# CALCULATION OF FAMILIES OF SOLITARY WAVES ON DISCRETE LATTICES

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ABSTRACT.

We extend the iterative method suggested by Hochstrasser et al. by using spectral collocation methods coupled with path-following techniques. The resulting scheme is very accurate and efficient, even for narrow pulses, and makes it possible to calculate a whole family of solitary wave solutions as a parameter (such as the velocity of the pulse) is varied.

## I. INTRODUCTION

In a recent paper [4], Hochstrasser et al. have put forward an iterative scheme based on Fourier transforms for the calculation of narrow solitary wave excitations on atomic chains. We suggest here modifications and extensions to their method based on spectral-collocation [1] and path-following [8] techniques. The advantages of this approach are twofold: (a) the linearly convergent iteration scheme of [4] is replaced by a quadratically convergent iteration, and (b) the use of continuation methods enable a whole family of solutions to be quickly generated, as an external parameter such as the soliton velocity is varied. As a by-product of our analysis, we also present numerical evidence that the spectral methods give super-algebraic convergence [1] as the number of spatial points is increased.

For conciseness we will treat here only the two cases treated in detail by [4], namely the Toda lattice and the lattice with potential $V(u) = \frac{1}{2}(u^2 + \beta u^4)$, with $\beta > 0$. However the methods we describe can be extended in a straightforward way to models with other nonlinear potentials, to coupled discrete lattice models such as those described by Pnevmatikos et al. [6], to other discrete systems supporting solitary waves such as myelinated nerve axons [7], or indeed to many continuous systems. Work on such applications is underway and will be reported elsewhere.

As discussed in [4], we consider a nonlinear monotonic chain of unit mass particles with nearest neighbour couplings, leading to a Lagrangian of the form

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

where $\alpha_n$ is the displacement of the $n$th particle from its equilibrium position. If the relative displacement of the $n$th bond is defined to be $u_n = \alpha_{n+1} - \alpha_n$, then the equation of motion becomes

$$\ddot{u}_n - \{V'(u_{n+1}) - 2V'(u_n) + V'(u_{n-1})\} = 0. \tag{2}$$

We are interested in travelling waves, i.e. in solutions of the form $u_n(t) = u(n - vt) = u(z)$. With this ansatz, (2) becomes

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

with $F(z) = V'\{u(z)\}$. By multiplying both sides by $z^2$ and integrating by parts, it is straightforward to show that

$$v^2 \int_{-\infty}^{\infty} u(z)dz = \int_{-\infty}^{\infty} F(z)dz \tag{4}$$

providing $u(z) = o(1/z)$ and $u_z(z) = o(1/z^2)$ as $|z| \to \infty$. This identity can also be obtained as the $q \to 0$ limit of the Fourier Transform of (3), as shown in [4], and turns out to be very useful.

## II. NUMERICAL METHODS

In [4], solutions of (3) are obtained by taking Fourier Transforms and solving the resulting equation in $q$ space by a linear iteration modified by the constraint (4). This procedure, when it converges, gives one of the infinite-dimensional solitary wave solutions of (2), but there is no way of proscribing the velocity in advance. By varying the starting point of the iterations, a number of solutions for different $v$ can be obtained, and a solution for a proscribed $v$ can then be obtained by interpolation.

Our technique, although also based on spectral methods, uses a quadratically convergent Newton-Raphson iteration, together with continuation methods to generate a whole path of solutions as a function of $v$. Any solutions required for specific values of $v$ can quickly be generated to high accuracy. Similar techniques for the study of stationary solutions of single and coupled reaction diffusion equations have been proposed in [2, 3].

To be specific, we approximate the exact solution $u(z)$ by a finite cosine series over a finite interval $L$.

$$u(z) \approx U(z) = \sum_{j=0}^{n-1} c_j \phi_j(z), \tag{5}$$

where $\phi_j(z) = \cos(2\pi jz/L)$. This will give us solutions of (3) with period $L$: in the large $L$ limit we expect to get good approximations to solitary waves which have infinite period.

The unknown coefficients are then fixed by inserting (5) into (3) and requiring that the resulting equations be satisfied on the $n-1$ collocation points $z_i = iL/2(n-1)$, with $i = 0, \ldots, n-2$. This gives the equations

$$-(2\pi v/L)^2 \sum_{j=0}^{n-1} j^2 c_j \phi_j(z_i) \;=\; F(U(z_i+1)) - 2F(U(z_i)) + F(U(z_i-1)) \quad (6)$$
$$i = 0, \ldots, n-2.$$

In addition we require one further equation: this is given by the trapezoidal rule approximation to (4) over the set of points $\{z_i, i = 0, \ldots, n-1\}$, where $z_{n-1} = L/2$:

$$v^2 c_0 = \frac{1}{2}F(z_0) + F(z_1) + \ldots + F(z_{n-2}) + \frac{1}{2}F(z_{n-1}). \quad (7)$$

Although these are mostly standard spectral collocation techniques, some further explanation is necessary. The cosine functions are chosen because the solution $u(z)$ can be chosen to be symmetric about the point $z = 0$. The collocation points are chosen to lie in $[0, L/2)$ because the cosines are symmetric about $L/2$. Finally the constraint equation (4) is chosen to pick out the "solitary" wave family of solutions from the two dimensional sheet of periodic solutions of (3). Without this constraint equation we may converge to another solution which does not satisfy the requirement that $u(z) \to 0$ as $|z| \to \infty$. The trapezoidal rule approximation to (4) has high accuracy for periodic functions [5].

