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Solitary waves on a strongly anisotropic KP lattice

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We consider a strongly anisotropic 2D atomic lattice model which in a continuum limit becomes the Kadomtsev–Petviashvili equation. Solitary waves on this lattice are studied by a variety of analytic and numerical techniques.

1. Introduction

In this paper we study a strongly anisotropic 2D atomic lattice model with Hamiltonian given by

$$H=\sum_{i,j}\left[\tfrac{1}{2}\dot{u}_{i,j}^2+\tfrac{1}{2}(u_{i+1,j}-u_{i,j})^2 + \tfrac{1}{2}\epsilon^2(u_{i,j+1}-u_{i,j})^2+\tfrac{1}{3}a\epsilon(u_{i+1,j}-u_{i,j})^3\right] . \qquad (1)$$

Here $\epsilon \ll 1$ is a small parameter and a is an O(1) parameter. The lattice has a weak nonlinearity along the i axis and has weak linear coupling in the j direction. For general coefficients, this is about the simplest strongly anisotropic lattice that can be studied. It models, for example, lattices which are made up of weakly coupled nonlinear 1D chains. With the specific coefficients given here (and in the special case $a=\frac{1}{4}$), we recover the Kadomtsev–Petviashvili (KP) equation [1] in a particular continuum limit. This enables us to compare results with a well-studied continuum model with many nice properties.

The basic question we seek to answer in this paper is the following: does the model (1) support exact plane solitary waves, i.e. plane waves which travel across the lattice without losing energy, the lattice analogue of the well-known exact solitary wave solutions of the KP equation? Although we have no analytic proof, we shall see that the numerical results strongly affirm a positive reply to this question.

We first discuss the continuum limit that leads to the (KP) equation. The equation of motion is

$$\ddot{u}_{i,j}=u_{i+1,j}-2u_{i,j}+u_{i-1,j} +\epsilon^2(u_{i,j+1}-2u_{i,j}+u_{i,j-1}) +a\epsilon[(u_{i,j}-u_{i-1,j})^2-(u_{i+1,j}-u_{i,j})^2] . \qquad (2)$$

To get a continuous model, we expand all terms around (i, j) in the usual way to get

$$u_{tt}=u_{xx}+\tfrac{1}{12}u_{xxxx}+\dots+\epsilon^2(u_{yy}+\tfrac{1}{12}u_{yyyy}+\dots) +a\epsilon(-2u_x u_{xx}+\dots) . \qquad (3)$$

Now changing variables, $z=\epsilon(x-t)$, $w=\epsilon y$, $\tau=\epsilon^3 t$ so that the equation becomes to $O(\epsilon^6)$

$$24u_{z\tau}+2u_{zzzz}+12u_{ww}-24au_z u_{zz}=0 . \qquad (4)$$

Finally differentiate with respect to z and set $v=u_z$ to get

$$(24v_\tau-24avv_z+v_{zzz})_z+12v_{ww}=0 , \qquad (5)$$

which is the Kadomtsev–Petviashvili equation. In the original discrete model (2) we often find it convenient to introduce the difference variable

$$\epsilon v_{i,j} = u_{i,j} - u_{i-1,j} ,$$

which can easily be shown to satisfy the equation

$$\ddot{v}_{i,j} = v_{i+1,j} - 2v_{i,j} + v_{i-1,j} + \epsilon^2 (v_{i,j+1} - 2v_{i,j} + v_{i,j-1}) - a\epsilon^2 (v^2_{i+1,j} - 2v^2_{i,j} + v^2_{i-1,j}) . \qquad (6)$$

Eq. (6) can also be shown to reduce to (5) directly using a similar continuum limit as above.

2. Solitary wave solutions

The KP equation (5) has solitary wave solutions

$$v(z, w, \tau) = -\tfrac{1}{2}k^2 \operatorname{sech}^2[\tfrac{1}{2}(kz + lw - \omega\tau)] , \qquad (7)$$

provided $\omega = \frac{1}{24}k^3 + l^2/2k$ and $a = \frac{1}{4}$. This solution can be integrated to give a kink like solution in the variable u to (4)

$$u(z, w, \tau) = -k \tanh[\tfrac{1}{2}kz + \tfrac{1}{2}lw - (\tfrac{1}{48}k^3 + l^2/4k)\tau] . \qquad (8)$$

