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Recurrence phenomena in soliton propagation in a lattice with impurities

A D Mistriotis†, St Pnevmatikos† and N Flytzanis†‡

† Research Center of Crete, PO Box 1527, Heraklio 711 10, Crete, Greece
‡ Department of Physics, University of Crete, Heraklio 714 09, Crete, Greece

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Abstract. The scattering of a soliton from a mass impurity in a Morse or Toda one-dimensional lattice with periodic boundary conditions is studied numerically. The energy of the soliton as a function of time exhibits either a fast decay (chaotic behaviour) or a recurrence, or an intermediate 'metastable' behaviour, which consists of a time period when recurrence takes place, followed by a fast decay. A model is developed to explain the recurrence and predict the recurrence time. A semiquantitative argument is also presented to explain the 'metastable' case. Finally the generality of this type of behaviour is discussed.

1. Introduction

The study of non-linear lattice dynamics (Jackson 1978) was initiated by the numerical experiment of Fermi, Pasta and Ulam (FPU) (Fermi *et al* 1955) on one-dimensional lattices with polynomial interaction. Their work was motivated by Fermi's ideas about the relationship between non-linearity and irreversibility. Several attempts to explain the FPU recurrence 'paradox' were the origin of important new ideas. One of them was the discovery of solitons by Zabusky and Kruskal (1965) as a solution of the integrable KdV equation, which is the continuous limit of the FPU lattice. Among the many lattices studied (Toda 1975, Northcote and Potts 1964), the Toda lattice proved to be integrable (Hénon 1974, Flaschka 1974), even in the discrete case, and to accept soliton solutions. The Toda lattice became the subject of extensive studies (Holian *et al* 1981, Ferguson *et al* 1982).

Even though in a physical system there are always perturbations that tend to destroy the regular motion, the soliton concept is still useful because of the fundamental Kolmogorov-Arnold-Moser theorem (Arnold 1963). Briefly the main point of this theorem is that, when a Hamiltonian of an integrable system is slightly perturbed, the majority of the tori on which the trajectories of the integrable system lie are not destroyed but are only deformed. Hence the perturbed system will exhibit qualitatively the same behaviour with the corresponding integrable system. This consideration indicates that the scattering of a soliton by an impurity in a one-dimensional lattice, which accepts soliton solutions, does not necessarily imply the decay of the soliton. Notice that the theorem does not specify how weak the perturbation should be.

The work presented here has been particularly motivated by interesting computational results published by Rolfe and Rice (1980) without an interpretation of the mechanisms involved. They studied the decay of a soliton travelling in a one-dimensional chain of Morse oscillators where an impurity of slightly heavier mass was introduced (figure 1). They found, that this system 'displays several unusual features which are unexpected from the point of view of the perturbation theory of solitary wave scattering'. More specifically they produced a large number of diagrams presenting the rate at which the soliton loses its energy for different values of its initial energy, of the impurity mass, or of the lattice length (number of particles). The results showed the following three types of dynamical behaviour.

(i) The soliton decays and its energy decreases fast.

(ii) The soliton never (for the time length of the computations) decays and its energy oscillates back to its original value. This recurrence of the energy of the soliton recalls the well known FPU recurrence (Fermi *et al* 1955). Indeed there are similarities between these results and the FPU recurrence. In both cases we study systems which can be treated as perturbations of an integrable system. Actually for the FPU case perturbation methods were developed (Ford 1961, Jackson 1963), where the recurrence was interpreted as a 'resonance' between the non-linear normal modes. Similarly we will develop here a resonance mechanism, which predicts the recurrence time of the Rolfe–Rice system in the case when the soliton does not decay.

(iii) The soliton decays after a very long time. In other words, its energy oscillates back to its original value but the energy of the soliton decreases rapidly after this recurrence has been repeated several times.

The Morse lattice without defects can sustain soliton-like excitations but their collisions can be slightly inelastic. To avoid this extra complication we also studied the Toda lattice which is known to be completely integrable for the pure chain. For the Toda lattice with one impurity and periodic boundary conditions the same results were obtained as for the Morse lattice. Therefore this behaviour may be general for systems which are small perturbations of integrable systems. We will attempt to explain these results.

This paper is organised as follows. In § 2, we describe in detail our numerical experiments. In § 3, a model is presented which successfully describes the dynamics of the system for the cases (ii) and (iii) for the time period when the soliton does not

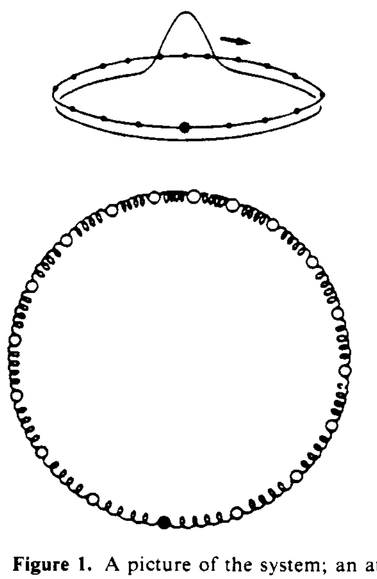


Figure 1. A picture of the system; an atomic ring with one impurity.

decay. By this method a prediction of the recurrence time of the energy of the soliton is made. The same model can be used to predict those values of the parameters of the system for which the decay of the soliton (case (i)) takes place. Finally in § 4 case (iii) is discussed and an argument is presented which justifies the metastable behaviour of the soliton in this case.

2. Numerical results

The first aim of our numerical calculations is to verify the results of Rolfe and Rice (1980). We also completed their numerical work by studying the dependance of their results on the mass of the impurity. The system they studied was a one-dimensional lattice of particles which interact only with their nearest neighbours with a Morse interaction:

$$V(r)=\tfrac{1}{2}A(e^{-br}-1)^2. \tag{1}$$

All particles have the same mass, which is taken to be unity, except one which has a different mass m. Periodic boundary conditions were considered. The parameters A and b were chosen equal to 16 and 0.25 respectively, such that the spring constant of the linear lattice is equal to unity. This choice does not influence the generality of our results.

