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Quasisoliton solutions in one-dimensional anharmonic lattices: I. Influence of the shape of the pair potential

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Abstract. We have investigated the influence of the shape of pair potentials on the existence and properties of soliton-like (quasisoliton) solutions in periodic one-dimensional lattices. The classical equations of motion were solved numerically for chains of 'atoms' with nearest-neighbour interactions. The class of pair potentials studied has the form $V_\sigma(r) \propto \exp(-2br) - 2\sigma \exp(-br/\sigma)$, $\sigma > 0$. For all σ's tested ($\sigma = 1, 5, 10, 15$), quasisoliton solutions were observed to propagate with essentially constant velocity and survived many collisions. Our most interesting conclusion is that long-lived quasisoliton solutions apparently exist for most systems with realistic anharmonic potentials. The conditions these potentials have to satisfy (a sufficiently steep, short-range repulsive part and an asymmetric ($V(r+r_0) \neq V(r-r_0)$, for all r_0) overall shape) are weak. The nature of the long-range part is unimportant. The initial conditions are more decisive; they determine the nature and behaviour of the quasisolitons created. Integrability of the Hamiltonian does not seem to be necessary for the existence of quasisolitons.

1. Introduction

In recent years interest has been focusing on finding soliton solutions of both integrable and non-integrable nonlinear differential equations (see Scott *et al* 1973, Makhankov 1978, Faddeev and Korepin 1978, Calogero and Degasperis 1976, 1977, Kaup and Newell 1978, and many others that can be traced through these). The soliton solutions of integrable systems retain their identity (Scott *et al* 1973), i.e. their widths, amplitudes and velocities remain invariant after collisions with other solitons (except for a possible shift in position or phase). Regarded as particles, they collide elastically and can be thought of as possessing infinite lifetimes. In contrast, solitons corresponding to non-integrable systems of equations can collide inelastically (Makhankov 1978), resulting in finite lifetimes. Although integrable systems of equations play an important role in mathematics and physics, it seems to be of great practical importance to find criteria that would help in identifying and characterising soliton-like (to be referred to as quasisoliton) solutions of arbitrary non-integrable systems of equations. For most realistic physical situations, the mathematical description of interactions of 'particles' with each other and with their environment is in terms of non-integrable differential equations (equations of motion). Quasisoliton solutions of such equations, if they exist, would have interesting features and important physical consequences, especially if they

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had lifetimes that were much longer than the longest *linear* (harmonic) relaxation time of the physical system.

Qualitative existence criteria for quasisoliton solutions that do *not* require the explicit solution of the equations (such as the Liapunov functions in the stability theory of differential equations) would, of course, be ideal. In the absence of any such criterion, numerical studies of the dependence of solutions on both local and global features of the system are the alternative. Candidates for such features include mass and/or force defects in an otherwise uniform chain, type, critical magnitude and range of the initial excitation, the number of interacting neighbours of a given unit in the chain, the nature of the boundary conditions, the form and range of both repulsive and attractive parts of the pair potential, the dimensionality of the system, etc. Many of these points have been considered in the literature (e.g. Currie *et al* 1977, Hasenfratz and Klein 1977); however, they all start with an integrable nonlinear partial differential equation (e.g. sine–Gordon or ϕ^4-field equation) which is known to have soliton solution, and 'perturb' it by discretisation or otherwise. In contrast, in this work we consider directly anharmonic one-dimensional periodic chains with nearest-neighbour interactions, and we study numerically their quasisoliton solutions. The Hamiltonians we consider are not known to be integrable, and so there is no guarantee that quasisoliton solutions exist. Their parametrisation enables us to concentrate mainly on the importance of the *shape* of the pair potential for soliton-like behaviour.

2. The Hamiltonians

We consider a class of Hamiltonians H_σ of an N-particle one-dimensional chain with nearest-neighbour interactions and unit masses:

$$H_\sigma = \sum_{n=1}^{N} \frac{p_n^2}{2} + \sum_{n=1}^{N} V_\sigma(r_n), \tag{1}$$

$$V_\sigma(r) = [A/(2\sigma - 1)][\exp(-2br) - 2\sigma \exp(-br/\sigma)], \tag{2}$$

$$r_n = y_n - y_{n-1}, \tag{3}$$

where p_n and y_n are the momentum and the displacement from equilibrium of the nth particle, respectively; A, b and σ are constants (for computational convenience (see below) we chose σ to be an integer $\geqslant 1$). Plots of the potential V_σ against r, with $b = 2{\cdot}828$ and $A = 1/2b$, are shown in figure 1. The curves 1, 2, 3 and 4 correspond to $\sigma = 1$, 5, 10 and 15 respectively. $V_\sigma(r)$ has its minimum at $r = 0$: $V_\sigma(0) = -A$. When $br > 0$ and $\sigma = 0$, $V_0(r)$ is closely related to the well-known exponential potential (Toda 1976); for $\sigma = 1$, $V_1(r)$ is the ubiquitous Morse potential. For larger values of σ, $V_\sigma(r)$ becomes longer in range (e.g. as measured by the value of the inflection point, $\mathrm{d}^2 V_\sigma/\mathrm{d}r^2|_{r=r_{\mathrm{infl}}} = 0$, $r_{\mathrm{infl}} \propto \sigma^2 \log \sigma$). The curvature of $V_\sigma(r)$ close to the equilibrium point is inversely proportional to σ: $\mathrm{d}^2 V_\sigma/\mathrm{d}r^2|_{r=0} = 2b^2 A/\sigma$. Thus the larger σ is, the flatter the potential.