We are interested in solitary wave solutions to the original discrete models (2) or (6). These have the form $u_{i,j}(t) = \phi(i\cos\theta + j\sin\theta - ct) \equiv \phi(z)$ for a wave at angle θ to the i axis [2]. With this ansatz, (2) becomes

$$c^2\phi_{zz} = \phi(z+\cos\theta) - 2\phi(z) + \phi(z-\cos\theta) + \epsilon^2[\phi(z+\sin\theta) - 2\phi(z) + \phi(z-\sin\theta)] + a\epsilon\{[\phi(z) - \phi(z-\cos\theta)]^2 - [\phi(z) - \phi(z+\cos\theta)]^2\} . \qquad (9)$$

Note that this differential-delay-advance equation is exact and is not a continuum approximation. It can be solved numerically using spectral and continuation methods as in the 1D lattice case [3], or approximated by a variety of continuum approximations. We mention in passing that these techniques can also be applied to other 2D or 3D lattices. In ref. [4] for example, we apply the methods described here to a weakly anisotropic nonlinear Klein–Gordon lattice.

Consider first a continuum approximation to (9) for slowly varying $\phi(z)$, corresponding to small c. It is convenient to scale z by $r\epsilon$, where r is a length scaling parameter. We write $\Phi(q) = \phi(q/r\epsilon)$ and express $\Phi(q)$ and c as formal power series in ϵ,

$$\Phi(q) = \Phi_0(q) + \epsilon^2\Phi_2(q) + O(\epsilon^4) ,$$

$$c = c_0 + \epsilon^2 c_2 + \epsilon^4 c_4 + O(\epsilon^6) . \qquad (10)$$

We can now insert this into (9) and expand in a Taylor series in ϵ around $\epsilon = 0$. Comparing coefficients of ϵ we get

$$c_0 = k/r ,$$

$$c_2 = \frac{k^3}{24r} + \frac{l^2}{2kr} ,$$

$$c_4 = \frac{k^5}{1920r} - \frac{kl^2}{48r} - \frac{l^4}{8k^3r} + \frac{l^4}{24kr} \qquad (11)$$

and

$$\Phi_0(q) = 2k(s-1) ,$$

$$\Phi_2(q) = \tfrac{1}{6}k^3 s(2s^2 + 3s - 4) + \frac{2l^4}{k^3}s + B(s^2 - s) , \qquad (12)$$

where $s \equiv s(q) = 1/(1+e^q)$ and B is an undetermined constant arising from the solution of the o.d.e. for Φ_2. Both $\Phi_0(q)$ and $\Phi_2(q)$ are "kink" shaped. Since $\Phi_0(q)$ is anti-symmetric about $q=0$, we choose $B = -k^3$ making $\Phi_2(q)$ anti-symmetric about $q=0$ also. This gives

$$\Phi_2(q) = \tfrac{1}{6}k^3 s(2s^2 - 3s + 1) + \frac{2l^4}{k^3}s . \qquad (13)$$

The kink height is then

$$H_{\text{kink}} = |\lim_{q\to\infty}\Phi(q) - \lim_{q\to-\infty}\Phi(q)| = |2k + \epsilon^2(\tfrac{1}{6}k^3 + 2l^4/k^3)| + O(\epsilon^4) , \qquad (14)$$

which is independent of the choice of B. We then define the relationship between kink height H_{kink} and wave speed S_{kink} for waves aligned at angle $\theta \in [0, \frac{1}{2}\pi)$ to the i axis parametrically by

$$H_{\text{kink}}(r) = 2k + \epsilon^2(\tfrac{1}{6}k^3 + 2l^4/k^3) + O(\epsilon^4) ,$$

$$S_{\text{kink}}(r) = k/r + \epsilon^2 c_2(r,\theta) + \epsilon^4 c_4(r,\theta) + O(\epsilon^6) , \qquad (15)$$

where $k = r\cos(\theta)$, $l = r\sin(\theta)$ and c_2, c_4 are defined above.

A similar calculation can be carried out for the "pulse" variable $v_{i,j}$. First define

$$v_{i,j}(t)=\psi(i\cos\theta+j\sin\theta-ct)\equiv\psi(z)\ . \tag{16}$$

Then rescale as before, $\Psi(q)=\psi(q/r\epsilon)$. We get finally to $O(\epsilon^4)$

$$\Psi(q)=2k^2(s^2-s)+\epsilon^2(s^2-s)\times[\tfrac{1}{12}k^4(5-18s+18s^2)+2l^4/k^2] \tag{17}$$

and

$$H_{\rm pulse}(r)=\tfrac{1}{2}k^2+\epsilon^2\frac{k^6+48l^4}{96k^2}+O(\epsilon^4) \tag{18}$$

and $S_{\rm kink}(r)$ as in (15).