It is known that the Morse lattice has an almost soliton solution, which is used as the initial condition in our numerical experiments. This initial condition is constructed by using a combination of analytical and numerical techniques. It is known that the continuum limit for the Morse lattice gives a Boussinesq-type equation (Flytzanis *et al* 1985) which can be solved. Therefore, using a continuum approximation one can find small-amplitude soliton solutions for the Morse lattice. It has also been proved numerically that even large-amplitude soliton-type solutions exist in the discrete Morse lattice. These are constructed numerically by letting an approximate soliton solution produced by solving the corresponding Boussinesq equation to propagate in a long discrete Morse lattice (Peyrard *et al* 1986). The amplitude–velocity relation in the large amplitude case is very different from the continuum result.

The energy of the soliton E_s is defined as the energy of n particles left and right of the particle with the highest velocity, where n is chosen large enough that E_s becomes independent of n. The energy of the soliton is determined after every collision of the soliton with the impurity at three different positions. The average of these three values is taken as the energy of the soliton, such that a possible abnormal contribution of the energy of the background motion to the energy of the soliton is avoided.

Figure 2 shows some typical numerical results of the energy of the soliton as a function of the number of the collisions for three different impurity masses, m_{imp}, while keeping constant the other parameters of the system, namely the energy of the soliton, E_s, and the length of the lattice, N. We conducted similar computations for several other combinations of these three parameters. Our results depend critically on the previous parameters, interchanging from regular to chaotic behaviour in agreement with the numerical results of Rolfe and Rice (1980). As explained earlier, the Morse lattice in the absence of impurities can sustain stable solitary waves. The lack of complete integrability, however, is reflected in the collision between narrow kinks, which is quasielastic (Flytzanis *et al* 1987). To avoid this effect and to check the generality of the coherent phenomena observed, we also studied the Toda lattice, which accepts soliton solutions.

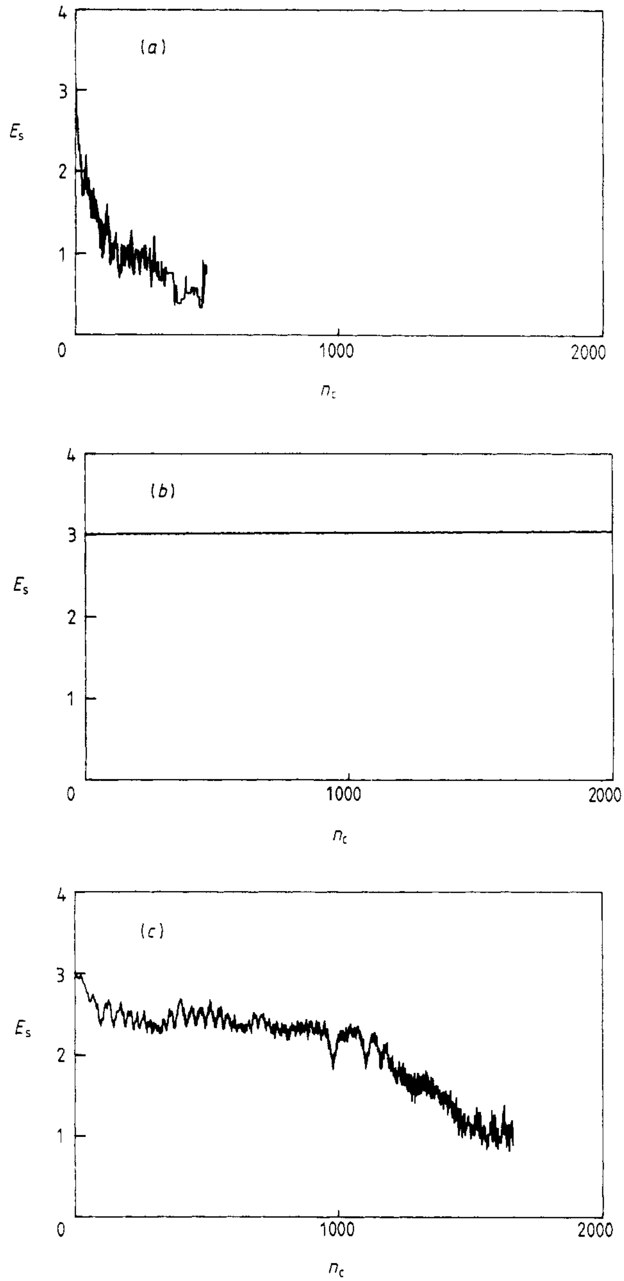


Figure 2. Graphs of the soliton energy E_s as a function of the number of collisions n_c of the soliton with the impurity for the Morse lattice. $E_s = 3.014$ and $N = 40$ for all three cases presented. The impurity mass is (*a*) 1.40, (*b*) 1.05 and (*c*) 1.15.

