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Approximations to solitary waves on lattices: II. Quasi-continuum methods for fast and slow waves

Jonathan A D Wattis
Department of Mathematics, Heriot-Watt University, Edinburgh, EH14 4AS, UK

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Abstract. A number of highly accurate analytic approximations to solitary waves on lattices are detailed, and the results of numerical tests presented. Two types of approximation are considered. The first set of approximations are generalizations of the continuum approximation, based around various Padé expansions of the operator. These are convergent to the exact solution in the limit of wavespeed $c \to 1$, or a dense lattice. We also consider ways of constructing approximations to fast solitary waves from a continuum-type theory. The two types are closely related. In both cases significant improvements are made on existing approximations. A symplectic Hamiltonian integration scheme is used to perform computer simulations. A new method of measuring the accuracy of a predicted waveform is also used on new and old approximations alike, to compare the various methods considered.

1. Introduction

This paper is concerned with forming highly accurate analytic expressions for the size and shape of solitary waves on lattices with non-harmonic interactions. We consider mainly simple polynomial potentials, such as those generated when Taylor-expanding a general potential around an equilibrium point. In general these lattices appear to support solitary waves which will propagate without changing form, but these do not form mathematical solitons. There are 'exact' numerical solutions: in the sense that it is possible to generate numerical solutions to the equations which propagate with no discernible change in form, and leave behind no measurable radiation. On collision, these do leave behind a small amount of radiation and emerge with slightly reduced energy. Hence we are only concerned with predicting the shape of a solitary wave. In particular we will be interested in predicting its speed–height characteristics. The term soliton will be used in this looser sense.

A typical lattice equation in one dimension is

$$\ddot{\phi}(t) = V'(\phi_{n+1}(t)) - 2V'(\phi_n(t)) + V'(\phi_{n-1}(t)). \tag{1.1}$$

where $V(\phi)$ is a potential energy function; e.g. $V(\phi) = \frac{1}{2}\phi^2 + \frac{1}{3}a\phi^3 + \frac{1}{4}b\phi^4$. Since we are interested in travelling waves, we seek solutions of the form $\phi_n(t) = \phi(n-ct) \equiv \phi(z)$. Equation (1.1) then becomes the nonlinear differential-delay equation

$$c^2\phi''(z) = V'(\phi(z+1)) - 2V'(\phi(z)) + V'(\phi(z-1)) \tag{1.2}$$

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The aim of this paper is to develop methods for finding approximate solutions to equation such as this, i.e. finding approximations to lattice solitons. These methods can then be used on more complex models. The results presented here can also be used to verify numerical simulations [1]. They can also be used to initialise numerical simulations, where it is often easier to start from an analytical approximation, than to numerically sum and/or iterate sequences to convergence. Our goal is to find highly accurate analytic approximations to properties of solitary waves. Such work has been carried out numerically by Eilbeck and Flesch [1]. Also some useful theory has been derived by Hochstrasser *et al* [2] but this is too complicated to be used in analytic approximations, and their results must really be considered as numerical work.

Our methods are based around Padé expansions. The notation (m, n) refers to the ratio of an mth degree polynomial by an nth degree polynomial. In some texts this is also written as P_n^m. As well as the method detailed below, most results can be derived via equations related to the Boussinesq equation: this suffers from a dispersion relation which is negative for large wave numbers. It is not claimed that such PDEs describe the time evolution of the lattice in some long wavelength approximation: we merely assert that a solitary wave will satisfy the appropriate travelling wave equation to some degree of accuracy.

In the remainder of this section, the results of the exactly integrable Toda lattice are quoted, and a simple piece of asymptotics is derived. The Toda potential is important, since it shows that exact solitons can exist on lattices. It also gives us an easy way to check our methods, by carrying out our methods on a potential where the exact results are known. The asymptotics will be referred to, to support some of the assumptions made in deriving the approximate methods.

In section two, we first quote the results already known, reviewing the work of Flytzanis, Pnevmatikos, Peyrard [3, 4], and Rosenau [5, 6]. We must also note the work of Druzhinin and Ostrovsky [7], and Hochstrasser *et al* [2]. in this subject area. Several new approximations are then derived, which extend this work. The section is purely concerned with the simplest lattice equation, that of a one-dimensional lattice with nonlinear nearest neighbour interactions.

In section three the earlier work is generalised to a two-dimensional lattice—the Kadomtsev–Petviashvili lattice. This has a highly non-isotropic potential, and has already been studied by Duncan *et al* [8]. Alternative methods of generating approximate wave forms for a variety of wave speeds have also been found. These highly accurate approximations are not based on expanding about a solution which is accurate the in limit of very large or very small speeds; but on the structure of the equations of motion. Details will be published in a subsequent paper [9].

1.1. Toda lattice

For comparison of the performance of differing continuum approximations, we shall use the Toda Potential

$$V(\phi) = ab^{-1}(\exp(-b\phi) + b\phi - 1) \tag{1.3}$$

which is integrable [10]. The solution of this is

$$y_n(t) = \frac{1}{b}\log\left(\frac{1+\exp 2(\kappa n - \kappa \pm \beta t)}{1+\exp 2(\kappa n \pm \beta t)}\right) + \text{constant} \tag{1.4}$$

where $\phi_n = y_{n+1} - y_n$. There is a one-parameter family of solutions, parametrised by κ, and $\beta = \sqrt{ab}\sinh\kappa$. The sequence $\{y_n\}$ forms a kink soliton, and $\{\phi_n\}$ a pulse; with peak height at $\kappa n = \beta t$, where $\phi = (2/b)\log\operatorname{sech}\kappa < 0$. The speed of such a pulse is $c = \beta/\kappa = \sqrt{ab}\sinh(\kappa)/\kappa$.