For fast solitary waves, $c\gg 1$, we can obtain a different formal expansion for $\psi(z)$ in powers of c^{-1},

$$\psi(z)=c^2[\psi_0(z)+c^{-2}\psi_2(z)+O(c^{-4})]\ . \tag{19}$$

Inserting this into the equation corresponding to (9) for v and neglecting higher powers of c^{-1} we get

$$\psi_0''(z)=a\epsilon^2[\psi_0^2(z+\cos\theta)-2\psi_0^2(z)+\psi_0^2(z+\cos\theta)] \tag{20}$$

and a linear equation for ψ_2 involving ψ_0. After some rescaling we find that

$$\psi_0(z)=\frac{1}{a\epsilon^2\cos^2\theta}Q(z/\cos\theta)\ , \tag{21}$$

where $Q(z)$ is a universal function satisfying

$$\frac{d^2}{dw^2}Q(w)=Q^2(w+1)-2Q^2(w)+Q^2(w-1)\ , \tag{22}$$

subject to the boundary conditions $Q(w)\to 0$ as $|w|\to\infty$.

Thus the height of the solitary wave is given by

$$\psi(0)=c^2\left(\frac{1}{a\epsilon^2\cos^2\theta}Q(0)+O(c^{-2})\right). \tag{23}$$

The function $Q(w)$ can be calculated by solving (22) using spectral methods, and we find $Q(0)\approx 1.397686$. Eq. (23) cannot, however, give a good fit for small c, especially since in this limit it does not give the continuum result $c\to\cos\theta$ as $H_{\rm pulse}\to 0$. We can introduce a constant correction to (23) which will not alter the asymptotic result and recover the small amplitude limit, to give

$$\psi(0)\approx\frac{c^2-\cos^2\theta}{a\epsilon^2\cos^2\theta}Q(0)\ . \tag{24}$$

Rather remarkably, this heuristic formula gives an excellent fit to the numerical results described below.

3. Numerical studies

One approach, already mentioned, is the numerical study of (9) or the corresponding equation for v using spectral and continuation methods [3]. Some results are shown in fig. 1 for $H_{\rm pulse}$ for the values of $\theta=0$, 0.1π, 0.2π, and 0.3π from right to left across the diagram. The solid lines correspond to the numerical calculation and the dashed line shows the "corrected" asymptotic formula (24). Note the fit between the two is surprisingly good for all ranges of c considered even for $c<1$. This is unexpected because the width of the solitary wave $\to\infty$ as $c\to\cos\theta$, whereas the width of the pulse solution of (22) is independent of c. By comparison, the continuum model results (not shown) only give a good fit to $H_{\rm pulse}$ for amplitudes close to zero.

Another approach is to integrate the original lattice equations (2) directly. If the initial conditions are chosen to coincide with a solitary wave given from the numerical solution of (9), the stability of such solutions can be tested over finite time scales. The method we use to integrate eqs. (2) and (6) is a symplectic ordinary differential equation solver (see ref. [5]). It is a fourth-order fixed-timestep method and is applicable to any system which can be written in separable Hamiltonian form, making it ideal for discrete lattice models. When applied to the Toda lattice model (for which there is an exact solution) the symplectic scheme produces better results more efficiently and easily than the commonly used Runge–Kutta method (see ref. [6] for further details). In addition, it is easy to code for parallel computers making the study of the 2D domains a great deal less costly.