The broken curve in figure 1 is a plot of $V_{\mathrm{HB}}(r^*)/2bV_{\mathrm{HB}}(r_{\mathrm{eq}})$, where

$$V_{\mathrm{HB}}(r^*) = \frac{12\,040}{r^{*12}} - \frac{4014}{r^{*10}} - \frac{11{\cdot}2365}{r^*}, \qquad r^* = r + r_{\mathrm{eq}}, \qquad r_{\mathrm{eq}} = 1{\cdot}836\,959\ \text{Å},$$

$$V_{\mathrm{HB}}(r_{\mathrm{eq}}) = -7{\cdot}136\,242\ \mathrm{kcal\ mol^{-1}}.$$

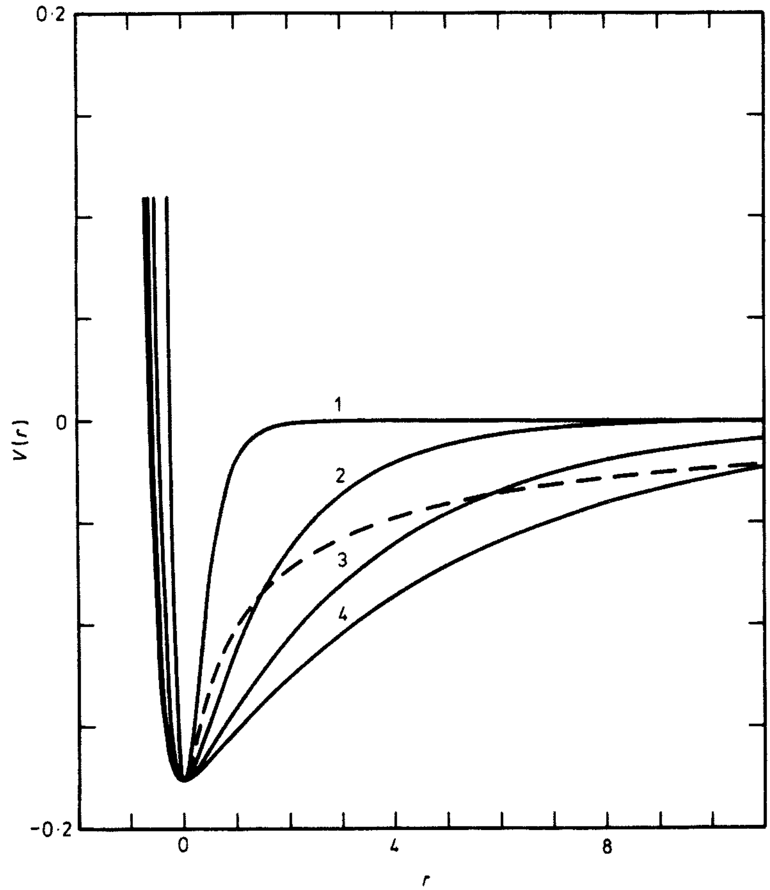

Figure 1. Plot of the potential $V_\sigma(r)$ against r, with $b = 2{\cdot}828$ and $A = 1/2b$. Curves 1, 2, 3 and 4 correspond to $\sigma = 1, 5, 10$ and 15. The broken curve is the normalised V_{HB} potential (see text).

The factor $1/2bV_{\mathrm{HB}}(r_{\mathrm{eq}})$ normalises $V_{\mathrm{HB}}(r^*)$ so that the latter coincides with $V_\sigma(r)$ at $r=0$ (i.e. $r^* = r_{\mathrm{eq}}$). The parameters in $V_{\mathrm{HB}}(r^*)$ correspond to a representative H···O hydrogen-bond potential (Momany *et al* 1974), to which we have added a typical electrostatic term. Note that the H-bond so modified is hardly distinguishable from $V_1(r)$ for $r<0$, although no value of σ can simulate it for all values of $r>0$.

The classical equations of motion for the chain are given by

$$\dot{y}_n = \partial H_\sigma / \partial p_n \tag{4}$$

and

$$\dot{p}_n = -\partial H_\sigma / \partial y_n. \tag{5}$$

Using equations (1)–(5) gives

$$\ddot{y}_n = [2bA/(2\sigma-1)][\exp(-2br_n) - \exp(-br_n/\sigma) - \exp(-2br_{n+1}) + \exp(-br_{n+1}/\sigma)]. \tag{6}$$

For the sake of computational efficiency we perform the change of variable

$$Z_n = \exp(-by_n/\sigma), \tag{7}$$

which transforms (6) into

$$\ddot{Z}_n = \dot{Z}_n^2/Z_n - [2Ab^2/\sigma(2\sigma-1)]Z_n(q_n^{2\sigma} - q_n - q_{n+1}^{2\sigma} + q_{n+1}), \tag{8}$$

where $q_n = Z_n/Z_{n-1}$.