1.2. Asymptotics

As a preliminary, we will consider a simple piece of asymptotics. Assuming a solitary wave exists, we want to know the form of its decay. We assume that for large z, ϕ is small and so the equation we consider is a linearisation of (1.2) about $\phi = 0$

$$c^2\phi''(z) = \phi(z+1) - 2\phi(z) + \phi(z-1). \tag{1.5}$$

This, being linear, has solutions of the form $\phi(z) = \exp(-\lambda z)$. Substituting this in, we can obtain the following equation for λ;

$$\tfrac{1}{2}c\lambda = \sinh\tfrac{1}{2}\lambda. \tag{1.6}$$

This has solutions with $\lambda > 0$ only if $c > 1$. It is already known that solitary waves exist only for $c > 1$, so we have found that solitary waves decay monotonically and exponentially. A similar result is easily obtained for the KP lattice.

2. One-dimensional lattice equation

2.1. Standard continuum approximation

From the single-dimensional lattice equation (1.1) with a general quartic polynomial potential, $V'(\phi) = \phi + a\phi^2 + b\phi^3$, the standard continuum approximation can be derived as in [3]. This reduces the system of ODEs to a PDE, the Boussinesq equation, and then seeks travelling wave solutions of this. The same results, however, can be arrived at in a different way, if we first assume that a travelling wave exists for the lattice equation (1.1), then write the differential delay equation (1.2) as an operator equation. We denote the derivative with respect to z by D

$$c^2D^2\phi(z) = [4\sinh^2(\tfrac{1}{2}D)]V'(\phi(z)) \tag{2.1}$$

using the fact that $\phi(z\pm1) = \phi(z) \pm D\phi(z) + \frac{1}{2}D^2\phi \pm \frac{1}{6}D^3\phi + \ldots = e^{\pm D}\phi$. Dividing the operator equation by D^2 corresponds to integrating the equation twice with both constants of integration being zero. We do not need to impose any additional constraints on a solitary wave, since we already expect it to decay to zero exponentially as $|z| \to \infty$.

The equation can now be written as $c^2\phi = \Lambda(D)V'(\phi)$. We can now form approximations by expanding $\Lambda(D)$. This can be justified more rigorously by taking Fourier Transforms of equation (1.2), denoting $V'(\phi(z))$ as $F(z)$

$$-c^2k^2\hat{\phi}(k) = -4\hat{F}(k)\sin^2\tfrac{1}{2}k \tag{2.2}$$

or $c^2\hat{\phi} = \hat{\Lambda}(k)\hat{F}$. Now approximating $\hat{\Lambda}(k)$ before inverting the transform, we obtain an equivalent approximation.

For the standard continuum approximation we expand $\Lambda(D)$ as $I+\frac{1}{12}D^2$, where I is the identity operator, to give

$$c^2\phi(z)=[I+\tfrac{1}{12}D^2][\phi+a\phi^2+b\phi^3]. \tag{2.3}$$

Now we assume that ϕ is small and slowly varying so that a product of ϕ with its derivative is negligible. The effect of this is that the D^2 operator only acts on the ϕ term. The ODE

$$(c^2-1)\phi-\tfrac{1}{12}\phi''-a\phi^2-b\phi^3=0. \tag{2.4}$$

is then easily obtained.

The results of this process are summarized below:

- In general the speed–height relationship is $c^2\phi_0^2=2V(\phi_0)$ with $\phi_0\neq 0$.
- For the pure cubic potential, $\phi(z)=\phi_0\,\mathrm{sech}^2(z\sqrt{3(c^2-1)})$, where $\phi_0=(3/2a)(c^2-1)$.
- For the pure quartic potential, $\phi(z)=\phi_0\,\mathrm{sech}(2z\sqrt{3(c^2-1)})$, where $\phi_0^2=(2/b)(c^2-1)$.
- For the Toda potential, $c^2=(2a/b\phi_0^2)(\mathrm{e}^{-b\phi_0}+b\phi_0-1)$. However to write it as $\phi_0=f(c)$ requires the solution of a transcendental equation. The waveform cannot be found in simple form.

2.2. (0,2) Padé continuum approximation

If we use the (0,2) Padé approximation to the operator, as suggested by Rosenau [5, 6]

$$\Lambda(D)\sim I+\tfrac{1}{12}D^2\sim[I-\tfrac{1}{12}D^2]^{-1} \tag{2.5}$$

then no further approximations are necessary to obtain explicit formulae. The operator acts on the left-hand side of the equation

$$c^2\phi(z)-\tfrac{1}{12}c^2\phi''(z)=V'(\phi(z)) \tag{2.6}$$

which is soluble in the case of pure cubic or pure quartic $V(\cdot)$, giving similar results to the standard continuum approximation. The speed–height relationships are exactly the same; however the (0,2) Padé approximation produces wider solitary waves. These are obtained by integrating the above, with the constant of integration being zero since at $\phi=0$ we also have $\phi'=0$. This equation can always be manipulated to give the solution in terms of an implicit integral. For the polynomial cases we are considering, explicit solutions are available.

- In general the speed–height relationship is $c^2\phi_0^2=2V(\phi_0)$ with $\phi_0\neq 0$. This gives the same speed–height relationships as above.
- The waveform in the cubic case is

$$\phi(z)=\frac{3(c^2-1)}{2a}\,\mathrm{sech}^2\left(\frac{z\sqrt{3(c^2-1)}}{c}\right).$$

- The waveform in the quartic case is

$$\phi(z) = \sqrt{\frac{2(c^2-1)}{b}} \operatorname{sech}\left(\frac{2z\sqrt{3(c^2-1)}}{c}\right).$$

In the proceeding sections further approximations will be described which generalise this idea. They provide new, more accurate approximations to the form of the solitary wave, and improved speed–height characteristics.

