PART III

LATTICE EXCITATIONS AND LOCALISED MODES

NUMERICAL STUDIES OF SOLITONS ON LATTICES

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Abstract

We use path-following methods and spectral collocation methods to study families of solitary wave solutions of lattice equations. These techniques are applied to a number of 1-D and 2-D lattices, including an electrical lattice introduced by Remoissenet and co-workers, and a 2-D lattice suggested by Zakharov, which in a particular continuum limit reduces to the Kadomtsev-Petviashvili equation.

1 Introduction

We consider here the study of solitary waves on lattices, as a special case of the more general problem of energy transport in lattice models. For example, consider the atomic lattice with Lagrangian

$$L = \sum_n \{\frac{1}{2}\dot{\alpha}_n^2 - V(\alpha_{n+1} - \alpha_n)\} \tag{1}$$

where α_n is the displacement of the nth particle from its equilibrium position, and $V(\alpha_{n+1} - \alpha_n)$ is some interaction potential. If the relative displacement of the nth bond is defined to be $u_n = \alpha_{n+1} - \alpha_n$, then the equation of motion becomes

$$\frac{d^2}{dt^2}u_n = V'(u_{n+1}) - 2V'(u_n) + V'(u_{n-1}). \tag{2}$$

In general no analytic solutions of this or similar lattice equations are known, except for some special cases such as the Toda lattice [1] or the Ablowitz-Ladik lattice [2]. If we look for solitary wave solutions of (2), i.e. solutions of the form $u_n(t) = u(n - ct) \equiv u(z)$, (2) becomes

$$c^2\frac{d^2u(z)}{dz^2} = F(z+1) - 2F(z) + F(z-1) \tag{3}$$

with $F(z) = V'\{u(z)\}$. Although we cannot solve this equation analytically, except in some special cases, it is possible to solve it numerically by a variety of methods. One technique which turns out to be efficient and accurate is the spectral collocation method [3]. If we use this together with path-following methods, we can generate a whole family of solutions to (3) as one of the parameters, such as the wave speed c, varies. A general survey of spectral methods can be found in [4]: for an introduction to continuation methods see

[5]. One important point to note is that (3) has a continuum of periodic solutions as well as a solitary wave solution, and that it is necessary to pick out the solitary wave by imposing an extra integral condition which ensures that $u(z) \to 0$ as $|z| \to \infty$ [3, 6].

Finding a solitary wave solution to (3) tells us nothing about the stability of such a pulse as a solution of the full time-dependent problem (2), nor whether it possesses approximate soliton properties on collision with other waves (we do not expect to find *exact* soliton properties except for some special cases as mentioned earlier). To investigate this question, we need to integrate (2) numerically. Conventionally this has been done using Runge-Kutta methods. Recently Duncan et al. [7] have developed symplectic solvers for lattice equations which conserve the Hamiltonian of the system to a high degree of accuracy. Their results should be read in conjunction with those described below.

Fig. 1 shows a numerical integration of (3) with two solitary waves as initial conditions, prepared by J A Wattis.

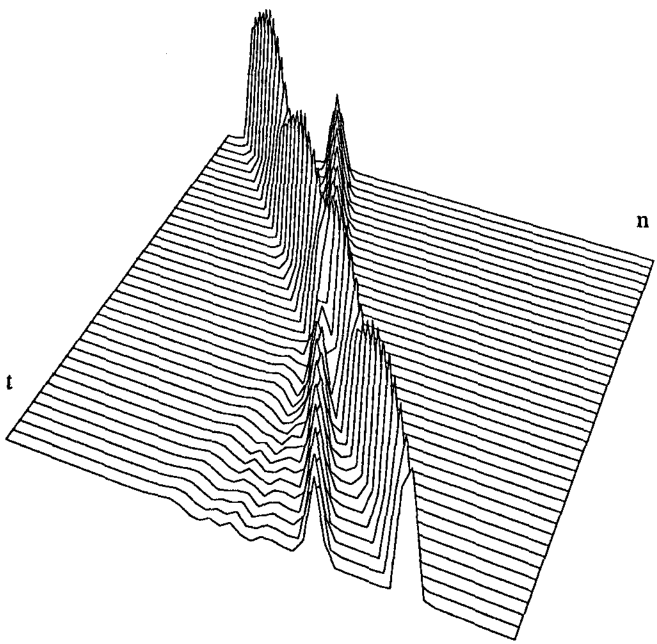

Figure 1: Collision of two solitary waves in the $V(u) = \frac{1}{2}(u^2 + u^4)$ lattice

The solitary waves emerge from the collision region with almost the same energy as before, with only a small oscillating tail left behind. For the rest of this paper we shall use the words "solitons" and "solitary waves" in a loose and interchangeable manner.