We have not been able to find an analytical solution of (6) (or of (8)). However, analytical solutions of some low-order continuum limit approximations to these discrete equations may exist and could reveal essential features. Thus we consider the continuum limits of equation (6) in order to determine whether there exist conditions for which soliton-like solutions may be expected.

3. Continuum limit approximation

Let $y_n = y(nh, t)$. Using the raising and lowering operators defined by (Toda 1976)

$$D_n^{\pm} f_n \equiv \exp(\pm\partial/\partial_n) f_n = f_{n\pm1}, \tag{9}$$

equation (6) becomes

$$\begin{aligned}\ddot{y}_n = [2bA/(2\sigma-1)][&\exp(-2by_n)D_n^- \exp(2by_n) - \exp(-by_n/\sigma)D_n^- \exp(by_n/\sigma)\\ &-\exp(2by_n)D_n^+ \exp(-2by_n) + \exp(by_n/\sigma)D_n^+ \exp(-by_n/\sigma)].\end{aligned} \tag{10}$$

Expanding equation (10) in a Taylor series and retaining terms through the fourth derivative, we obtain

$$\frac{\partial^2 y}{\partial t^2} = \left(1 + \alpha\frac{\partial y}{\partial x}\right)\frac{\partial^2 y}{\partial x^2} + \frac{\beta}{12}\left[\frac{\partial^4 y}{\partial x^4} + \frac{6b^2(4\sigma^2+2\sigma+1)}{\sigma^2}\frac{\partial^2 y}{\partial x^2}\left(\frac{\partial y}{\partial x}\right)^2\right],$$

$$\alpha = -(2\sigma+1)/(2\sigma A)^{1/2}, \qquad \beta = \sigma/2b^2A, \qquad x = (2b^2A/\sigma)^{-1/2} n. \tag{11}$$

It is convenient to change to the variables (Cercignani 1977)

$$\begin{aligned}&\xi = \epsilon(x-t), \qquad \tau = \epsilon^3\beta t, \qquad y = \epsilon u,\\ &\partial/\partial t = \beta\epsilon^3\partial/\partial\tau - \epsilon\partial/\partial\xi, \qquad \partial/\partial x = \epsilon\partial/\partial\xi,\end{aligned} \tag{12}$$

where ϵ is an 'ordering' parameter. Using the definitions in equation (12) reduces (11) to

$$\beta^2\epsilon^7\frac{\partial^2 u}{\partial\tau^2} - 2\beta\epsilon^5\frac{\partial^2 u}{\partial\tau\,\partial\xi} = \alpha\epsilon^5\frac{\partial u}{\partial\xi}\frac{\partial^2 u}{\partial\xi^2} + \frac{\beta}{12}\left[\epsilon^5\frac{\partial^4 u}{\partial\xi^4} + \frac{6b^2(4\sigma^2+2\sigma+1)}{\sigma^2}\epsilon^7\frac{\partial^2 u}{\partial\xi^2}\left(\frac{\partial u}{\partial\xi}\right)^2\right]. \tag{13}$$

Neglecting terms of order higher than ϵ^5 in equation (13), we obtain

$$\partial v/\partial\tau + \mu v\,\partial v/\partial\xi + \tfrac{1}{24}\partial^3 v/\partial\xi^3 = 0, \tag{14}$$

where

$$v = \partial u/\partial\xi, \qquad \mu = \alpha/2\beta = -b^2A(2\sigma+1)/\sigma(2\sigma A)^{1/2}. \tag{15}$$

Equation (14) is one form of the Korteweg–deVries (K–dV) equation which is known to be integrable and supports solitons. A soliton solution of (14) is given (Cercignani 1977) by

$$v = (3c/\mu)\,\mathrm{sech}^2[\sqrt{6}c(\xi - c\tau)],$$

where c is a constant. Thus if the discrete problem (6) is well represented by (11) for some A, b, σ, then this continuum limit of (6) suggests that the discrete lattice may well support at least soliton-like solutions. Of course, there is no *a priori* assurance that representing the discrete problem more accurately (by going to even higher-order continuum equations) will preserve the soliton-supporting features. Thus a direct study of the discrete lattice was undertaken, based on the expectation that soliton-like solutions will be found for physically reasonable A, b, σ.