2.3. (2,0) Padé continuum approximation

The first approximation to be generated is a more accurate form of the continuum approximation. A (2,0) Padé approximation is exactly the same as a Taylor expansion to $O(D^2)$. If we allow the D^2 term to act on the full form of $V'(\phi)$ and not just on the linear part, we obtain a second-order ODE

$$\begin{aligned} c^2\phi(z) &= [I + \tfrac{1}{12}D^2]V'(\phi(z)) \\ &= V'(\phi(z)) + \tfrac{1}{12}V''(\phi(z))\phi''(z) + \tfrac{1}{12}V'''(\phi(z))\phi'(z)^2 \end{aligned} \tag{2.7}$$

which can still be integrated to first-order

$$E = \tfrac{1}{24}V''(\phi(z))^2\phi'(z)^2 + \tfrac{1}{2}V'(\phi(z))^2 - c^2V'(\phi(z))\phi(z) + c^2V(\phi(z)). \tag{2.8}$$

For a solitary wave, from the asymptotics: $\phi = 0 \Rightarrow \phi' = 0, V = 0, V' = 0$, hence $E = 0$. To get a speed–height relationship we put $\phi' = 0, \phi_0 \neq 0$, to obtain the following results;

- The general speed–height equation: $c^2[\phi_0 V'(\phi_0) - V(\phi_0)] = \frac{1}{2}V'(\phi_0)^2$
- For a pure cubic potential, $V(\phi) = \frac{1}{2}\phi^2 + \frac{1}{3}a\phi^3$

$$c^2 = \frac{3(1+a\phi_0)^2}{3+4a\phi_0} \qquad \text{or} \qquad \phi_0 = \frac{1}{3a}(2c^2 - 3 + c\sqrt{4c^2-3}). \tag{2.9}$$

- For a pure quartic potential, $V(\phi) = \frac{1}{2}\phi^2 + \frac{1}{4}b\phi^4$

$$c^2 = \frac{2(1+b\phi_0^2)^2}{2+3b\phi_0^2} \qquad \text{or} \qquad \phi_0^2 = \frac{1}{4b}(3c^2 - 4 + c\sqrt{9c^2-8}). \tag{2.10}$$

- And for the Toda potential, just the one form is available

$$c^2 = \frac{ab(1-\mathrm{e}^{-b\phi_0})^2}{2(1-\mathrm{e}^{-b\phi_0} - b\phi_0\mathrm{e}^{-b\phi_0})} \tag{2.11}$$

since other equations are transcendental in nature.

The form of the solitary wave is somewhat harder to obtain. From equation (2.8) we find

$$\pm 2\sqrt{3}\,z = \int_0^z \pm 2\sqrt{3}\,\mathrm{d}z' = \int_{\phi_0}^{\phi} \frac{V''(u)\,\mathrm{d}u}{\sqrt{2c^2uV'(u) - 2c^2V(u) - V'(u)^2}}. \tag{2.12}$$

In the cases of cubic and quartic potentials, the integral can be calculated, but the solution can not be written in the explicit form $\phi = \phi(z)$, it has to be left as an implicit expression $z = z(\phi)$. To avoid much tedious algebra, we shall simply quote the results, and explain how to use them in setting up initial conditions.

2.3.1. Cubic Potential: $V(\phi)=\frac{1}{2}\phi^2+\frac{1}{3}a\phi^3$. Calculating the integral (2.12)

$$\pm 2\sqrt{3}\,z = 4\tan^{-1}(\Theta) - \frac{1}{\sqrt{c^2-1}}\log\left(\frac{1-\Theta\sqrt{\beta/a\phi_0}}{1+\Theta\sqrt{\beta/a\phi_0}}\right) \tag{2.13}$$

$$\Theta^2 = \frac{a(\phi_0-\phi)}{a\phi+\beta} \qquad \beta = \frac{1}{3}c\sqrt{4c^2-3}-\frac{2}{3}c^2+1. \tag{2.14}$$

To solve these equations for a fixed z, we first note that (2.13) can be rearranged to form a simpler implicit equation

$$\Theta = \sqrt{\frac{a\phi_0}{\beta}}\tanh[\sqrt{c^2-1}(\pm\sqrt{3}\,z-2\tan^{-1}(\Theta))]. \tag{2.15}$$

To start an iterative solution of this equation, we can use another approximation, e.g. the (0,2) Padé approximation with ϕ_0 supplied by the speed–height relation generated by this method, $\phi=\phi_0\operatorname{sech}^2(\kappa z)$, where ϕ_0 from equation (2.9), and $\kappa=(1/c)\sqrt{3(c^2-1)}$ from the (0,2) Padé approximation. This leads to an initial value of $\Theta^{(0)}$ which can be calculated numerically from

$$\Theta^{(0)} = \frac{\sinh(\kappa z)}{\sqrt{1+(\beta/a\phi_0)\cosh^2(\kappa z)}} \tag{2.16}$$

followed by a carefully chosen iteration method, making sure that convergence is guaranteed for all z.

Once the iteration has converged, $\phi(z)$ can easily be found from Θ. However $\mathrm{d}\phi/\mathrm{d}z$ needs a little more work to find. We differentiate (2.13) with respect to z, to find (after some rearrangement)

$$\frac{\mathrm{d}\Theta}{\mathrm{d}z} = \frac{\pm\sqrt{3}(1+\Theta^2)(a\phi_0-\beta\Theta^2)}{(1+\Theta^2)+2(a\phi_0-\beta\Theta^2)}. \tag{2.17}$$

Note that

$$\frac{\mathrm{d}\phi}{\mathrm{d}z} = \frac{-2\Theta(a\phi_0+\beta)}{a(1+\Theta^2)^2}\frac{\mathrm{d}\Theta}{\mathrm{d}z} \tag{2.18}$$

$$= \frac{-2\Theta\sqrt{3}(a\phi_0+\beta)(a\phi_0-\beta\Theta^2)}{a(1+\Theta^2)[(1+\Theta^2)+2(a\phi_0-\beta\Theta^2)]} \tag{2.19}$$

and we can calculate all necessary quantities to initialise a solitary wave.