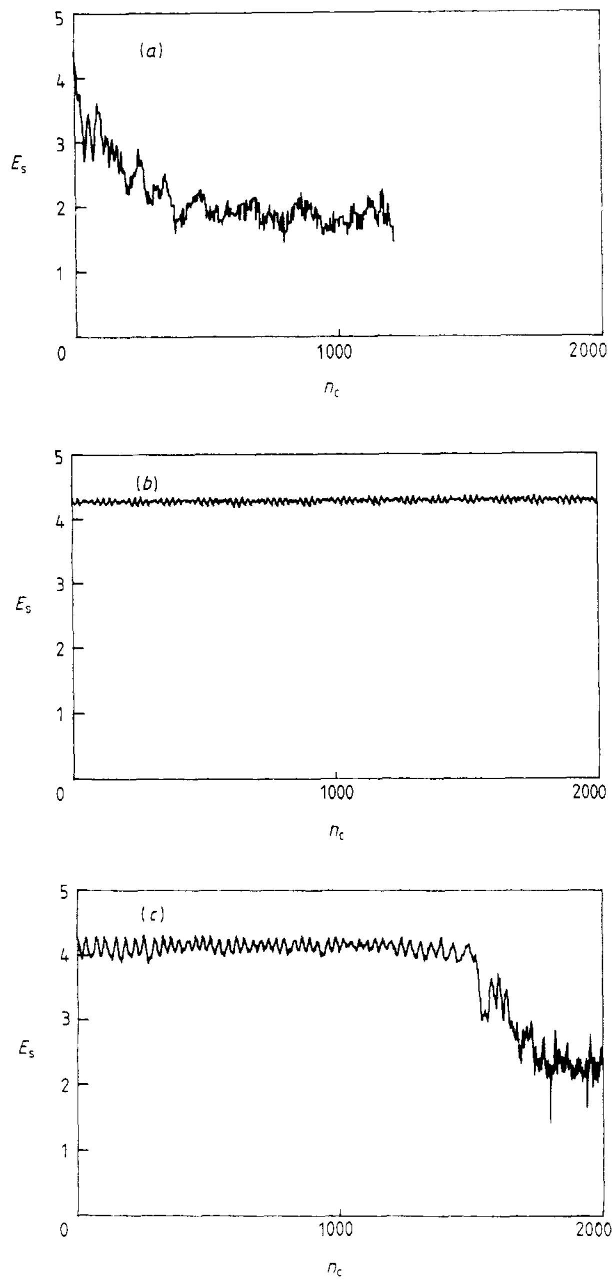


Figure 3. Graphs of the soliton energy E_s as a function of the number of collisions n_c of the soliton with the impurity for the Toda lattice. $E_s = 4.409$ and $N = 40$ for all three cases presented. The impurity mass is (*a*) 0.5, (*b*) 0.6 and (*c*) 0.5075.

The scattering of a soliton in a Toda lattice from an impurity, has been studied (Yoshida and Sakuma 1987, Nakamura 1978, Klinker and Lauterborn 1983) by inverse scattering techniques. Geist and Lauterborn (1986) studied the decay of a soliton when it is scattered by an impurity in a Toda lattice with periodic boundary conditions, but for a range of parameters where the soliton decays after a few collisions. In all these cases, no coherent behaviour was observed as studied by Rolfe and Rice (1980). In the Toda case the interaction between the first neighbours is of the type

$$V(r)=\frac{C}{d}\,e^{-dr}+Cr-\frac{C}{d}. \tag{2}$$

In our computations $C=\frac{16}{3}$ and $d=\frac{3}{8}$. The initial conditions were constructed to satisfy the soliton solution of the Toda lattice, which can be solved analytically even in the discrete case.

Figure 3 shows typical results of the numerical calculations of the energy of the soliton for the Toda lattice. The soliton energy was computed in the same fashion as in the Morse lattice. The energy of the soliton as a function of time was calculated also for several other combinations of the impurity mass, the soliton energy and the lattice length. These results show that the behaviour observed in the Morse lattice also appears in the Toda lattice.

The qualitative characteristics of the dynamical behaviour of the impurity system can be summarised and distinguished in the following three cases which were also briefly presented in the introduction.

(i) Figures 2(*a*) and 3(*a*) present two typical examples of a fast decaying soliton in a Morse or Toda lattice respectively. The decay of the soliton takes place in an irregular way. Any regular characteristics cannot be recognised in the function $E_s(t)$.

(ii) In this case, contrary to case (i), the energy of the soliton behaves as a periodic function of time without decaying. In other words $E_s(t)$ can be presented as a superposition of trigonometric functions. Figures 2(*b*) and 3(*b*) correspond to Morse and Toda lattices, respectively, and are two typical examples of this case. The periodic behaviour of function $E_s(t)$ shown in figure 3(*b*) is demonstrated better in figure 4, where its power spectrum is presented. This power spectrum mainly consists of two discrete peaks; therefore it is a spectrum of a periodic function.

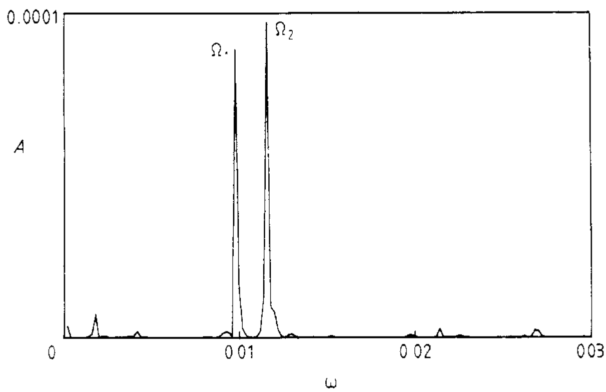


Figure 4. Power spectrum of the soliton energy for a Toda lattice where $E_s=4.409$, $N=40$ and $m_{imp}=0.6$. The two large peaks are at $\Omega_1=0.010$ and $\Omega_2=0.012$.

(iii) The third case shown in figures 2(c) and 3(c) corresponds to an intermediate situation between cases (i) and (ii). The function $E_s(t)$ behaves periodically with time for a long period of time, after which it exhibits a fast decay. It is also possible that this decay brings the energy of the soliton to a new plateau where the motion is periodic until a new decay occurs.

Several examples of all these three cases for the Morse lattice can be found in the paper of Rolfe and Rice (1980), where the question of the numerical accuracy was also examined. In our calculations, we have used a fourth-order Runge-Kutta numerical scheme to integrate the equations of motion. The error in conservation of the lattice energy was used as a test of the accuracy of the numerical results. We used an integration step such that this error was smaller than 10^{-5}.