4. Computations and results

Here we present the method used to solve equation (6) via equation (8), and the results of the computations. The set of differential equations (8), with periodic boundary conditions

$$Z_{N+k} = Z_k, \qquad \text{i.e. } r_{N+k} = r_k, \qquad y_{N+k} = y_k,$$

where N is the total number of particles in the chain, was solved using a fourth-order explicit Runge–Kutta scheme with fixed step size h (Abramowitz and Stegun 1965, equation 25.5.20). The step size ranged from 0·0005 to 0·01 time units in order to maintain conservation of the total energy E to at least seven significant figures during the numerical run. To achieve this accuracy, smaller step sizes were needed for larger E (σ constant) or for larger σ (E constant). The initial values (at $t = 0$) of y_n and $\dot{y}_n$ (and hence of Z_n and $\dot{Z}_n$) were chosen to be those corresponding to a Toda soliton placed at the $N/2$ lattice site. Their explicit forms at $t = 0$ are

$$r_j(0) = y_j(0) - y_{j-1}(0) = \lambda \ln(1 + \omega^2 \operatorname{sech}^2 x_j), \tag{16}$$

$$\dot{r}_j(0) = \dot{y}_j(0) - \dot{y}_{j-1}(0) = 2\lambda\omega^2 \exp(r_j) \tanh x_j \operatorname{sech}^2 x_j, \tag{17}$$

with

$$\lambda = \pm 1, \qquad \omega = \sqrt{b} \sinh(\kappa), \qquad \kappa = \text{constant}$$

and

$$x_j = \kappa(N/2 - j), \qquad j = 1, 2, \ldots, N.$$

In figures 2–5(a) we show plots of f_j as functions of time, where the force at site j is

$$f_j = [\exp(-2br_j) - \exp(-br_j/\sigma)]/(2\sigma - 1), \qquad \forall j. \tag{18}$$

Figure 5(b) is a plot of the velocity $\mathrm{d}y_j/\mathrm{d}t$, in the centre-of-mass coordinate system of the chain. The relevant parameters and some results corresponding to the figures are collected in table 1. Note that except for the Morse case, figure 2, all initial velocities were set to zero. In figure 2, $\dot{y}_j$ was chosen according to equation (17).

Some comments are in order on the definition and/or meaning of the displayed quantities. N, σ, E, f_j have already been defined and κ is a constant that governs the amplitude (and hence the total energy) of the initial excitation. The parameter λ determines whether on excitation the separation between two adjacent masses of the chain increases ($\lambda = 1$, dilatation) or decreases ($\lambda = -1$, compression). At equilibrium, $r_j = 0$. $f^{\max}$ is the maximum amplitude of the local force f_j at $t = 0$, attained anywhere in the chain. For $\lambda = -1$, this is at $j = N/2$ (i.e. where the excitation occurred). For $\lambda = 1$, it is at $j = N$. The soliton amplitudes f_j, $\dot{y}_j$ in figures 2–5 were scaled differently, merely for convenience in plotting. Note that for figure 5(b) the maximum modulus of the

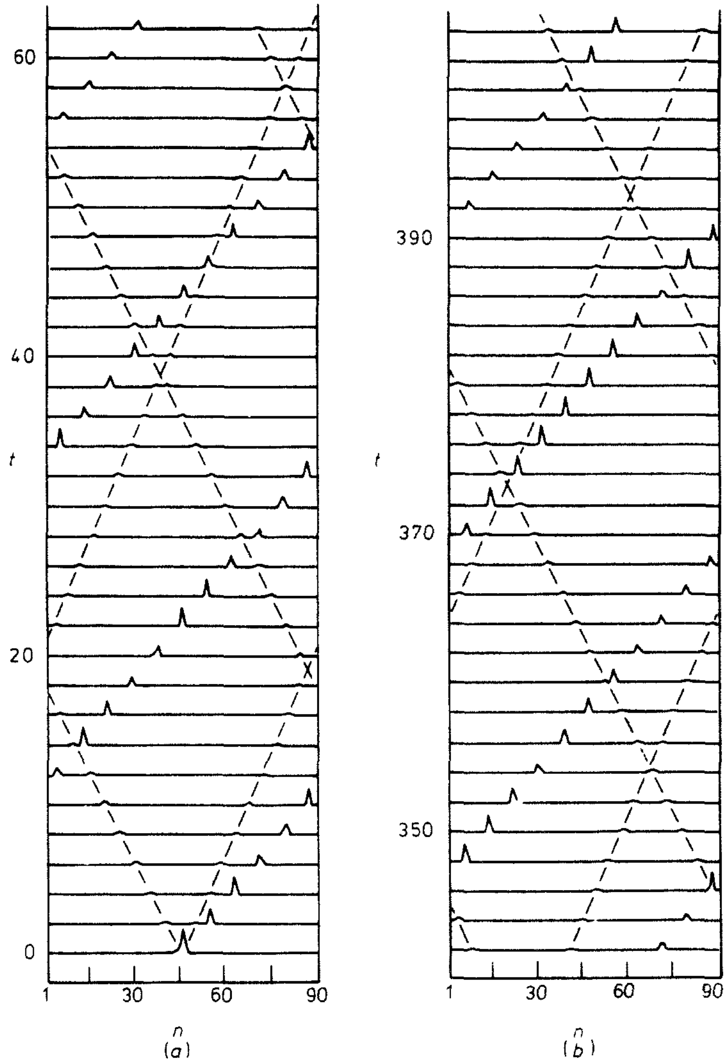

Figure 2. Plot of $f_j(t)$ (equation (22)) as a function of t and j. See table 1 for values of the parameters. The broken lines indicate the approximate positions of the two small pulses.