2.3.2. Quartic potential: $V(\phi)=\frac{1}{2}\phi^2+\frac{1}{4}b\phi^4$. Results for this potential are shown in table 2. Again calculating the integral in (2.12)

$$\pm 2\sqrt{3}\,z = 3\tan^{-1}(\Theta) - \frac{1}{2\sqrt{c^2-1}}\log\left(\frac{1-\Theta\sqrt{\beta/b\phi_0^2}}{1+\Theta\sqrt{\beta/b\phi_0^2}}\right) \tag{2.20}$$

$$\Theta^2 = \frac{b(\phi_0^2-\phi^2)}{b\phi^2+\beta} \qquad \beta = \frac{1}{4}c\sqrt{9c^2-8}-\frac{3}{4}c^2+1. \tag{2.21}$$

Note that the definitions of β and Θ are different to those used in the cubic case. A simpler implicit equation is

$$\Theta = \sqrt{\frac{b\phi_0^2}{\beta}} \tanh\left(\sqrt{c^2-1}\,(\pm 2\sqrt{3}\,z - 3\tan^{-1}(\Theta))\right). \tag{2.22}$$

If, as before, we use a form of the (0,2) Padé approximation to start the iteration, then $\phi = \phi_0 \operatorname{sech}(\kappa z)$, with ϕ_0 from equation (2.10), and $\kappa = (2/c)\sqrt{3(c^2-1)}$. This leads to an initial value of Θ given by

$$\Theta^{(0)} = \frac{\sinh(\kappa z)}{\sqrt{1 + (\beta/b\phi_0^2)\cosh^2(\kappa z)}}. \tag{2.23}$$

From (2.20)

$$\frac{d\Theta}{dz} = \frac{\pm 2\sqrt{3}\,(1+\Theta^2)(b\phi_0^2 - \beta\Theta^2)}{3(b\phi_0^2 - \beta\Theta^2) + (1+\Theta^2)} \tag{2.24}$$

so

$$\frac{d\phi}{dz} = \frac{-2\Theta(b\phi_0^2 + \beta)}{[3(b\phi_0^2 - \beta\Theta^2) + (1+\Theta^2)]}\sqrt{\frac{3(b\phi_0^2 - \beta\Theta^2)}{b(1+\Theta^2)}}. \tag{2.25}$$

2.4. (2,2) Padé approximation

If we seek more accurate approximations to the travelling waves, we have to find a fourth-order accurate form for $\Lambda(D)$, which will still allow us to solve the resulting ODE. The simplest way to do this is to use a (2,2) Padé approximation for $\Lambda(D)$, so we still get a second-order differential equation.

$$4\sinh^2 \frac{1}{2}D \sim I + \frac{1}{12}D^2 + \frac{1}{360}D^4 \sim \frac{I + \frac{1}{20}D^2}{I - \frac{1}{30}D^2}. \tag{2.26}$$

Then, $c^2\phi = \Lambda(D)V'(\phi)$ becomes

$$c^2[I - \tfrac{1}{30}D^2]\phi(z) = [I + \tfrac{1}{20}D^2]V'(\phi(z)). \tag{2.27}$$

This leads to equations very similar to those obtained in the (2,0) Padé method, and the same tools are sufficient to solve them. We multiply by $[2c^2 + 3V''(\phi(z))]\phi'(z)$ and integrate

$$E = \tfrac{1}{2}[2c^2 + 3V''(\phi(z))]^2\phi'(z)^2 - 30\,W \tag{2.28}$$

$$W = 2c^4\phi(z)^2 + 6c^2\phi(z)V'(\phi(z)) - 10c^2V(\phi(z)) - 3V'(\phi(z))^2. \tag{2.29}$$

Again for a solitary wave, when $\phi = 0$; $\phi' = 0$, $V = 0$ and $V' = 0$, so $E = 0$. Hence the speed–height relationship is given by $E = 0, \phi' = 0, \phi \neq 0 \Rightarrow W = 0$

$$c^2 = \frac{1}{2\phi_0^2}\left(5V(\phi_0) - 3\phi_0V'(\phi_0) + \sqrt{10V(\phi_0)^2 + 15(\phi_0V'(\phi_0) - V(\phi_0))^2}\right). \tag{2.30}$$

In the case of cubic and quartic potentials this relation can be inverted and ϕ_0 found as a function of c

- For a cubic potential

$$\phi_0 = \frac{1}{9a}\left(4c^2 - 9 + c\sqrt{5(14c^2-9)}\right). \tag{2.31}$$

- For a quartic potential

$$\phi_0^2 = \frac{1}{12b}\left(7c^2 - 12 + c\sqrt{5(29c^2-24)}\right). \tag{2.32}$$

- For the Toda potential

$$c^2 = \frac{1}{2b\phi_0^2}\Big[3ab\phi_0 e^{-b\phi_0} + 2ab\phi_0 - 5a + 5ae^{-b\phi_0} + a\sqrt{5}(5e^{-2b\phi_0} - 10e^{-b\phi_0} \\ -2b\phi_0 e^{-b\phi_0} + 5 - 4b\phi_0 + 2b^2\phi_0^2 + 6b\phi e^{-2b\phi_0} + 3b^2\phi_0^2 e^{-2b\phi_0})^{1/2}\Big]. \tag{2.33}$$

An expression for the waveform is again complicated, but possible to find in terms of an implicit equation. From (2.28), we obtain the relation

$$\sqrt{60}\,\mathrm{d}z = \frac{2c^2 + 3V''(\phi)}{\sqrt{W}}\,\mathrm{d}\phi \tag{2.34}$$

which can then be integrated. The tricks used to perform this are identical to those used earlier, in deriving the (2,0) Padé approximation; and so will be omitted here. The end results are:

2.4.1. Cubic potential: $V(\phi) = \frac{1}{2}\phi^2 + \frac{1}{3}a\phi^3$. Integrating (2.34)

$$\pm 2\sqrt{15}\,z = 4\sqrt{3}\,\tan^{-1}(\Theta) - \frac{2c^2+3}{\sqrt{3a\phi_0\beta}}\log\left(\frac{1-\Theta\sqrt{\beta/a\phi_0}}{1+\Theta\sqrt{\beta/a\phi_0}}\right) \tag{2.35}$$

$$\Theta^2 = \frac{a(\phi_0 - \phi)}{a\phi + \beta} \qquad \beta = \frac{1}{9}c\sqrt{5(14c^2-9)} - \frac{4}{9}c^2 + 1. \tag{2.36}$$

