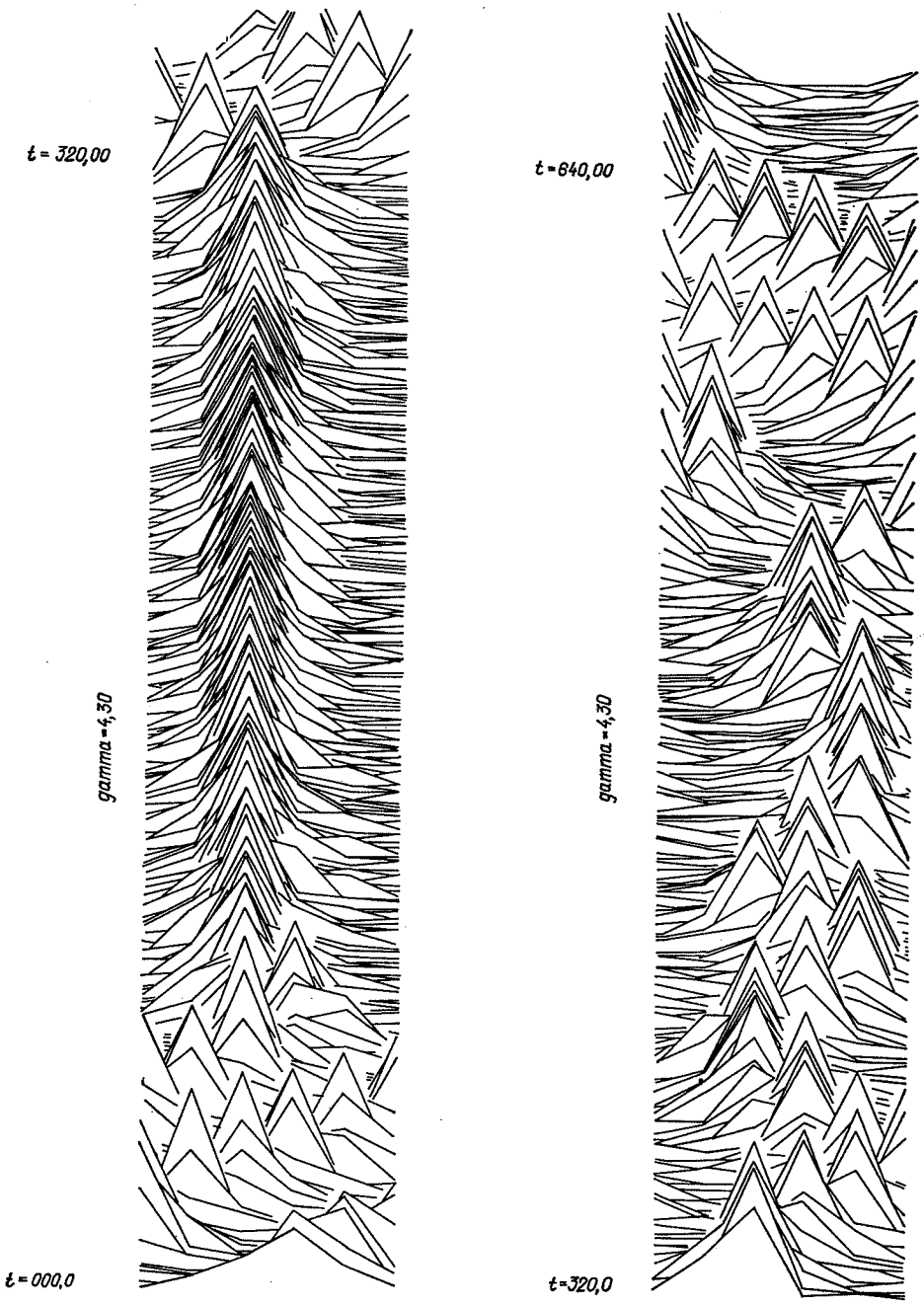

Fig. 5. As Fig. 4, with $\gamma = 4.3$.

red to check the accuracy of the numerical intergration: if N deviated by more than a fraction of a percent from unity the calculation was repeated with a smaller value of the time step.

The results of some these calculations are displayed in Fig. 2—5 for $\gamma = 1.8, 2.8, 3.8, 4.3$, respectively. In each figure time is advancing from bottom to top: the left hand plot shows a plot of $|A_i|^2$ for the time range $0 \leqslant t \leqslant 320$ and the right hand plot shows the continuation diagram for $320 \leqslant t \leqslant 640$. The horizontal axis is the six lattice sites.