3. A model explaining the recurrence in the energy of the soliton

In this section we will explain the appearance of a recurrence in the energy of the soliton which was observed in case (ii) of the last section. The numerical results show that in this case the soliton retains a large percentage of its energy such that the following two assumptions are true.

(a) The shape of the soliton does not change drastically due to scattering. Hence this slightly deformed soliton rapidly readapts to a new solution of the pure lattice. Therefore the soliton loses energy mainly at the impurity. Furthermore its velocity is almost constant.

(b) The energy which is transferred into the lattice, because of the collisions of the soliton with the impurity, is small so the harmonic approximation can successfully describe the background motion.

If this second assumption is correct the coupling between the normal modes, because of the non-linearity, can be neglected. Hence the dynamics of the system can be reduced to the motion of a single effective harmonic oscillator, which moves under the influence of a periodic square pulse $F(t)$ with period T and amplitude a, and pulse duration τ (figure 5). This external force represents the periodic kicks of the impurity by the soliton. The motion of this system can be studied analytically. The

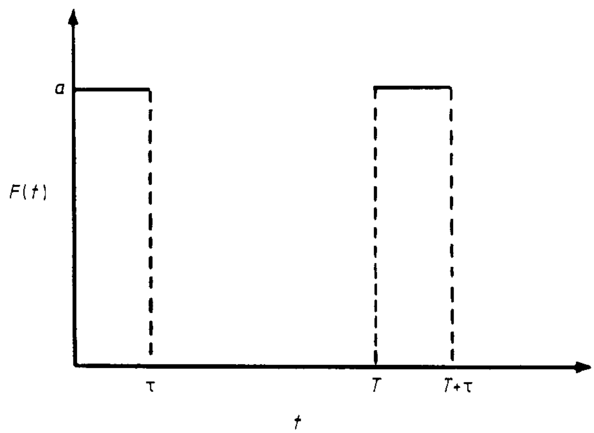


Figure 5. Description of the external force $F(t)$.

equation of motion of the system is

$$\ddot{x} = -\omega_0^2 x + F(t) \tag{3}$$

where ω_0 is the frequency of the effective oscillator. The general solution of (3) is

$$x(t) = C\cos(\omega_0 t) + D\sin(\omega_0 t) + A_0 + \sum_{n=1}^{\infty} [(A_n \cos(n\omega t) + B_n \sin(n\omega t)] \tag{4}$$

where $\omega = 2n/T$ and

$$\begin{aligned} A_0 &= a\tau / T\omega_0^2 \\ A_n &= a\sin(n\omega\tau)/nT\omega(\omega_0^2 - n^2\omega^2) \\ B_n &= -a\cos(n\omega\tau)/nT\omega(\omega_0^2 - n^2\omega^2). \end{aligned} \tag{5}$$

Because of the form of A_n and B_n we can keep only the terms A_{n_0} and B_{n_0} for which $n_0\omega \approx \omega_0$. Therefore $n_0\omega/\omega_0 \approx 1$ and $(n_0\omega - \omega_0) \approx 0$. Notice that $(n_0\omega - \omega_0)t$ is not necessarily small because t can be large. The choice of initial conditions for the effective oscillator can change the results only up to a phase and for simplicity we choose $x(0) = 0$ and $\dot{x}(0) = 0$:

$$x(t) = -\frac{2A_{n_0}}{\sin(n_0\omega\tau)} \sin[\tfrac{1}{2}(n_0\omega - \omega_0)t] \cos(\omega_0 t + n_0\omega\tau). \tag{6}$$

Then it is easy to show that the energy which has been transferred to the effective oscillator is

$$E(t) = \tfrac{1}{2}(\dot{x}^2 + \omega_0^2 x^2) = \left(\frac{a}{T(\omega_0^2 - n_0^2\omega^2)}\right)^2 [1 - \cos(n_0\omega - \omega_0)t]. \tag{7}$$

As a consequence, in the case of a harmonic lattice interacting with a square pulse, the ith normal mode will be excited, if $(n_i^2\omega_s^2 - \omega_i^2)$ is small, ω_i is the eigenfrequency of the ith mode, and $\omega_s = 2\pi v_s/N$, where v_s is the velocity of the soliton and N is the number of the particles in the lattice. Hence the time dependence of the energy of the soliton is of the form

$$E_s(t) = E_s(0) - \sum_i \left(\frac{a}{T(\omega_i^2 - n_i^2\omega_s^2)}\right)^2 [1 - \cos(n_i\omega_s - \omega_i)t] \tag{8}$$

where $E_s(0)$ is the initial soliton energy.

Therefore we expect to find the frequencies $(n_i\omega_s - \omega_i)$ in the spectrum of the energy. Hence, if the soliton is approximated by a square pulse, its energy exhibits a recurrence such that the recurrence times are the periods corresponding to these frequencies.

To test this idea we will find the eigenfrequencies ω_i of the lattice using a perturbation method. The frequency ω_s corresponding to the time between two successive collisions of the soliton with the impurity is determined numerically. Therefore the $(n_i\omega_s - \omega_i)$ can be determined and the modes which will be excited most can be predicted. The results of this model can be compared with the numerically produced spectrum of the velocity of a particle in the lattice. A second check is to find the smallest $(n_i\omega_s - \omega_i)$ to be the frequencies in the spectrum of the energy of the soliton.