To solve these equations for a fixed z, we first note that (2.35) can be rearranged to give

$$\Theta = \sqrt{\frac{a\phi_0}{\beta}}\tanh\left(\frac{3\sqrt{a\phi_0\beta}}{2c^2+3}(\pm\sqrt{5}\,z - 2\tan^{-1}(\Theta))\right) \tag{2.37}$$

and to start the iteration process, we can use (0,2) Padé approximation as before, i.e. $\phi = \phi_0\,\mathrm{sech}^2(\kappa z)$; with ϕ_0 supplied by the speed–height relation generated by this method (2.31), and $\kappa = (1/c)\sqrt{3(c^2-1)}$. This leads to an initial value of Θ given by

$$\Theta^{(0)} = \frac{\sinh(\kappa z)}{\sqrt{1 + (\beta/a\phi_0)\cosh^2(\kappa z)}}. \tag{2.38}$$

Once the iteration has converged $\phi(z)$ can easily be found from Θ and $\mathrm{d}\phi/\mathrm{d}z$ after differentiating (2.35) with respect to z

$$\frac{\mathrm{d}\Theta}{\mathrm{d}z} = \frac{3\sqrt{5}\,(1+\Theta^2)\,(a\phi_0 - \beta\Theta^2)}{6(a\phi_0 - \beta\Theta^2) + (2c^2+3)(1+\Theta^2)} \tag{2.39}$$

then

$$\frac{\mathrm{d}\phi}{\mathrm{d}z} = \frac{-6\sqrt{5}\,\Theta(a\phi_0 + \beta)\,(a\phi_0 - \beta\Theta^2)}{a(1+\Theta^2)[6(a\phi_0 - \beta\Theta^2) + (2c^2+3)(1+\Theta^2)]}. \tag{2.40}$$

2.4.2. Quartic potential: $V(\phi) = \frac{1}{2}\phi^2 + \frac{1}{4}b\phi^4$. We follow the same procedure as above

$$\pm\, 2\sqrt{15}\, z = 3\sqrt{3}\tan^{-1}\Theta - \frac{2c^2+3}{2\sqrt{3b\phi_0^2\beta}}\log\left(\frac{1-\Theta\sqrt{\beta/b\phi_0^2}}{1+\Theta\sqrt{\beta/b\phi_0^2}}\right) \tag{2.41}$$

$$\Theta^2 = \frac{b(\phi_0^2 - \phi^2)}{b\phi^2 + \beta} \qquad \beta = \frac{1}{12}c\sqrt{5(29c^2-24)} - \frac{7}{12}c^2 + 1. \tag{2.42}$$

The equation to be solved is then

$$\Theta = \sqrt{\frac{b\phi_0^2}{\beta}}\tanh\left(\frac{3\sqrt{a\phi_0^2\beta}}{2c^2+3}\left(\pm 2\sqrt{5}\,z - 3\tan^{-1}(\Theta)\right)\right). \tag{2.43}$$

An initial value for the iteration is

$$\Theta^{(0)} = \frac{\sinh(\kappa z)}{\sqrt{1 + (\beta/b\phi_0^2)\cosh^2(\kappa z)}} \tag{2.44}$$

which is generated from $\phi = \phi_0 \operatorname{sech} \kappa z$, $\kappa = (2/c)\sqrt{3(c^2-1)}$, and ϕ_0 from (2.32). The final result we need is

$$\frac{\mathrm{d}\phi}{\mathrm{d}z} = \frac{6\sqrt{5}\,\Theta(b\phi_0^2 + \beta)\sqrt{b\phi_0^2 - \beta\Theta^2}}{\sqrt{b}\sqrt{1+\Theta^2}[9(b\phi_0^2 - \beta\Theta^2) + (2c^2+3)(1+\Theta^2)]}. \tag{2.45}$$

2.5. Global approximation of the operator in Fourier space

We can state the lattice soliton problem in Fourier space as

$$c^2\hat{\phi}(k) = \hat{\Lambda}(k)\hat{F}(k) \qquad \hat{\Lambda}(k) = \frac{4\sin^2\frac{1}{2}k}{k^2}. \tag{2.46}$$

In aiming to produce a good approximation to the solitary wave, the initial objective is to find a good approximation of the operator $\hat{\Lambda}(k)$ which still allows the equations to be solved. The continuum approximations already considered achieve this by a Taylor expansion about $k = 0$. This gives good approximations provided the final solution has a small high frequency component. However, large fast solitary waves become quite narrow (2 or 3 lattice spacings wide) and so do contain a considerabley high frequency component. Hence to obtain good approximations to these solitary waves, we need an approximation to $\hat{\Lambda}(k)$ which is uniformly valid for all k.

We also note, from considering the (0,2) Padé approximation, that, approximations of the form

$$\hat{\lambda}(k) = \frac{1}{\alpha + \beta k^2} \tag{2.47}$$

lead to equations which are easily soluble, and enable us to write the final solution as $\phi = \phi(z)$. We shall consider approximations of the above form, and attempt find α, β giving a good global fit to $\hat{\Lambda}(k)$.

Five different expressions have been considered, to find equations relating α and β: minimising the L^1, L^2, L^∞ norms of the difference, $\hat{\Lambda}(k) - \hat{\lambda}(k)$; forcing equality at $k = 0$, or forcing equality in an averaged sense as $\lambda \to \infty$. Minimising the L^1 and L^∞ norms is not simple, but can be attempted numerically, or heuristically (as we have done for the L^∞ case). Of all the possible combinations left, forcing equality at $k = 0$ together with minimising the L^2 norm of the difference gives the best results. To minimise the L^2 norm, we follow an Euler–Lagrange formulation and expand around the minimum $\hat{\lambda}_0$, where $\hat{\lambda}(k) = \hat{\lambda}_0(k) + \epsilon(k)$

$$I(\hat{\lambda}) = I(\hat{\lambda}_0) + \int_0^\infty \epsilon(k)[\hat{\Lambda}(k) - \hat{\lambda}(k)]\,\mathrm{d}k + \mathrm{O}(\|\epsilon\|^2). \tag{2.48}$$

By making $\epsilon(k)$ sufficiently small, and of one sign on $[0,\infty)$, we find a condition for the minimum to be attained. This is $\int_0^\infty \hat{\Lambda}(k)\mathrm{d}k = \int_0^\infty \hat{\lambda}(k)\mathrm{d}k$. Now, $\int_0^\infty \hat{\Lambda}(k)\mathrm{d}k = \pi$, and $\int_0^\infty \hat{\lambda}(k)\mathrm{d}k = \pi/2\sqrt{\alpha\beta}$. Hence $\alpha\beta = \frac{1}{4}$. Making $\hat{\lambda}(k) = \hat{\Lambda}(k)$ at $k = 0$ produces $\alpha = 1$; so $\beta = \frac{1}{4}$.