velocity amplitude is recorded; $\max|\dot{y}_j|$ was attained at $t = 1{\cdot}676$. The penultimate column of table 1 contains the final time t_{fin} to which the equations of motion were integrated out. The last column lists the longest finite linear relaxation time τ_1 of the chain. This was obtained by retaining only the linear term in the equations of motion for the chain, equation (6). Then we have

$$\ddot{y} = (2b^2A/\sigma)\mathbf{D}\mathbf{y},$$

where $\mathbf{D}$ is the $N \times N$ symmetric matrix with non-vanishing matrix elements $d_{jj} = -2$, $d_{j,j+1} = d_{1,N} = 1, \forall j$. The eigenvalues μ_k of $(2b^2A/\sigma)\mathbf{D}$ are (Björck and Golub 1977)

$$\mu_k = -(4b^2A/\sigma)[1 - \cos(2\pi k/N)], \qquad k = 0, 1, \ldots, N-1,$$

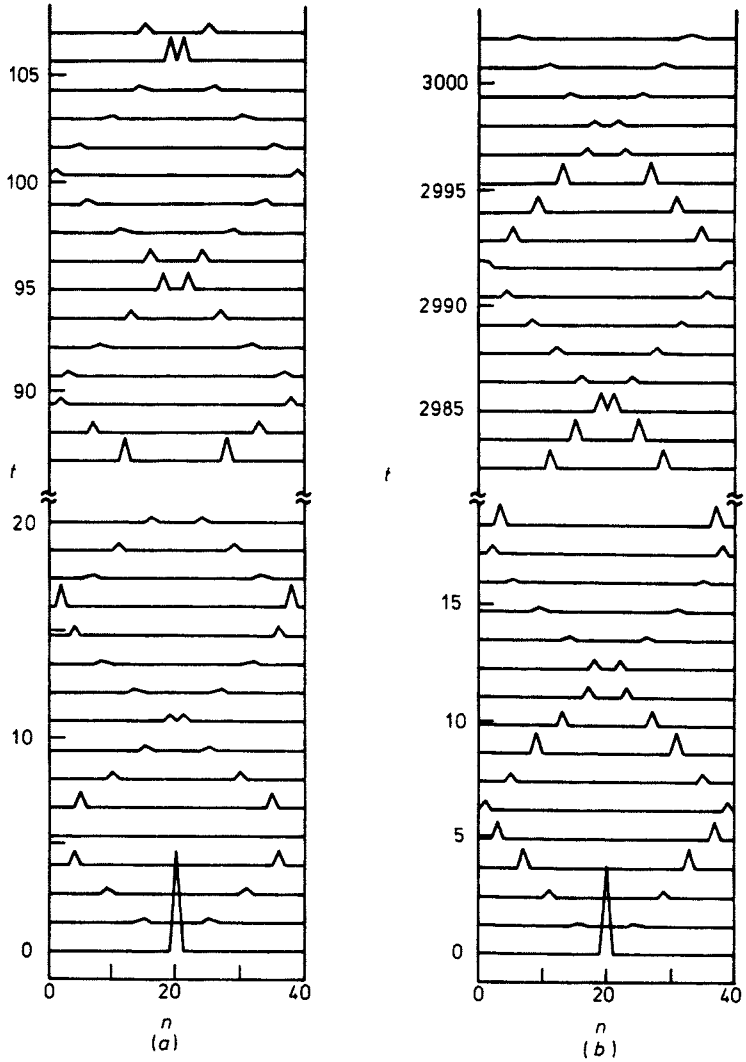

Figure 3. Plots of $f_j(t)$ against t and j. See table 1 for values of the parameters. (a) corresponds to $\sigma = 5$, (b) to $\sigma = 10$.

and the linear relaxation times are defined by $\tau_k = 1/|\mu_k|$. Apart from τ_0, which corresponds to the relaxation time of the chain as a whole, the longest finite value is given by τ_1. Its comparison with t_{fin} enables us to state whether the duration of soliton behaviour can be considered as meaningfully long. In tables 2 and 3, characteristics of the quasisoliton solutions are presented. Table 2 contains results for the Morse potential (figure 2). The initial conditions lead to the creation of three quasisolitons. Their velocities, initial directions of travelling, the total number of pair collisions in t_{fin}, and the times between successive collisions are listed. In table 3 we collect the results for the other potentials (figures 3–5). All five cases are characterised by the creation of a soliton pair, members of which travel with identical velocities but in opposite directions. The velocities, times between collisions and the total number of collisions are recorded.