The perturbation method used to find the ω_i is as follows. The displacement q_i of the ith particle can be considered the sum of the displacement because of the soliton s_i and the displacement because of the background motion u_i:

$$q_i = s_i + u_i. \tag{9}$$

We suppose that u_i is small. Hence the equations of motion

$$m_i\ddot{q}_i = F(q_{i+1} - q_i) - F(q_i - q_{i-1}) \tag{10}$$

can be linearised with respect to u_i. These linearised equations of motion for u_i are

$$m_i\ddot{u}_i = \frac{\partial F(q_{i+1} - q_i)}{\partial(q_{i+1} - q_i)}\bigg|_{(s_{i+1} - s_i)} (u_{i+1} - u_i) - \frac{\partial F(q_i - q_{i-1})}{\partial(q_i - q_{i-1})}\bigg|_{(s_i - s_{i-1})} (u_i - u_{i-1}). \tag{11}$$

The constants

$$\frac{\partial F(q_i - q_{i-1})}{\partial(q_i - q_{i-1})}\bigg|_{(s_i - s_{i-1})} \tag{12}$$

can be determined from the initial form of the solution. Therefore a set of eigenfrequencies and their corresponding eigenvectors can be determined. Notice that we considered a soliton sufficiently wide that its position in the lattice does not much influence these eigenvalues. The values of these frequencies can be compared to the values found in the numerically produced spectrum of the velocity of a particle in the lattice. We found only a fair agreement between these two values. For this reason another technique was used to improve the value of the eigenfrequencies.

This improvement takes into account also the non-linearity of the equations of motion, in the following way. Using the matrix of the eigenvectors a_{ij} which were calculated by the aproximation presented in the last paragraph we make the transformation to new coordinates x_i

$$q_i = \sum_j a_{ij}x_j \tag{13}$$

such that the linearised equations of motion become uncoupled in the new coordinates. q_i and $p_i = m_i\dot{q}_i$ are replaced by the corresponding expansions (13) in the exact Hamiltonian of the lattice. If the coupling between the non-linear 'normal modes' is weak we can assume that only one of the x_i is non-zero. In this case the Hamiltonian $H(x_i, m_i\dot{x}_i)$ is reduced to a Hamiltonian with only one degree of freedom. Therefore the relationship between energy and frequency can be found analytically and so a corrected value for the frequency is determined. These new values of the eigenfrequencies were found in good agreement with the numerical results for both types of interaction we examined.

This is shown in tables 1 and 2 for Morse and Toda lattices respectively. The first column of each of these tables shows the eigenfrequencies of the corresponding lattice which were calculated by taking into account only the existence of an impurity in the lattice but not of the soliton. The second column shows the corrected eigenfrequencies after the influence of the soliton was considered. The third column shows the improved eigenfrequencies where also the non-linearity of the potential was introduced into the perturbation method. The fourth column shows the numerical values of the eigenfrequencies which were found in the power spectrum of the velocity $v(t)$ of the impurity. Figure 6 shows an example of a spectrum of $v(t)$ corresponding to the case shown in figure 3(b) and the energy power spectrum of figure 4. The fifth column shows the multiples of the frequency corresponding to the time at which the soliton covers the length of the lattice. The sixth column shows the differences between the fifth column and the closest values of the third column, while the seventh shows the differences between the values of the fifth and the fourth columns. Finally the eighth column shows the values of the frequencies found in the spectrum of the energy of the soliton. There is a good agreement between the sixth, seventh and eighth column for both the

Table 1. A comparison between the eigenfrequencies obtained by the perturbation method of § 3 with the numerical values found in the power spectrum of the velocity of the impurity (column 4) for a Morse lattice with $E_s = 3.014$, $m_{imp} = 1.11$ and $N = 40$. A comparison is also made between the theoretically predicted and the numerically calculated frequencies found in the spectrum of the soliton energy (columns 6-8). See text for further explanation.

ω_0	ω'_{per}	ω_{per}	ω_{num}	$n\omega_s$	$\lvert n\omega_s - \omega_{per}\rvert$	$\lvert n\omega_s - \omega_{num}\rvert$	Ω_{en}
0.1565	0.1569	0.1579					
0.1569	0.1627	0.1642		0.1830	0.0188		
0.3120	0.3140	0.3160					
0.3129	0.3237	0.3266		0.3660	0.0394		
0.4656	0.4692	0.4721					
0.4669	0.4832	0.4873		0.5490	0.0617		
0.6163	0.6233	0.6271					
0.6180	0.6378	0.6431					
0.7633	0.7757	0.7804		0.7320	0.0484		
0.7654	0.7864	0.7926					
0.9055	0.9207	0.9263	0.928	0.9150	0.0113	0.013	0.014
0.9080	0.9326	0.9397					
1.0421	1.0597	1.0662					
1.0450	1.0724	1.0804		1.0980	0.0176		
1.1724	1.1955	1.2030					
1.1756	1.2022	1.2106					
1.2953	1.3216	1.3299		1.2810	0.0489		
1.2989	1.3268	1.3358					
1.4104	1.4364	1.4456					
1.4142	1.4455	1.4554	1.455	1.4640	0.0086	0.009 }	
1.5167	1.5456	1.5555					0.0085
1.5208	1.5514	1.5612					
1.6136	1.6451	1.6557	1.655	1.6470	0.0087	0.008 }	
1.6180	1.6476	1.6580					
1.7007	1.7298	1.7309					
1.7053	1.7372	1.7371					
1.7772	1.8065	1.8179					
1.7820	1.8118	1.8236	1.823	1.8300	0.0064	0.007	0.007
1.8428	1.8713	1.8834					
1.8478	1.8751	1.8874					
1.8971	1.9198	1.9317					
1.9021	1.9293	1.9420					
1.9398	1.9587	1.9725					
1.9447	1.9655	1.9803					
1.9707	1.9862	2.0018					
1.9754	1.9883	2.0110					
1.9901	1.9968	2.0122	2.0130	0.0008			
1.9938	2.0872	2.1388	2.1960	0.0572			
1.9990	2.5934	2.6357	2.5620	0.0737			

cases we present here. Similar results were also found for all other combinations of the values of the parameters of the system we examined.