Solving the resultant equations to find $\phi(z)$, we find for the cubic and quartic potentials respectively

$$\begin{aligned} \phi_3(z) &= \frac{3}{2a}(c^2-1)\,\mathrm{sech}^2\left(z\sqrt{\frac{c^2-1}{c^2}}\right) \\ \phi_4(z) &= \sqrt{\frac{2}{b}(c^2-1)}\,\mathrm{sech}\left(2z\sqrt{\frac{c^2-1}{c^2}}\right). \end{aligned} \tag{2.49}$$

2.6. *Results of numerical tests*

Numerical tests have been carried out using a fourth-order symplectic Hamiltonian scheme [11]. The scheme has been extensively tested and found to be useful tool for investigating large systems of ODEs [12]. The Hamiltonian itself is not exactly conserved as one of these, but is 'almost conserved'. It oscillates around its initial value with a small, non-increasing amplitude. The scheme is more efficient than an equivalent Runge–Kutta scheme since it requires fewer evaluations of the potential energy gradient. Over extended periods it is much more accurate, since it does not suffer from in-built damping, as Runge–Kutta schemes do.

The accuracy percentage quoted in the following tables is calculated by inserting the predicted waveform into the integrator described above, and integrating forward in time until the solitary wave has separated from radiation. The energy in the soliton is then measured again and divided by the total energy in the system. This gives the proportion of the initial condition which actually forms a soliton. Tables have been compiled with $dt = 0.01, (a, b) = (2, 0), (0, 2)$. The energy is measured in the seven points centred around the point with maximal dispacement. Some of the energy in very wide solitary waves will be neglected, this accounts for some of the inaccuracy at low speeds.

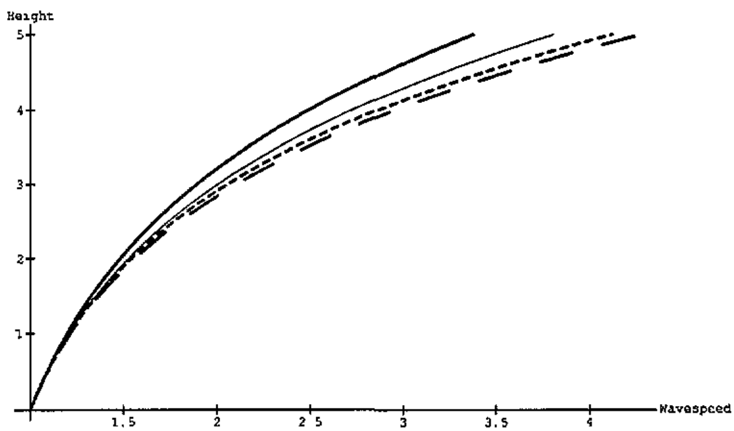

Figure 1. The figure shows height versus speed for the Toda potential. The narrow line represents the exact solution; the thick line the standard continuum/(0,2) Padé; the dashed line is the full continuum and the dotted line the (2,2) Padé approximation.

Note, also the graph showing how each of the various methods compares when used to predict the speed–height characteristics for the Toda potential.

2.6.1. *Cubic potential.*

Results for this potential are shown in table 1. Where no percentage is shown the initial condition degenerated before a soliton could separate from radiation (small amplitude linear waves). The degeneration is due to the error in the initial conditions being large enough to push some lattice nodes over the potential barrier at $\phi = -1/a$. These nodes have then escaped from the potential well, and the system is doomed.

The (0,2) Padé approximation will not produce a wave at speed $c = 2.0$ due to the errors being too large. The (2,2) Padé approximation can produce waves up to $c = 2.8$ without the errors becoming catastrophic.

Table 1. Results for numerical tests with a cubic potential. See text for details

	Wave speed c				
	1.1	1.3	1.5	1.9	2.5
Standard continuum	99.3% $H = 0.051$	93% $H = 0.380$	81% $H = 1.177$	N/A	N/A
(2,0) Padé continuum	99.89% $H = 0.060$	99.7% $H = 0.630$	99.6% $H = 2.44$	99.5% $H = 15.4$	99.4 $H = 101$
(0,2) Padé continuum	99.87% $H = 0.055$	99.20% $H = 0.526$	98.4% $H = 1.894$	97.0% $H = 11.13$	N/A
(2,2) Padé continuum	99.97% $H = 0.058$	99.993% $H = 0.602$	99.98% $H = 2.332$	99.94% $H = 14.86$	99.89% $H = 99.4$
Global approximation to Fourier operator	95.7% $H = 0.095$	95% $H = 0.919$	96.3% $H = 3.41$	97.5% $H = 20.6$	98.1% $H = 133$

2.6.2. *Quartic potential.* With a quartic potential, there is no problem with nodes escaping over a potential barrier and all methods can be considered at any speed. For the case $c = 100$, $\mathrm{d}t$ was reduced to 0.001.

Table 2. Results of numerical tests with a quartic potential. See text for details.