We have integrated both a 1D version of the equations (i.e. $\theta=0$) and a fully two-dimensional version ($\theta\neq 0$) in domains with periodic boundary conditions and several different sets of initial conditions corresponding to different choices of c. In all cases the solitary waves are propagating almost undis-

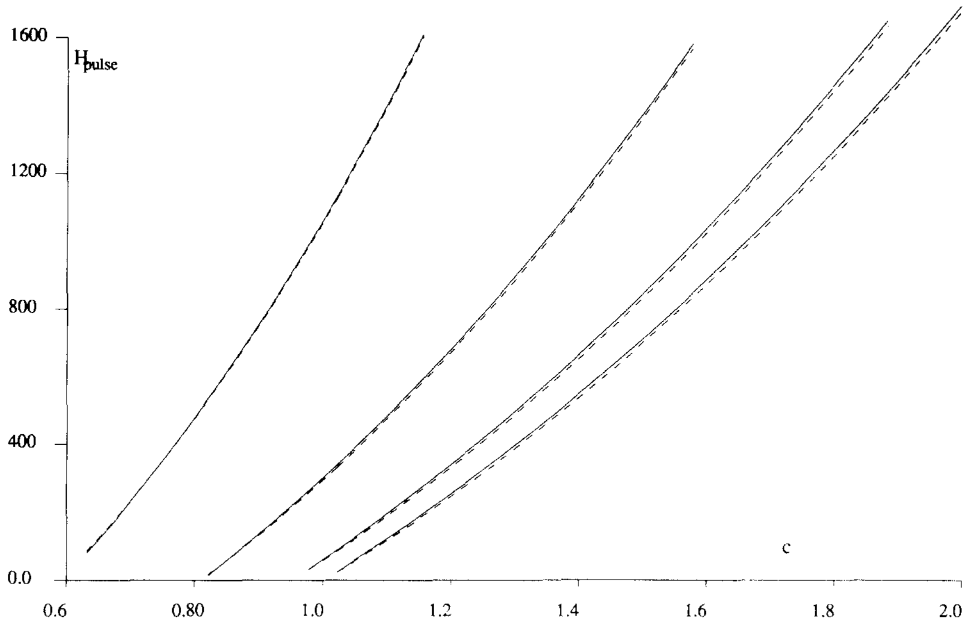

Fig. 1. Plot of H_{pulse} against c, see text for details.

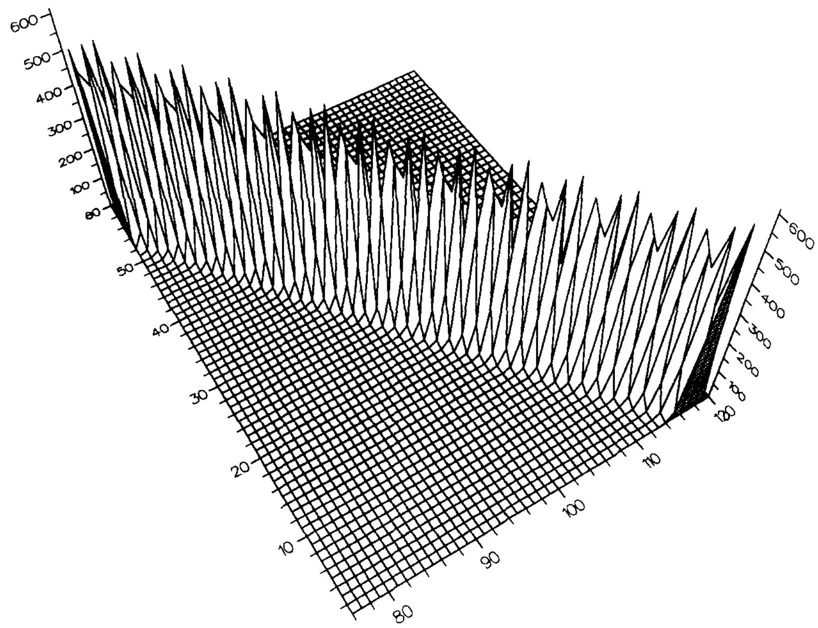

Fig. 2. Plot of solitary wave $v_{i,j}$, see text for details.

torted with good conservation of the Hamiltonian, although with a very tiny "tail" of ripples. For example, for $\tan\theta=\frac{3}{4}$, $c=1.15458$, timestep size $h=\frac{1}{64}$ and times up to $t=1000$, the solitary wave amplitude is about 616, the amplitude of the ripples is less than 0.0003 and the Hamiltonian is conserved to at least six significant figures. It is thought that this "tail" of ripples arises from truncation of the Fourier series when determining the initial conditions. Fig. 2 shows a section of the domain with the solitary wave passing through it at time $t=600$. The initial conditions (not shown) are indistinguishable from this figure at this resolution, except of course for a translation. Note that the solitary wave is quite sharp in this example, being appreciably nonzero over only a small number of lattice points.

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