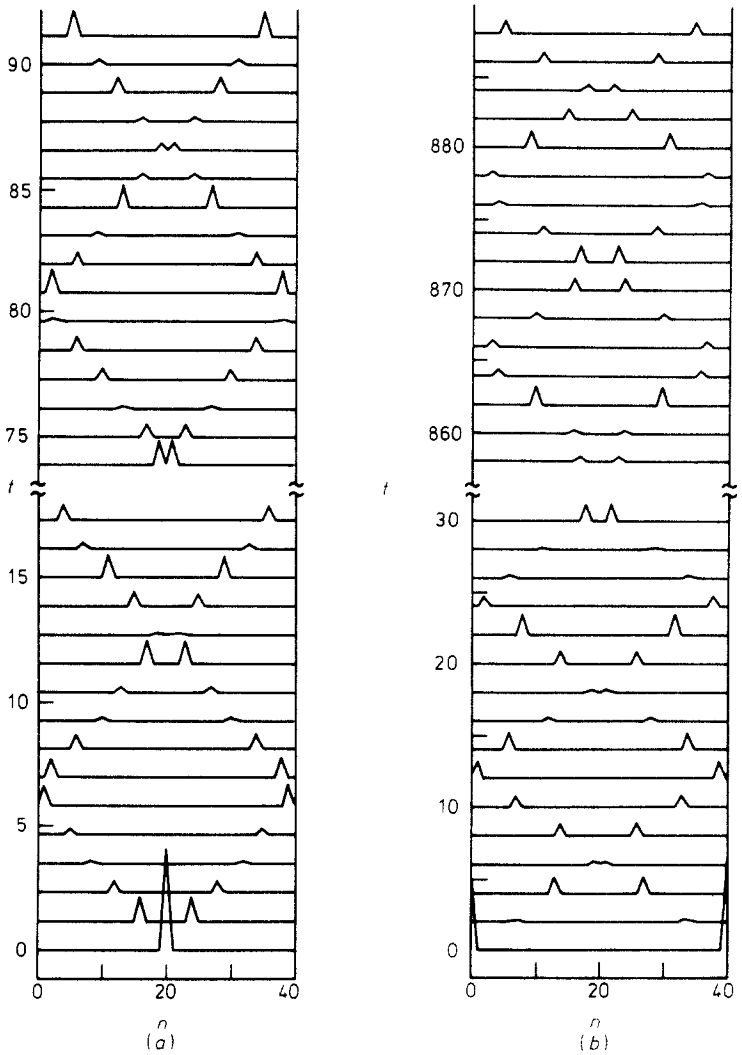

Figure 4. Plots of $f_j(t)$ against t and j. (a) corresponds to $\lambda = -1$, (b) to $\lambda = 1$. For other parameters see table 1.

All computations were carried out in double precision on IBM computers. The shorter runs were done on a 360/67, the long ones on the 370/3031.

5. Discussion

Quasisoliton solutions should be quasi stable. That is, the pulse(s) associated with a given total energy and momentum should propagate without appreciable decay. As a consequence, the energy (or charge or whatever physical property of interest is 'carried' by the pulse) would take relatively long times to dissipate into the surroundings. To be of interest, these decay times should be comparable to, or much longer than, the longest relaxation time of the linearised system. Inspection of the figures and table 1 indicates

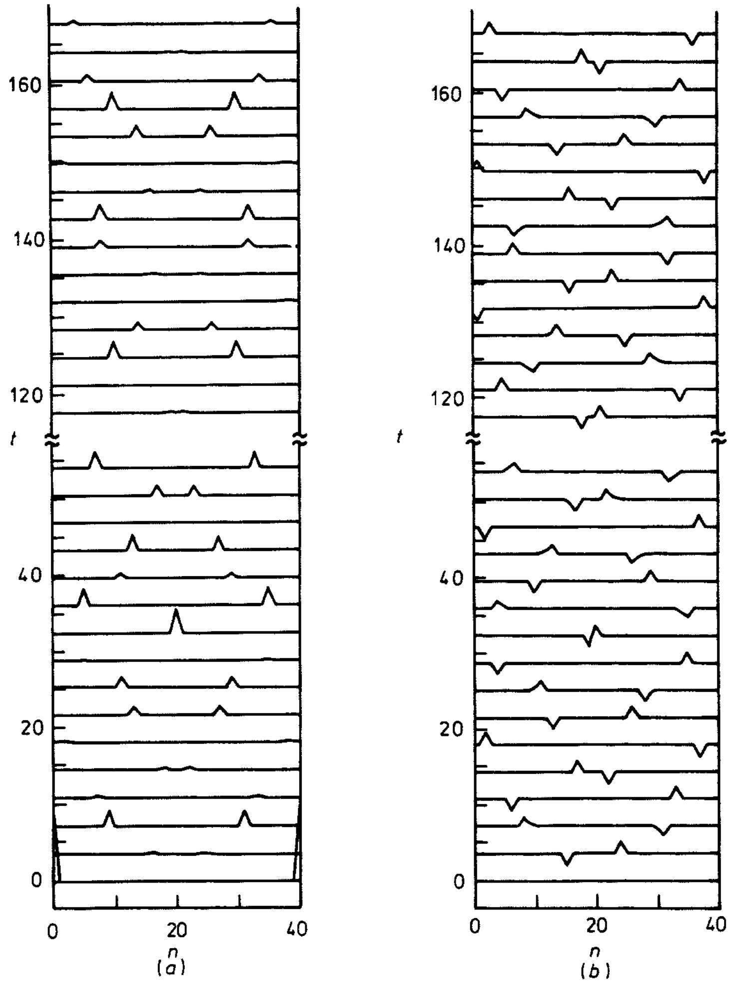

Figure 5. (*a*) Plot of $f_j(t)$ against t and j. $\sigma = 5$, other parameters in table 1. (*b*) Plot of $\dot{y}_j(t)$ against t and j. $\sigma = 5$, other parameters in table 1. This is the velocity plot corresponding to (*a*).