	Wave speed c				
	1.1	1.5	2.5	4.0	100.0
(2,0) Padé continuum	99.7% $H = 0.410$	97.8% $H = 3.32$	95.8% $H = 38.0$	95.3% $H = 276$	91.8% $H = 1.3\mathrm{e}+8$
Standard continuum	97.7% $H = 0.308$	52% $H = 1.484$	28% $H = 16.4$	32% $H = 120$	33% $H = 1.7\mathrm{e}+7$
(0,2) Padé continuum	99.1% $H = 0.343$	88% $H = 1.924$	78.5% $H = 18.9$	76% $H = 134$	74% $H = 5.5\mathrm{e}+7$
(2,2) Padé continuum	99.98% $H = 0.390$	99.6% $H = 2.90$	98.7% $H = 31.0$	98.2% $H = 224$	97.9% $H = 9.3\mathrm{e}+7$
Global approximation to the Fourier operator	93.5% $H = 0.598$	97.0% $H = 3.49$	98.4% $H = 31.7$	98.4% $H = 217$	98.3% $H = 8.7\mathrm{e}+7$

For speeds above 2.5 the method based on a global approximation to the operator in Fourier space is seen to out-perform the (2,2) Padé approximation. The former approximation also gives the waveform explicitly, so is much more useful at these higher speeds. However, it is not so accurate at lower speeds, and the (2,2) Padé approximation is much more of a uniform approximation for the shape and size of solitary waves.

3. The Kadomtsev–Petviashvili lattice

The second equation we consider is the discrete Kadomtsev–Petviashvili equation as derived in [8]

$$\begin{aligned}\ddot{v}_{ij} = v_{i+1,j} - 2v_{i,j} + v_{i-1,j} + \epsilon^2(v_{i,j+1} - 2v_{i,j} + v_{i,j-1}) \\ - a\epsilon^2(v_{i+1,j}^2 + v_{i,j}^2 + v_{i-1,j}^2). \end{aligned} \tag{3.1}$$

The travelling wave ansatz, $v_{i,j} = \phi(i\cos\theta + j\sin\theta - ct) \equiv \phi(z)$, transforms this to

$$\begin{aligned} c^2\phi''(z) &= \phi(z+\cos\theta) - 2\phi(z) + \phi(z-\cos\theta) \\ &\quad - a\epsilon^2[\phi^2(z+\cos\theta) - 2\phi^2(z) + \phi^2(z-\cos\theta)] \\ &\quad + \epsilon^2[\phi(z+\sin\theta) - 2\phi(z) + \phi(z-\sin\theta)]. \end{aligned} \tag{3.2}$$

The most obvious way to group the terms is in ϕ and ϕ^2 on opposite sides of the equation, to obtain

$$\begin{aligned} &[c^2D^2 - 4\sinh^2(\tfrac{1}{2}D\cos\theta) - 4\epsilon^2\sinh^2(\tfrac{1}{2}D\sin\theta)]\phi(z) \\ &\qquad = [-4a\epsilon^2\sinh^2(\tfrac{1}{2}D\cos\theta)]\phi^2(z). \end{aligned} \tag{3.3}$$

We then define the operator so that $\Lambda(D)\phi(z) = \phi(z)^2$. Results such as

$$\begin{aligned} |\phi_0| &= \frac{3}{2}\left(\frac{c^2 - \cos^2\theta - \epsilon^2\sin^2\theta}{a\epsilon^2\cos^2\theta}\right) \\ |\phi_0| &= \frac{4}{3}\left(\frac{c^2 - \cos^2\theta - \epsilon^2\sin^2\theta}{a\epsilon^2\cos^2\theta}\right) \end{aligned} \tag{3.4}$$

are easily obtained for the (0,2) and (2,0) Padé approximations (respectively). Numerics show that these are reasonable results, but that better can be achieved with a little more thought. (In the results table, these approximations are described as being from the first approach.)

In the second, more accurate approach, rather than group the functions ϕ and ϕ^2, we are concern ourselves more with the direction that the differences are taken in. There is a nonlinear potential acting in one direction, and not in the other, so we attempt to keep the effects of differences in the i and j directions separate. Defining $V'(\phi) = \phi - a\epsilon^2\phi^2$, we see that equation (3.2) can be written as

$$c^2D^2\phi(z) = [4\sinh^2(\tfrac{1}{2}D\cos\theta)]V'(\phi(z)) + \epsilon^2[4\sinh^2(\tfrac{1}{2}D\sin\theta)]\phi(z). \tag{3.5}$$

This can be rearranged to the form

$$\phi(z) = A(D)V'(\phi(z)) \qquad A(D) = \frac{4\sinh^2(\tfrac{1}{2}D\cos\theta)}{c^2D^2 - 4\epsilon^2\sinh^2(\tfrac{1}{2}D\sin\theta)}. \tag{3.6}$$

It is possible to expand all terms as a power series in D, we divide out the common factor of D^2 as usual. To enable us to see through the complexities of the calculation we will use the simplifying notation $\alpha = \cos^2\theta, \beta = \sin^2\theta, \gamma = c^2 - \epsilon^2\sin^2\theta$, to write the operator as

$$A(D) \sim \frac{\alpha + \frac{1}{12}\alpha^2D^2 + \frac{1}{360}\alpha^3D^4}{\gamma - \frac{1}{12}\beta^2\epsilon^2D^2 - \frac{1}{360}\beta^3\epsilon^2D^4}. \tag{3.7}$$

3.1. (2,0) Padé approximation

For the (2,0) Padé approximation, we expand $A(D)$ to $O(D^2)$ in a Taylor series

$$A(D) \sim \left[\alpha + \frac{1}{12}\alpha D^2\right]\left[\gamma - \frac{1}{12}\beta^2\epsilon^2 D^2\right]^{-1} \sim \frac{\alpha}{\gamma} + \frac{\alpha}{12\gamma}(\alpha\gamma + \beta\epsilon^2)D^2 \tag{3.8}$$

$$\stackrel{\text{def}}{=} P + QD^2. \tag{3.9}$$

The differential equation is then (after an integration)

$$\phi V'(\phi) - V(\phi) = \tfrac{1}{2}PV'(\phi)^2 + R\phi'^2 V''(\phi)^2 - E. \tag{3.10}$$

For a solitary wave, $\phi, \phi' \to 0$, and so $E = 0$. The height of the solitary wave is then independent of Q; and substituting for P gives

$$\frac{\gamma}{\alpha} = \frac{V'(\phi_0)^2}{\phi_0 V'(\phi_0) - V(\phi_0)}. \tag{3.11}$$