2 Some Applications

In [3] we considered the Toda lattice as a numerical test, and a lattice with $V(u) = \frac{1}{2}(u^2 + u^4)$. A more complicated example we consider below is the "electrical" lattice model worked on by Remoissenet and Michaux [8]. This is an electrical transmission line, which in the absence of loss terms has the equation (in dimensionless coordinates)

$$\frac{d^2}{dt^2}Q(V_n) = V_{n+1} - 2V_n + V_{n-1}, \tag{4}$$

where the charge Q is a nonlinear function of the voltage V.

The original motivation for our interest in lattices was a study of Davydov solitons on protein molecules [9]. A typical lattice equation from the semi-classical theory for such models is

$$\begin{aligned} i\hbar\frac{d}{dt}a_n &= E_0 a_n - J(a_{n+1} - a_{n-1}) + \chi(\beta_{n+1} - \beta_{n-1})a_n \\ M\frac{d^2}{dt^2}\beta_n &= w(\beta_{n+1} - 2\beta_n + \beta_{n-1}) + \chi(|a_n|^2 - |a_{n-1}|^2) \end{aligned} \tag{5}$$

Here $|a_n(t)|^2$ is the probability of finding a quantum of bond energy at site n, $\beta_n(t)$ is the longitudinal displacement of the nth amino acid in the protein, $E/\hbar$, J, χ, M and w are real physical constants. We have not yet developed the code to treat coupled systems of equations of this complexity, but this presents no problems in principle, except as discussed below. A simpler approximation to this system which has been studied by various authors is the so-called Discrete Self-Trapping (DST) equation [10], which with nearest neighbour couplings becomes a discrete Nonlinear Schrödinger (DNLS) equation

$$i\frac{d}{dt}A_n + \gamma|A_n|^2 A_n + \epsilon(A_{n+1} + A_{n-1}) = 0 \tag{6}$$

Here $A_n(t)$ is complex, and γ and ϵ are real parameters (not necessarily small). Finding travelling waves for this system is more difficult that the normal lattice equations, since in general a travelling wave will be a travelling wave *envelope* modulating a carrier wave travelling at a different velocity. This problem is treated by Feddersen elsewhere [11]. Solving the Davydov equations will be even more involved.

A more straightforward extension of the basic method described in the Introduction is to treat simple 2D problems. For example, we can generalise (2) to a 2D square lattice

$$\frac{d^2}{dt^2}u_{n,m} = V'(u_{n+1,m}) + V'(u_{n-1,m}) + V'(u_{n,m+1}) + V'(u_{n,m-1}) - 4V'(u_n). \tag{7}$$

Looking for a travelling wave solution, with wave front at an angle θ to the $m-$axis, we use $u_{n,m}(t) = u(n\cos\theta + m\sin\theta - ct) \equiv u(z)$ to get the equation corresponding to (3) (c.f. [12])

$$c^2\frac{d^2u(z)}{dz^2} = F(z+\cos\theta) + F(z-\cos\theta) + F(z+\sin\theta) + F(z-\sin\theta) - 4F(z) \tag{8}$$

This can be solved with the same techniques as above. It is straightforward to show that $u(z)$ satisfies the same integral constraint as in the 1-D case, i.e.

$$c^2\int_{-\infty}^{\infty} u(z)\,dz = \int_{-\infty}^{\infty} F(z)\,dz \tag{9}$$

Another, more anisotropic 2D lattice, is the following, first suggested by Zakharov [13]

$$\begin{aligned}\frac{d^2}{dt^2}v_{n,m} &= v_{n+1,m} - 2v_{n,m} + v_{n-1,m} + \epsilon^2(v_{n,m+1} - 2v_{n,m} + v_{n,m-1}) \\ &\quad -a\epsilon^2(v_{n+1,m}^2 - 2v_{n,m}^2 + v_{n-1,m}^2) \qquad (10)\end{aligned}$$

