ON THE QUASI-CONTINUOUS APPROXIMATION OF THE TODA LATTICE ☆

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We study the viability of an analytic procedure for deriving a partial differential equation approximating the dynamics of a lattice, with an arbitrary interparticle potential, in close to continuum conditions. The comparison is made through a computer study of the Toda lattice. Although the exact integrability is not preserved by the approximation, the shape of the colliding solitons is extremely well preserved after many collisions.

Consider a one-dimensional chain of interacting particles as represented by the hamiltonian

$$H=\sum_{n=1}^{N-1}\left[\frac{m}{2}\left(\frac{\mathrm{d}Y_n}{\mathrm{d}t}\right)^2+P\left(\frac{Y_{n+1}-Y_n}{h}\right)\right], \tag{1}$$

where Y_n is the displacement coordinate along the chain axis for the nth particle and P is the interaction potential between adjacent mass points with mass m, separated in equilibrium by a distance h.

The equation for the relative change in the displacement, $U_n=(Y_n-Y_{n-1})/h$, is

$$hm\frac{\mathrm{d}^2U_n}{\mathrm{d}t^2}=T(U_{n+1})-2T(U_n)+T(U_{n-1})\,. \tag{2}$$

Here $T(u)\equiv\partial_u P(u)/h$ is the tension function of the corresponding continuum limit. The continuum limit as $n\uparrow\infty$ and $h\downarrow 0$ for the solution $U_n(t)=u(nh,t)$ and particle mass $m=h\rho$ is

$$\rho\frac{\partial^2 u}{\partial t^2}=\frac{\partial^2}{\partial x^2}T[u(x,t)]\,, \tag{3}$$

where ρ is the density of the continuum. Unless T is linear, eq. (3) is a nonlinear wave equation and discontinuities will, in general, form in a finite time.

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We have shown in refs. [1] and [2] that if the leading effects due to the discreteness are properly accounted the solution of eq. (2) is better approximated by

$$\rho\frac{\partial^2 u}{\partial x^2}=\frac{\partial^2}{\partial x^2}T[u(x,t)]+\frac{\rho h^2}{12}\frac{\partial^4 u}{\partial x^2\partial t^2}, \tag{4}$$

than by eq. (3). Eq. (4) describes long wave phenomena of the discrete dense lattice to fourth order and regularizes the solution when shocks would form in eq. (3). In the derivation of eq. (4), $T(u)$ was assumed to be an arbitrary smooth function and no limitation was made on the magnitude of u.

The main objective of this letter to study numerically the relationship between the solutions to eqs. (2), (3), and (4) in the Toda lattice [3] where

$$T(U_n)=a\exp(-b_0U_n),\quad a, b_0 \text{ constants}\,. \tag{5}$$

This nonlinear tension function is especially interesting because the resulting eq. (2) is integrable [3]. Our study will consist of testing how well an exact solution of the discrete Toda lattice is preserved by the flow generated by the approximate eqs. (3) and (4).

The one-soliton solution [3] to eq. (2) with the Toda potential (5) is

$$U_n=-\frac{1}{b_0}\ln(1+f_n/a_0)\,, \tag{6a}$$

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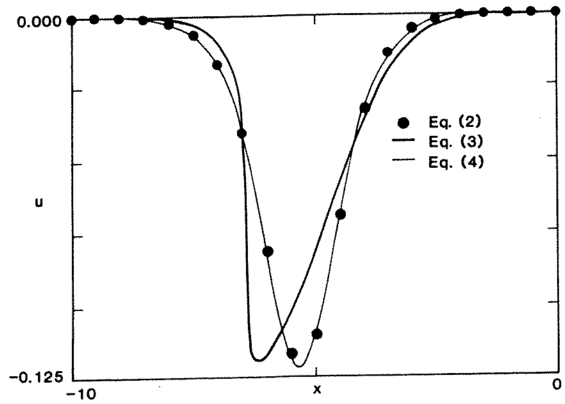

Fig. 1. The evolution of the one-soliton solution (6) under eqs. (2), (3) and (4). The parameters were $a_0=1$, $h=1/2$, $\delta=5$, $p_0=1$, $b_0=2$ and $\rho_0=1$. Note eq. (4) is an excellent approximation of eq. (2) while the solution of eq. (3) breaks into a shock.