Substituting now for α, γ, V; and putting $T \stackrel{\text{def}}{=} \gamma/\alpha = (c^2 - \epsilon^2 \sin^2\theta)\sec^2\theta$

$$|\phi_0| = \frac{1}{3a\epsilon^2}[2T - 3 + \sqrt{T(4T-3)}]. \tag{3.12}$$

3.2. (0,2) Padé approximation

In this approximation, the differential operator acts on ϕ, and not on the nonlinear function, $V'(\phi)$. Using the same notation $(\alpha, \beta, \gamma, P, Q)$ in the previous subsection

$$A(D)^{-1} \sim [P + QD^2]^{-1} \sim \frac{1}{P}\left[1 - \frac{Q}{P}D^2\right] \tag{3.13}$$

then $P\phi - Q\phi'' = P^2 V'(\phi)$ can be integrated to

$$\tfrac{1}{2}P\phi^2 - \tfrac{1}{2}Q\phi'^2 = P^2 V(\phi) - E. \tag{3.14}$$

For a soliton solution, $\phi, \phi' \to 0$ in the large z limit, so $E = 0$. For the speed–height curve, we set $\phi'(0) = 0$, to find $\phi_0^2 = 2PV(\phi_0)$. Substituting back, we find that

$$|\phi_0| = \frac{3}{2}\left(\frac{c^2 - \cos^2\theta - \epsilon^2\sin^2\theta}{a\epsilon^2\cos^2\theta}\right). \tag{3.15}$$

3.3. (2,2) Padé approximation for the KP lattice

We expand (3.7) to $O(D^4)$, write $A(D)$ as

$$A(D) \sim \frac{\alpha + RD^2}{\gamma + SD^2}. \tag{3.16}$$

Equating coefficients in the corresponding expansions gives

$$S = \frac{-(2\alpha^2\gamma^2 + 5\alpha\beta^2\epsilon^2\gamma + 2\beta^3\epsilon^2\gamma + 5\beta^4\epsilon^2)}{60(\alpha\gamma + \beta^2\epsilon^2)} \tag{3.17}$$

$$R = \frac{\alpha}{\gamma}\left[S + \frac{1}{12}(\alpha\gamma + \beta^2\epsilon^2)\right]. \tag{3.18}$$

We solve the differential equation, $[\gamma + SD^2]\phi = [\alpha + RD^2]V'(\phi)$ to obtain

$$\tfrac{1}{2}\alpha RV'(\phi_0)^2 - \gamma R(\phi_0 V'(\phi_0) - V(\phi_0)) - \alpha SV(\phi_0) + \tfrac{1}{2}\gamma S\phi_0^2 = 0 \tag{3.19}$$

as a speed–height relation. This is not a function of R, S, α, γ independently, but only the ratios, $U \stackrel{\text{def}}{=} R/S, T \stackrel{\text{def}}{=} \gamma/\alpha$ (T as defined earlier). After some manipulation we arrive at the quadratic

$$0 = U(a\epsilon^2\phi_0)^2 + (\tfrac{2}{3} - 2U + \tfrac{4}{3}TU)(a\epsilon^2\phi_0) + (T + U - 1 - TU). \tag{3.20}$$

The solution is then

$$|\phi_0| = \frac{2TU + 1 - 3U + \sqrt{(1-TU)(1-4TU+3U)}}{3Ua\epsilon^2}. \tag{3.21}$$

3.4. Comparison of results

Table 3 shows the percentage errors in the speed–height curves when the height of the exact solution (calculated numerically by a spectral method) reached $\simeq 1600$, with parameters $\epsilon = 0.1, a = 0.25$. All methods converge to the exact solution as height $\to 0$.

Table 3. Percentage errors in the speed–height curves. See text for details.

	Angle θ		
	$\pi/10$	$\pi/5$	$3\pi/10$
(2,0) Padé-first approach	+6.20%	+6.00%	+4.80%
(2,0) Padé—second approach	−3.90%	−3.90%	−3.90%
(2,2) Padé—either approach	−1.21%	−1.20%	−1.17%
Asymptotic expansion in [8]	−1.03%	−0.88%	−0.43%

Note the (0,2) Padé approximation gives the same results as the (2,0) Padé—first approach. Use of the asymptotic result derived in [8] still requires the solution of a nonlinear differential delay equation, which has to be carried out numerically.

4. Discussion and conclusions

We have used various continuum approximations to model solitary waves in a discrete system—a lattice with various forms of non-harmonic interaction. In all cases the (2,2) Padé method is seen to be more accurate than any other. The accuracy at high speeds shows a significant improvement on other methods, allowing much faster solitary waves to be initiated in the cubic potential than was previously possible. A speed–height relationship is very simple to find in all cases, however the complete waveform sometimes is non-trivial.

The method of testing accuracy that has been used here measures how the initial wave form adapts to the grid. It does not compare the predicted speed with the actual speed of propagation in the lattice. However this can be done, and the fit is found to be reasonably good. In the case of a lattice with quartic interaction potential and the initial conditions given by the (2,2) Padé approximation at speed $c = 2.0$, the actual speed of the wave generated is $c \simeq 2.07$, an error of 3–4%. Hence we can conclude that the speed of the wave generated is very close to the predicted value.

Of the three methods which give an explicit waveform, the (0,2) Padé method gives the best results, but even its accuracy tails off for larger speeds ($c > 1.5$). Its relative accuracy is due to the fact that it relies on fewer approximations than the other two methods. The standard continuum method uses the approximation $\mathrm{d}^2V'(\phi(z))/\mathrm{d}z^2 \simeq \mathrm{d}^2\phi/\mathrm{d}z^2$. This is seen to be valid only in a very small region above $c = 1$, ($c \lesssim 1.3$).

The method based on a global approximation to the operator in Fourier space works just as well for the two-dimensional lattice as for one. The integrals can still be calculated analytically. For the KP lattice, the integrals are not solvable explicitly, although they are well defined. A numerical calculation can be carried out, or they can be calculated by asymptotic methods. An expansion of the discrete KP operator in Fourier space assuming ϵ to be small can lead to an infinite power series in ϵ with coefficients given by calculable integrals. The details of these results are left to the reader.

In summary we see that it is possible to derive analytic results with much greater accuracy than those obtained by the straightforward continuum approximation.

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