Here $\epsilon \ll 1$ is a small parameter and a is an $O(1)$ parameter. The lattice has a weak non-linearity along the n-axis and has weak linear coupling in the m direction. It can be shown that in a particular continuum limit this lattice becomes the Kadomtsev-Petviashvili (KP) equation.

$$(24v_\tau - 24avv_z + v_{zzz})_z + 12v_{ww} = 0, \qquad (11)$$

3 The "electrical" lattice

The simplest version of the model (4) is to take $Q(V) = V - aV^2$. Since a can be taken out of the calculation by a rescaling of V, we take $a = 1$. The solution of the equation corresponding to (3) proceeds in a similar way to the cases described in [3], and Fig. 2 shows the results of the calculation. In this figure, the solid line shows the height of the

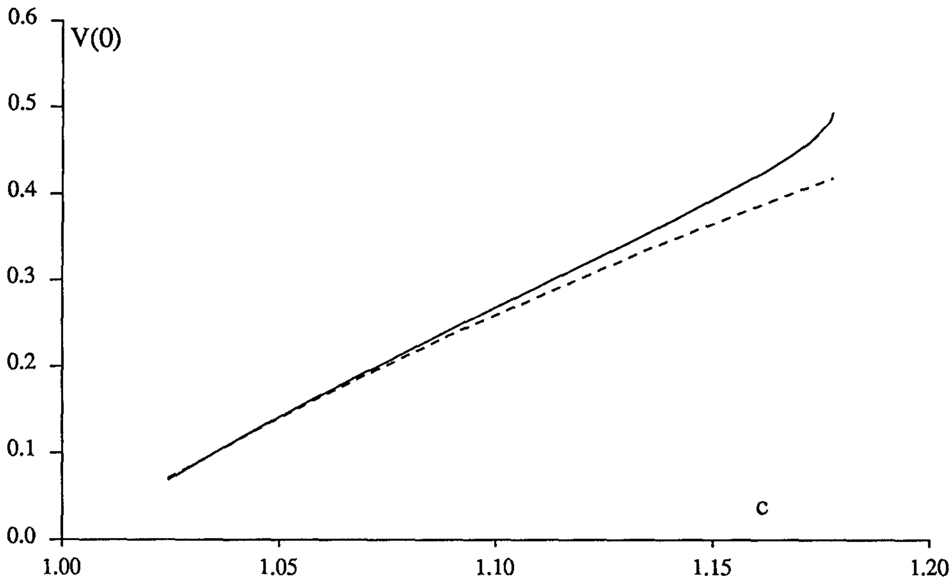

Figure 2: $V(0)$ v. c for the quadratic electrical lattice.

soliton as a function of c from the numerical calculation, and the dashed line shows the continuum approximation to the solution, which takes the form $V(0) = \frac{3}{2}(1 - 1/c^2)$ for the given $Q(V)$. For small amplitudes the agreement between the two is seen to be good. When the velocity is close to 1, the numerical calculation fails, because the soliton width is of the same order as that of the periodic boundary conditions (this could easily by cured by working on a larger interval). However the program also failed near the upper end of the curve, where $V(0)$ gets close to $\frac{1}{2}$. In this region the number of Fourier modes required to ensure accuracy grows very large, and eventually for large enough c, above $c \approx 1.172$, no solution can be found. If the solutions are plotted out for various values of c, the cause of the problem becomes obvious. Fig. 3 shows such a plot, for solitons corresponding to $c \approx 1.024$, 1.068, and 1.172 respectively.

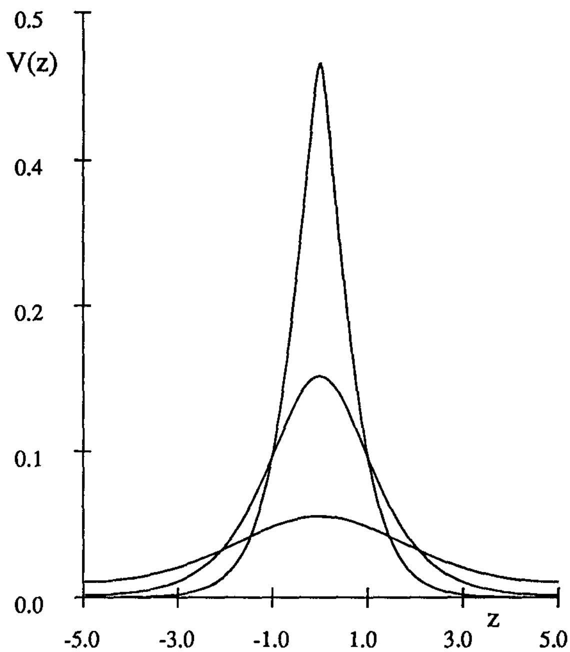

Figure 3: $V(z)$ for various values of c for the quadratic electrical lattice.