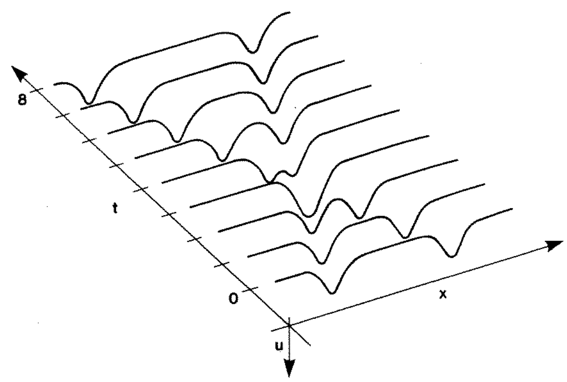

Fig. 2. Collision time history of two solitons satisfying eq. (4). Note that there is very little radiation after the collision. (Same parameters as fig. 1.).

where

$$f_n=a_0\Omega^2\,\mathrm{sech}^2(p_0hn+v_0t+\delta),\quad \delta=\mathrm{const}\,, \tag{6b}$$

and

$$v_0=\pm(a_0b_0/\rho_0)^{1/2}\Omega/h\,,$$

$$\Omega=\sinh(p_0h)\,,\quad p_0=\mathrm{const}\,. \tag{6c}$$

Eq. (4) was derived under the assumption of small, but finite, h. Thus the small amplitude wide (that is, long wavelength) discrete solitons should be well approximated in the quasicontinuum;

$$U_n\simeq -f_n/b_0a=\mathrm{O}(h^2)\,. \tag{7}$$

In fig. 1 we compare the evolution of the one-soliton solution (6) taken as an initial datum for eqs. (2), (3) and (4). It is clear from fig. 1 that the shape of the small-amplitude Toda soliton is preserved by the solution to eq. (4) but, as expected, a shock forms in the solution to eq. (3) in finite time.

In fig. 2 the collision history of two solitons exactly satisfying eq. (2) is described. Fig. 3 compares the shapes of two-soliton solutions to eqs. (2) and (4) after nine collisions in a periodic system. While, evidently, the collisions under eq. (4) are slightly inelastic, the solitons have preserved their original shape and only very minor radiation is present. This radiation did not increase noticeably as the number of collisions was increased to twenty (not shown).

The numerical approximations were performed with the MOLID integration package [4]. The spatial derivatives were approximated by a psuedo-spectral discrete Fourier transform method and the time integration used a variable order, variable time step Adams–Bashford–Moulton method. The time accuracy was varied between 10^{-6} and 10^{-10} per unit time and the number of spatial grid points was varied between 128 and 512 to insure the solutions were well converged.

These studies have shown that for long wavelength solutions with spatial scales large compared with the characteristic spacing of the lattice, the solutions of eq. (4) approximate well the behavior of the discrete lattice solutions, eq. (2), and certainly much better

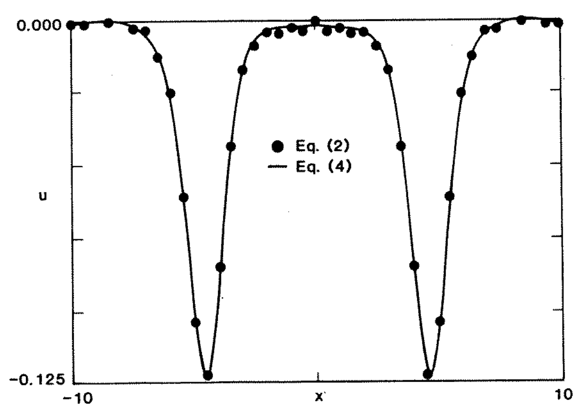

Fig. 3. The two solitons (eq. (4)) shown in fig. 2, are displayed with the discrete Toda solution (eq. (2)) after 9 collisions in a periodic system. Note the close agreement between the continuous and discrete models. (Same parameters as fig. 2.)

than the solutions of eq. (3). Since the Toda lattice is highly nonlinear, the very successful performance of eq. (4) leads us to believe in its universal ability to study one-dimensional chains with an arbitrary interparticle potential. Finally, we note that the method leading to the derivation of eq. (4) was recently generalized to multidimensional lattices [5].

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