The set of equations (6-7) are nonlinear in the unknowns $c_j$ and are soved by a Newton-Raphson iteration. This requires a suitable starting guess, which can be obtained in a number of ways, i.e. exact solutions (where known), exact solutions of continuum approximations, numerical solutions of nearby solutions in parameter space. The continuation method works by using the last of these in an Euler-type predictor scheme [8]. Usually convergence to the solutions of (6-7) to machine accuracy at each step is reached in three or four iterations.

## III. RESULTS

We first tested the scheme on the Toda lattice [9]. Here $V(u) = a(1 - \exp(-bu))$, and analytic solutions are known for both the periodic case and the infinite line. For a given solution to (3), other solutions can be constructed by the transformation $u \to u' + u_0, v^2 \to (v')^2 \exp(bu_0)$, where $u_0$ is a constant. From the exact solutions on the periodic lattice [9], solutions satisfying the constraint (4) can be constructed by this transformation, to test the numerical scheme. In Fig. 1 we show graphs of the errors in two cases, (a) $L = 3, k^2 = 0.9$, corresponding to $v \approx 1.55268$, and (b) $L = 10, k^2 = 0.9999$, corresponding to $v \approx 1.257097$. Here $L = \lambda$ is the period of the lattice,

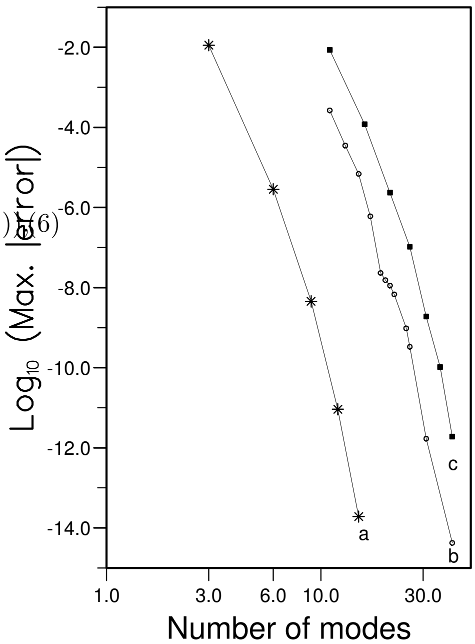


FIG. 1: Curves of maximum error as a function of $n$, for the cases discussed in the text.

and $k$ is the modulus of the dn functions appearing in the analytic solution (eqn. (2.3.1) in [9]). In both cases we took $a = b = 1$. The error is defined to be the maximum absolute error, i.e. $\max_{z\in[0,L]} |u_{exact}(z) - U(z)|$ . For the $L = 3$ case we need only 9 points to achieve 8 decimal place accuracy, whereas for the $L = 10$ case we can achieve the same accuracy with 21 points. The graph of the errors clearly suggest superalgebraic convergence, i.e. convergence faster than any power of $1/n$ [1]. Next we consider the lattice with potential $V(u) = \frac{1}{2}(u^2 + \beta u^4)$. In this case only solutions to the continuum approximation are available [4]. The error curves for a solution in the case $L = 10, \beta = 1, v = 2$ are also shown in Fig. 1 as curve (c). Here we define the "exact" solution as the numerical solution with a large value of $n$. The rate of convergence is similar to the Toda case. In Fig. 2 we show the path of a family of solutions in this case as $v$ is varied, where we plot the height of the solitary wave against velocity. This curve and the resulting solutions take only a few seconds to calculate on a Sun Sparcstation 1. The inset in Fig. 2 shows some of the resulting waveforms at various points on this curve.

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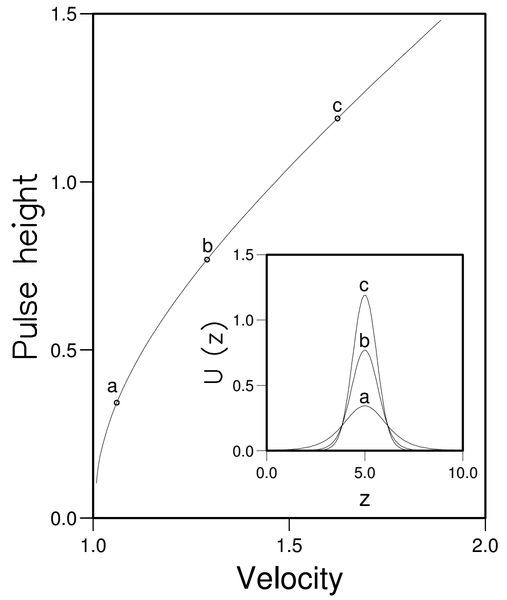


FIG. 2: Path of travelling pulse solutions as a function of $v$, as discussed in the text, and corresponding wave forms.


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