Note that in tables 1 and 2 the lowest eigenfrequency, which corresponds to a simple rotation of the particles in the lattice and is equal to zero, has been omitted. Note also that the perturbation method, which is presented in this section, does not correctly determine the three highest eigenfrequencies of the lattice, because these are particularly influenced by the assumption that the soliton is a static deformation of

Table 2. As table 1 but for a Toda lattice with $E_s = 4.4$, $m_{imp} = 0.6$ and $N = 40$.

ω_0	ω'_{per}	ω_{per}	ω_{num}	$n\omega_s$	$\lvert n\omega_s - \omega_{per}\rvert$	$\lvert n\omega_s - \omega_{num}\rvert$	Ω_{en}
0.2219	0.2227	0.2230					
0.2242	0.2286	0.2291	0.227	0.2367	0.0076	0.010	0.010
0.4425	0.4436	0.4442					
0.4469	0.4564	0.4574		0.4734	0.0160		
0.6603	0.6678	0.6688					
0.6669	0.6752	0.6768		0.7101	0.0333		
0.8740	0.8843	0.8855					
0.8828	0.8944	0.8958		0.9468	0.0510		
1.0824	1.0909	1.0924					
1.0932	1.1117	1.1139		1.1835	0.0696		
1.2841	1.2984	1.3004					
1.2969	1.3137	1.3162					
1.4778	1.4989	1.5015		1.4202	0.0813		
1.4925	1.5078	1.5099					
1.6625	1.6809	1.6834		1.6569	0.0265		
1.6789	1.7011	1.7041					
1.8369	1.8572	1.8598					
1.8548	1.8782	1.8813	1.881	1.8936	0.0123	0.012	0.012
2.0000	2.0245	2.0272					
2.0193	2.0417	2.0440					
2.1508	2.1752	2.1758		2.1303	0.0482		
2.1711	2.1966	2.1998					
2.2882	2.3128	2.3160					
2.3095	2.3360	2.3399		2.3670	0.0271		
2.4116	2.4380	2.4350					
2.4333	2.4589	2.4633					
2.5201	2.5455	2.5485					
2.5418	2.5686	2.5723		2.6037	0.0314		
2.6131	2.6368	2.6407					
2.6342	2.6597	2.6639					
2.6900	2.7138	2.7177					
2.7095	2.7310	2.7351					
2.7503	2.7697	2.7740					
2.7672	2.7873	2.7917					
2.7936	2.8067	2.8109					
2.8062	2.8196	2.8251					
2.8197	2.8308	2.8365		2.8404	0.0039		
2.8259	3.0861	3.1154		3.0771	0.0383		
3.0861	3.1827	3.2028		3.3138	0.1110		

the lattice. Therefore the resonances of the soliton with these high eigenfrequencies which are shown in tables 1 and 2 should not be taken into account.

This theory not only explains well why the soliton retains most of its energy and describes the mechanism which permits the soliton to regain the energy it lost, but can also predict for which values of the parameters of the system the decay of the soliton occurs. Formula (8) shows that when $(n_i^2\omega_s^2 - \omega_i^2)$ is small the energy of the background becomes large and the soliton is destroyed. In other words the decay of the soliton takes place when a resonance of the type $(n_i\omega_s - \omega_i) \approx 0$ exists. Note that the relationship between the appearance of these resonances and the values of the parameters of the system cannot be described by a simple rule, as one can also see in the figures of the paper by Rolfe and Rice (1980).

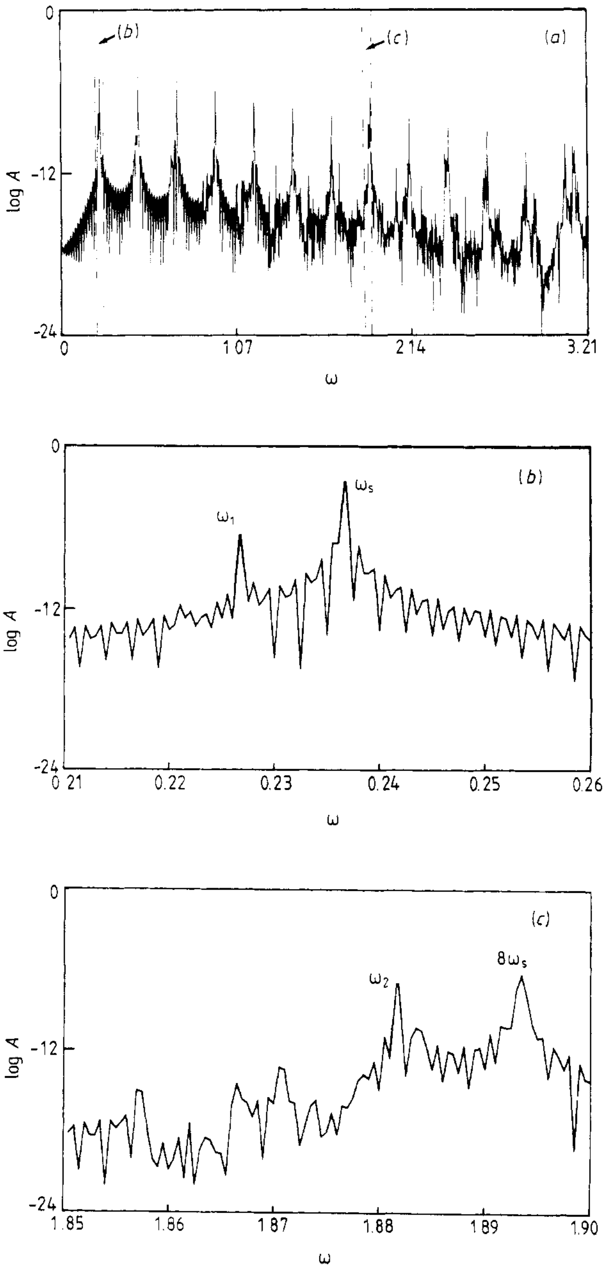


Figure 6. Power spectrum of the velocity of the impurity for a Toda lattice where $E_s = 4.409$, $N = 40$ and $m_{imp} = 0.6$. Regions (*b*) and (*c*) of spectrum (*a*) are magnified in parts (*b*) and (*c*) respectively. Notice that $\Omega_1 = \omega_s - \omega_1$ and $\Omega_2 = 8\omega_s - \omega_2$.