It is clear that, as the soliton gets bigger (and faster), it develops a sharp peak. In other words the calculations suggest that second derivative of V at $z = 0$ is blowing up as $V(0) \to \frac{1}{2}$, and above this height and corresponding velocity, no solutions of the travelling wave equation exist. It is suggestive that the blowup occurs at a value of V corresponding to a maximum of $Q(V)$. Also a solution of the form $V \sim \frac{1}{2} - C|z|$ for some constant C has the right type of singularity, and the corresponding Q is well-behaved at this point. However, we have not yet succeeded in proving any firm results along these lines.

Although of mathematical interest, this behaviour may not be physically relevant, since the approximation $Q(V) \approx V - aV^2$ is invalid at these values of V. We repeated the calculation with a better approximation, $Q(V) = V - 0.18V^2 + 0.021V^3 - 0.0021V^4$ (constants supplied by M. Remoissenet). The results were qualitatively the same as those shown in Figs. 2 and 3, with blowup near $c \approx 1.216, V(0) \approx 3.98$, close to the value of V (≈ 4.11) at which $Q(V)$ has a maximum for these parameters. In a final effort to avoid blowup, Remoissenet supplied an even more accurate fit to Q, $Q(V) = V - aV^2 + bV^3 - cV^4 + dV^5 - eV^6$, with $a = 0.19086, b = 0.0223199, c = 0.00166791, d =$

$0.749668 \times 10^{-4}, e = 0.159795 \times 10^{-5}$. When the program was rerun with this new $Q(V)$ we again recorded a blowup phenomena similar to Figs. 2 and 3, this time at $c \approx 1.433, V(0) \approx 9.265$, again close to the value of V (≈ 9.86) at which $Q(V)$ has a maximum. However, these values of the scaled variable V lie outside the physical range of the electrical components involved in the network.

4 2-D results

4.1 The $V(u) = \frac{1}{2}(u^2 + u^4)$ lattice

We can solve (7) with a simple extension of the methods used in 1D (of course the resulting advance-delay equation (8) is still one-dimensional, but there are now two delay constants and two advance constants). One interesting point revealed by (8) is that when $\theta = \pi/4$, the equation reduces to the usual 1-D model except that z is scaled by $\sqrt{2}$. This means that any solitary wave solution of the 1-D equation will also propagate at $\pi/4$ to the axes with the same velocity and height but with a width reduced by a factor of $\sqrt{2}$.

For fixed θ, the curves of $u(0)$ v. c look very like the 1-D case, c.f. Fig. 2 in [3]. For values of θ between 0 and $\pi/4$, the height of the solitary wave is slightly greater than for one travelling along an axis with the same velocity. Fig. 4 shows a graph of $u(0)$ v. θ for solitary waves with fixed $c = 2$.