Table 1. Input parameters, identification and some results of the various V_σ considered.

Case no.	Figure no.	Quantity plotted	Input parameters N	λ	σ	κ	E	$f^{max}(t=0)$	t_{fin}	τ_1
1	2	f_j	90	−1	1	1·0	−10·9582	19·16	404	72·58
2	3(*a*)	f_j	40	−1	5	1·93711	15·4137	125·5	107	71·80
3	3(*b*)	f_j	40	−1	10	2·12316	15·4137	126·2	3006	143·6
4	4(*a*)	f_j	40	−1	15	2·22861	15·4137	126·5	91	215·4
5	4(*b*)	f_j	40	+1	15	1·0	15·4137	127·3	887	215·4
6	5(*a*)	f_j	40	+1	5	1·5	743·906	4249	168	71·80
7	5(*b*)	$\dot{y}_j$	40	+1	5	1·5	743·906	27·03†	168	71·80

† Maximum modulus of amplitude for $\dot{y}_j$, attained at $t = 1·676$

Table 2. Computed characteristics of the quasisoliton solutions for the $\sigma = 1$ (Morse potential) case.

Case no.	Soliton no.	Direction of travel	Soliton velocity (site/unit time)	Soliton–soliton collision	Time between collisions	No. of collisions in t_{fin}
	1	Forward	4·11	1–2	44·78	9
1	2	Forward	2·10	2–3	19·52	20
	3	Backward	2·51	1–3	13·60	29

Table 3. Computed characteristics of quasisoliton solutions for the potentials tested.

Case no.	Soliton velocity (site/unit time)	Time between collisions	No. of collisions in t_{fin}
2	3·68	10·87	9
3	3·31	12·08	250
4	3·30	12·12	7
5	3·11	12·86	68
6	4·25	9·41	17

that we have carried out our integrations to satisfy this criterion. In all cases the pulses survive and propagate essentially unchanged, even for the two weakest solitions of the Morse case. This is the more remarkable since during these integrations there were from 7 to 250 pair collisions suffered by the various solitons (tables 2 and 3). Our potentials V_σ can be considered as modifications of the exponential (Toda) potential V_0, which is integrable and has soliton solutions (Toda 1976). Since we observed soliton-like solutions for all σ values we tested, and for a wide range of total (excitation) energies, there was the possibility that the class of Hamiltonians H_σ is integrable. (The continuum limit K–dV equation for the velocities was particularly suggestive.) To check this, we repeated the run for case 3 (figure 3(*b*)) with identical initial conditions, except for $y_1(0)$ which was changed to $y_1'(0) = y_1(0) + 10^{-6}$. Thus initially the two trajectories in the 80-dimensional phase space were separated by 10^{-6}, i.e. $D(0) = 10^{-6}$, with

$$D^2(t) = \sum_{i=1}^{N} [(y_i(t) - y_i'(t))^2 + (p_i(t) - p_i'(t))^2],$$

where $p_i(t)$ is the momentum of particle i at t.

If the system were integrable, then two trajectories initially very close together in phase space would separate linearly as the system evolves. For a non-integrable system, this separation would *eventually* be exponential (Casati and Ford 1975, 1976). In our test run, log $D(t)$ against t gives a linear plot, i.e. $D(t)$ increases exponentially, and thus this particular trajectory pair originates in a stochastic region of phase space. This is suggestive of non-integrability. (A more definite statement cannot be made in view of some evidence (Benettin *et al* 1977) that local exponential divergence does not necessarily imply global instability.†)

The possibility of non-integrability is, in fact, a much more interesting result than if we could have shown integrability (the latter is a far more arduous task, since numerical results can only be suggestive and the ultimate proof has to be analytic). If the system were in fact non-integrable, then it is remarkable that the creation and stability of quasisolitons may not even require that the initial conditions correspond to a non-stochastic region of phase space! This suggests that quasisoliton existence–stability cannot be related in a simple fashion to non-ergodicity.

A closer scrutiny of the figures reveals that the quasisolitons possess more complex temporal behaviour than true solitons, even when far away from the collision regions. The most striking aspect is the rather regular waxing and waning of the force amplitudes. The smaller amplitudes reflect expansion ($r>0$), while the larger correspond to contraction ($r<0$) of the chain. This behaviour is qualitatively similar, whether initially the chain was stretched ($r>0$, $\lambda=1$) or compressed ($r<0$, $\lambda=-1$). Interestingly, the amplitudes of the velocities‡ $\dot{y}_i$ are much more nearly constant in time (compare figures 5(*a*) and (*b*)). This is supported by the continuum limit analysis which indicates the possibility of soliton-like behaviour for the velocities.