Unfortunately the above resonant mechanism which is presented in this section does not explain the strange metastable behaviour of case (iii) in the introduction. We study this case in the next section.

4. The case of a metastable soliton

Even though the theory presented in the last section offers a satisfactory explanation of the recurrence of the energy of the soliton, it fails to explain why the plateau of the energy of the soliton sometimes breaks in a sudden and 'unpredictable' way. In other words, our analysis cannot distinguish between cases (ii) and (iii).

One can ask whether the breaking of the energy plateau is a result of the numerical accuracy of the computations. As an answer to this we recall that in our calculations the total energy of the system was conserved with an accuracy of at least 10^{-5} and that Rolfe and Rice (1980), who also used similar precautions, found the same behaviour in many cases. Therefore, even if the accuracy of the numerical integration of the system influences the breaking of the energy plateau, this behaviour can only be interpreted as the result of a highly unstable situation.

How can such an unstable behaviour arise? In the previous section we did not consider at all the non-linear coupling between the normal modes of the lattice. This assumption is true only if the energy of the background motion is small. In the case that the amplitude of the oscillations of the soliton energy is large the energy of the background motion can become large during the time periods which correspond to the minima of the energy of the soliton. Hence several other normal modes will be excited. These normal modes retain their energy because they are not in resonance with the soliton, as explained in the last section. This process will make the soliton slower. Therefore a new stronger resonance with a normal mode is possible. In this case the soliton decays.

Figures 7 and 8 give a pictorial demonstration of the idea described in the last paragraph. Figure 7 shows how the energy of the soliton decays in a case where the number of particles is 40, the type of interaction is Morse, the energy of the soliton is 3.014 and the mass of the impurity is 1.13. Figure 8 shows the power spectrum of the velocity of the impurity taken over a time period of length $T=2500$ time units at the four different times (t_0, t_1, t_2, t_3) shown in figure 7. Clearly there is a gradual widening of the lines in the power spectrum as the soliton decays.

This 'metastability' is a more general behaviour and is observed in all nearly integrable systems. It corresponds to trajectories which initiate in the chaotic component of the phase space of the nearly integrable system, but close to its boundary with the regular component. Therefore these trajectories behave almost regularly for a long but finite period of time before they start to behave in a clearly chaotic way.

This idea is demonstrated in figure 9. There a Poincaré surface of section for the Hénon–Heiles model (Hénon and Heiles 1964) is shown. The energy is taken as 0.155 and the initial conditions are $q_1=0$, $q_2=0.6143$, $p_1=0.291\,65$, $p_2=-0.046$. This trajectory produces 67 points near the central regular island (figure 9(a)) before it leaves to fill the whole chaotic component of the phase space (figure 9(b)).

The persistence of regular behaviour near the boundaries between the chaotic and the regular regime of a nearly integrable system can also be detected in systems with more degrees of freedom than the simple Hénon–Heiles model. In the case we examine, namely the one-dimensional Morse or Toda lattice, this can be done by computing

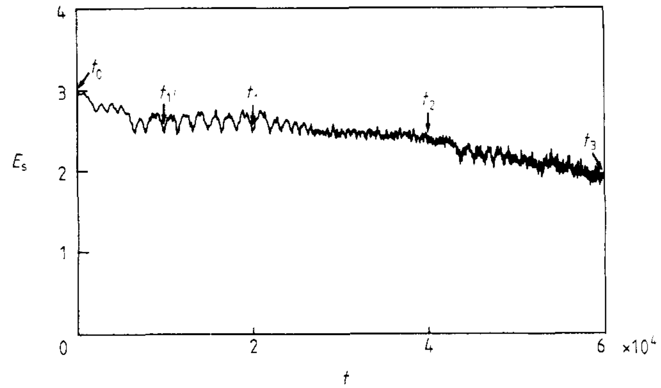


Figure 7. Graph of the soliton energy as a function of time for a Morse lattice where $E_s = 3.014$, $N = 40$ and $m_{imp} = 1.13$. $t_0 = 0$, $t_{1'} = 10^4$, $t_1 = 2 \times 10^4$, $t_2 = 4 \times 10^4$, $t_3 = 6 \times 10^4$.

the divergence between two trajectories close to each other in the phase space. Figure 10 shows the distance, $D(t)$, between two trajectories in the phase space of the lattice which was presented earlier in this section. One of the trajectories in figures 10(a) and 10(b) has initial conditions which correspond to the times $t_{1'}$ and t_1 of figure 7 respectively. The second trajectory initiates at a distance 10^{-7} from the first. Notice that figure 10(a) which coresponds to a plateau of the energy of the soliton shows a clear linear divergence with time between the trajectories (regular behaviour). In contrast, figure 10(b), which corresponds to a time period during which the plateau breaks, shows an irregular behaviour of the distance between the two trajectories, which appears at about the same time with the breaking of the plateau. The perfectly linear character of the graph shown in figure 10(a), which does not present any fluctuations, is a special characteristic of the Morse lattice with a large number of oscillators.