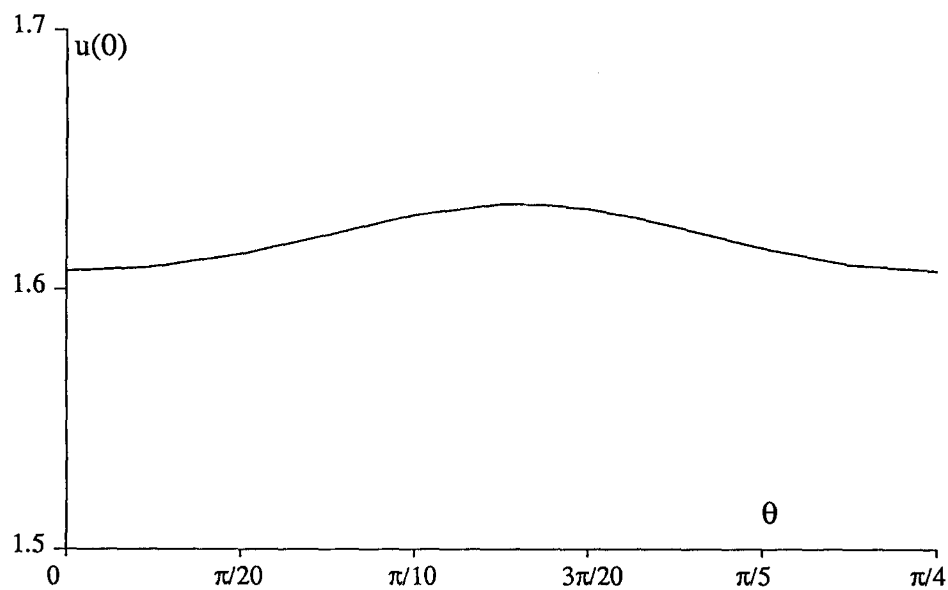

Figure 4: $u(0)$ v. θ for the $V(u) = \frac{1}{2}(u^2 + u^4)$ lattice, $c = 2$.

This graph is symmetric around $\theta = \pi/4$ and periodic with period $\pi/2$. The graph is not quite symmetric around $\pi/8$: a study of a continuum expansion shows the same qualitative features. Another interpretation is that solitary waves travelling at angles between 0 and $\pi/4$ with fixed *height* will travel slightly slower than those travelling along an axis or a diagonal.

4.2 KP lattice

For the problem (10), the 1-D technique again carries over simply to the 2-D case. This time there is no symmetry except the trivial one for rotations through π. In the limit $\theta \to \pi/2$, where θ is the direction of propagation relative to the "nonlinear" n-axis, we expect no solutions, since the equation reduces to a linear 1-D problem. For $\theta = 0$ the equation reduces to a 1-D problem with $V(v) = v^2 + kv^3$.

A continuum calculation suggest that $c \to \cos\theta$ as the pulse amplitude $\to 0$. Fig 5, taken from [13], shows the results of calculations giving a plot of pulse height against c for various angles of propagation to the n-axis. The solid line shows the numerical result,

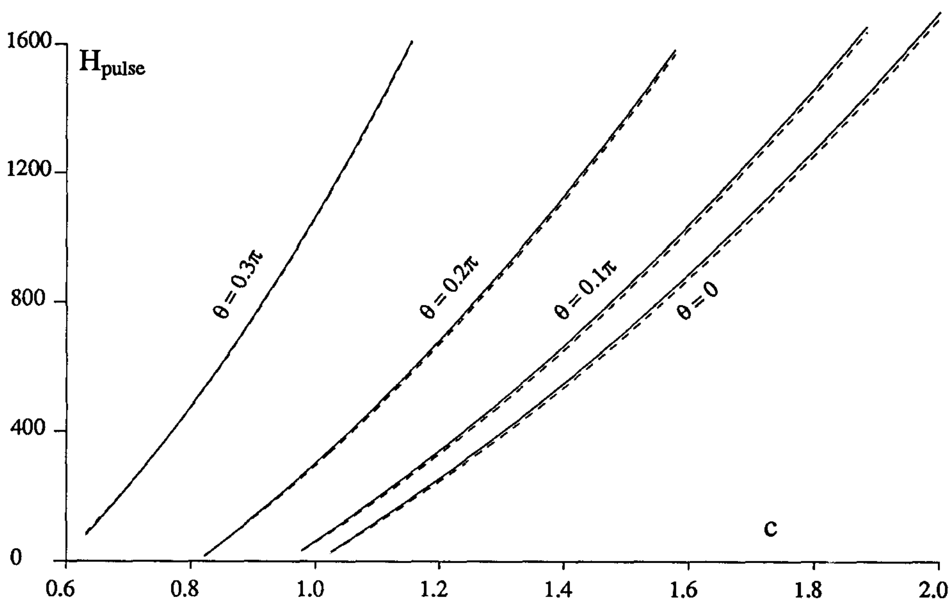

Figure 5: H_{pulse} v. c for the KP lattice

whereas the dashed line shows a heuristic formula $v(0) \approx (c^2 - \cos^2\theta)Q(0)/a\epsilon^2\cos^2\theta$, where $Q(w)$ is a universal function with $Q(0) \approx 1.3977$. This fit to the pulse height, derived from a modified asymptotic formula, is surprising good, although the corresponding pulse shapes are not accurate, except in the limit $c \to \infty$.

Acknowledgements

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