For low values of γ, as in Fig. 2, the solution quickly evolves into a shallow progressive wave which travels round the ring, but with a small chaotic component. For $\gamma = 2.8$, more interesting structures emerge, with chao-

tic switching between different modes. In Fig. 3 the initial pulse quickly settles down to a wave which peaks at only two of the six lattice sites, essentially a soliton which hops from site 2 to site 5 and back again. This apparently stable mo 'e suddenly switches at $t \approx 250$ into a running soliton mode which travels round the ring in a regular fashion for the rest of the period of calculation. For other values of γ in this band (not shown), there is also a «hopping mode» where the soliton peaks at every alternate site instead of every third site. Both the type of mode exhibited and the switching between the modes are very sensitive to the value of γ chosen and the initial conditions.

For a larger value of γ, such as $\gamma = 3.8$ as shown in Fig. 4, the soliton structure is much more pronounced, but the dynamics of this pulse is much more irregular. Several different modes can be identified: running modes, the soliton moving round the ring peaking at each site in turn, with the direction of motion switching from clockwise to anticlockwise or vice versa at irregular intervals (cf. $t \approx 100$—150); pseudostationary modes, where the soliton remains at one site for several time periods before moving off to another site (cf. $t \approx 90$—100); and regular and irregular «hopping modes» where the soliton dissolves and reforms on another adjacent or distant site.

For still larger values of γ, such as the $\gamma = 4.3$ calculation shown in Fig. 5, all these modes are still present, with the additional feature that the soliton spends much more time in a «stationary» mode ($t \approx 90$—290 and $t \approx 600$—640). Similar results are found for higher values of ν (calculation up to $\nu = 5.9$ have been carried out) with the proportion of «stationary state» time apparently increasing with increasing γ.

More studies are required to quantify the time spent in different modes and to investigate the apparently chaotic switching between these modes.

4. Conclusions

The studies reported here show that the $n = 6$ case has a varied and interesting set of solutions, both in the stationary solution case and the time dependent case. It acts as a bridge between the low n case, which is relatively well understood, and the large n case, where the continuum limit is a useful model. The time-dependent calculations show an interesting set of different evolutionary modes, often with internal chaotic components, as well as irregular switching between these different modes.

Further studies are required to relate these results to the physics of the benzene molecule, and to quantify the various chaotic effects observed here.

Biggs N. (1974) «Algebraic graph theory», Cambridge University Press: Cambridge.
Carr J. and *Eilbeck J. C.* (1985) «Stability of stationary solutions of the discrete self-trapping equation», Physics Letters, **109A**, 201—204.
Dodd R. K., Eilbeck J. C., Gibbon J. D. and *Morris H. C.* (1982) «Solitons and nonlinear wave equations», Academic Press: London.
Eilbeck J. C., Lomdahl P. S. and *Scott A. C.* (1984) «Soliton structure in crystalline acetanilide», Phys. Rev., **B30** 4703—4712.
Eilbeck J. C., Lomdahl P. S. and *Scott A. C.* (1985a) «The discrete self-trapping equation», Physica, **16D**, 318—338.
Eilbeck J. C., Lomdahl P. S. and *Scott A. C.* (1985b) «Stationary solitons on finite lattices», Proceedings of the III International Symposium on Selected Topics in Statistical Mechanics, Dubna, USSR, 22—26 August 1984, vol. II, 328—339.
Eilbeck J. C. (1985) «Numerical simulations of the dynamics of polypeptide chains and proteins», to be published in the Proceedings of the conference «Computer Analysis for Life Science — Progress and Challenges in Biological and Synthetic Polymer Research», July 9—12, 1985, Okayama, Japan.
Jensen J. H., Christiansen P. L., Elgin J. N., Gibbon J. D. and *Skovgaard O.* (1985) «Correlation exponents for trajectories in the low-dimensional discrete self-trapping equation», Physics Letters, **110A**, 429—431.
Kuprievich V. A. (1985) «On autolocalization of the stationary states in a finite molecular chain», Physica, **14D**, 395—402.
Nussbaum I. and *Fischer S. F.* (1986) «Analytical treatment of localized, stationary states of the discrete self-trapping equation», Physics Letters, **115A**, 268—270.
Scott A. C. and *MacNeil L.* (1983) «Binding energy versus nonlinearity for a 'small' stationary soliton», Physics Letters, **98A**, 87—88.

Scott A. C., Lomdahl P. S. and *Eilbeck J. C.* (1985) «Between the local-mode and normal-mode limits», Chem. Phys. Letters, **113**, 29—36.
Scott A. C. and *Eilbeck J. C.* (1986a) «On the CH stretch overtones of benzene», Heriot-Watt preprint.
Scott A. C. and *Eilbeck J. C.* (1986b) «The quantized discrete self-trapping equation», Heriot-Watt preprint.
Wheatley J., Buchanan D. S., Swift G. W., Migliori A. and *Hofler T.* (1985) «Nonlinear natural engine: model for thermodynamic processes in mesoscale systems», Proc. Natl. Acad. Sci. USA, **82**, 7805—7809.

Department of Mathematics
Heriot-Watt University Riccarton,
Edinburgh EH14 4AS, UK

Received 07.07.86