Similarly to true solitons, the quasisolitons suffer displacement upon collision, in our examples usually by about a lattice separation. However, after collision, the quasisolitons seem to accelerate for a time, then slow down again to the velocity they had before collision. As in the case of true solitons, quasisolitons with larger velocities have, on the average, larger force amplitudes.

The most interesting finding of this work is that under very weak restrictions on the shape of the pair potentials, reasonably long-lived quasisoliton solutions can exist in one-dimensional chains of particles with nearest-neighbour interactions. Qualitatively, what seems to be needed is a sufficiently steep repulsive part and some anharmonicity (nonlinearity) that makes the potential asymmetric (i.e. there is no x_0 such that $V(x_0-x)=V(x_0+x)$). (We have integrated the equations of motion for symmetric potentials of the forms $V(x)=x^{2m}$, $m\geqslant 2$, and lost the initial pulse very quickly and irretrievably.) A very recent finding of Valkering (1978) supports this idea. He proved that the necessary conditions a pair potential has to satisfy in order for periodic permanent waves to exist in the chain are that it has vertical and horizontal asymptotes and an inflection point. It is important to emphasise that the existence of quasisoliton solutions has not been proven: this would need proof that two or more pulses with different velocities are stable under small perturbations and, in particular, survive interaction (collisions). Our numerical results indicate that this may well be the case.

In order to eliminate the possibility that quasisoliton solutions are peculiar to V_σ, we have also solved the equations of motion for V_{HB} (broken curve in figure 1). Again, we found that quasisoliton solutions exist.

All these results point to the conclusion that, given physically reasonable pair potentials, it is the *initial conditions* that really determine whether the excitation leads to quasisoliton solutions, and if it does, how many there are and how they behave. It is not difficult to create quasisolitons. What is more difficult is to produce them with specific properties (e.g. it is not straightforward to choose those initial conditions that

† We thank one of the referees for bringing this important paper to our attention.

‡ This study was essentially completed when we became aware of two earlier uses (Dancz and Rice 1977, Hardy and Karo 1977) of the Morse ($\sigma=1$) potential in connection with soliton solutions of equations of motion. Based on our velocity plot, we reach the same conclusion as Hardy and Karo.

would create a single quasisoliton with a particular velocity, propagating in a prescribed direction). Note that the initial conditions do not have to be as simple as the ones we used in most of our tests. In fact, five equal pulses placed at sites 8, 16, 24, 32 and 40 initially, with zero initial velocities, produce five quasisoliton pairs that remain equally spaced and recur periodically with essentially undiminished amplitudes.

None of our runs was long enough to tell us what the lifetimes of our quasisolitons might be. Assuming that the finite lifetime of quasisolitons is due to coupling with phonons of the lattice, one could estimate numerically how much of the soliton energy 'leaks' into the lattice as the system evolves. However, this would involve the dubious and poorly defined separation at any given time of sites into two classes: soliton-bearing and phonon-bearing. If this could be done (e.g. if one could exclude times when soliton–soliton interaction is large), then one could extrapolate to times when the average phonon energies are comparable with the average soliton energies, i.e. when one could not distinguish between solitons and phonons. These times could be considered as measures of quasisoliton lifetimes. Even then, the possibility of recurrence phenomena (characteristic of many nonlinear systems with soliton solutions) makes the value and reliability of extrapolation problematic.

A more promising approach is to use singular perturbation techniques (e.g. Kaup and Newell 1978, Weiland *et al* 1977, Karpman 1978), starting with the Toda solution (V_0) as the unperturbed system, and deriving differential equations for the time dependence of both soliton amplitudes and velocities. Solutions of these would help us elucidate the complex temporal behaviour of quasisolitons analytically or semi-analytically, and would provide quantitative lifetime estimates. Such an analysis is in progress and will be reported.

6. Addendum

Since this work was submitted, a paper (Rolfe *et al* 1979) has appeared which, with its different aims, complements our work rather nicely. The authors have studied large-amplitude motion on nearest-neighbour chains of Morse and Lennard–Jones oscillators, with both fixed and cyclic boundary conditions. They find that the shape and behaviour of the Morse or Lennard–Jones solitons is very similar to that of the Toda solitons. Furthermore, they studied the effect of mass impurities on quasisoliton stability for different mass ratios. The point of overlap with our study is their conclusion (stated somewhat differently) about some of the necessary conditions the pair potentials have to satisfy in order to be soliton-bearing. We agree on these. However, their claim that the Morse and Lennard–Jones lattices support only compressional solitons is in disagreement with our findings. This discrepancy has to be attributed to different boundary conditions; we have always used cyclic boundary conditions, while their arguments seem to be based on free end boundary conditions.

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