Therefore the 'metastability', which was observed in the numerical results presented in § 2, is a generic behaviour and should be detected in other dynamical systems which are small perturbations of integrable systems. Indeed similar behaviour was also reported in other dynamical systems (Caponi *et al* 1982). In a more general approach, the possibility of persistence of the regular behaviour for trajectories initiating in the chaotic regime of the phase space of a weakly perturbed integrable system is discussed by Benettin *et al* (1984) in relation to Nekhoroshev's theorem (Nekhoroshev 1977).

5. Conclusions

We studied the behaviour of a soliton travelling in a one-dimensional non-linear (Morse or Toda) lattice with periodic boundary conditions having one impurity. Our numerical studies not only verified the results of Rolfe and Rice (1980) in the Morse lattice, but also showed similar behaviour in the Toda lattice. In addition, the behaviour of the system was studied when the impurity mass changes, while Rolfe and Rice kept this parameter constant. We have also developed an interpretation of these numerical results.

The recurrence of the energy of the soliton, which was observed when the mass of the impurity is close to the mass of the other particles in the chain, is explained as the

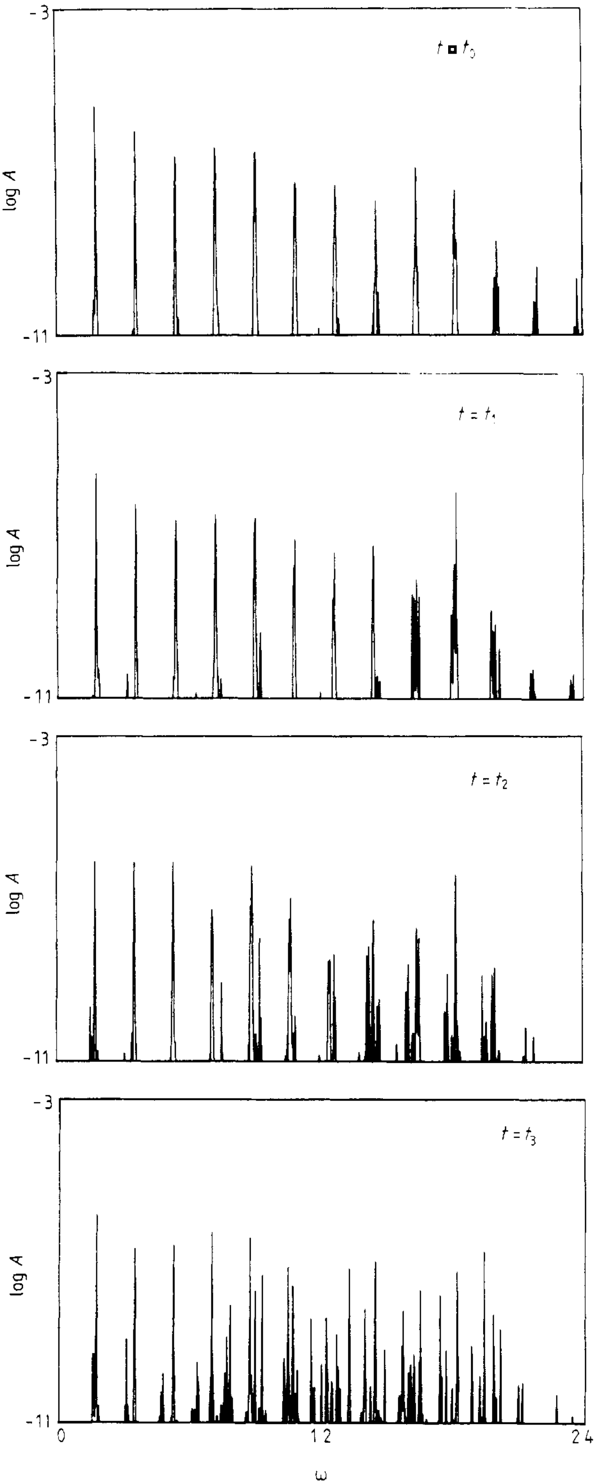


Figure 8. Power spectra of the velocity of the impurity in a Morse lattice where $E_s = 3.014$, $N = 40$ and $m_{imp} = 1.13$, taken at t_0, t_1, t_2 and t_3 of figure 7.

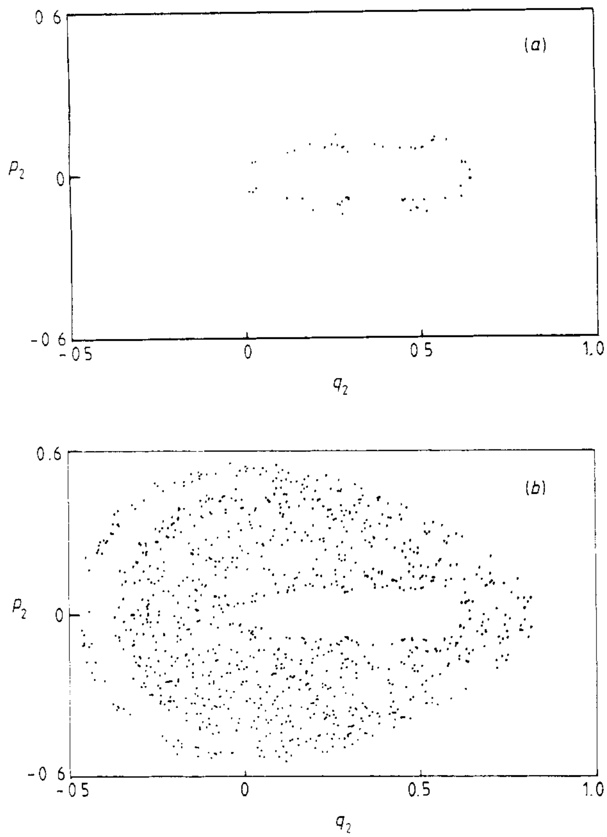
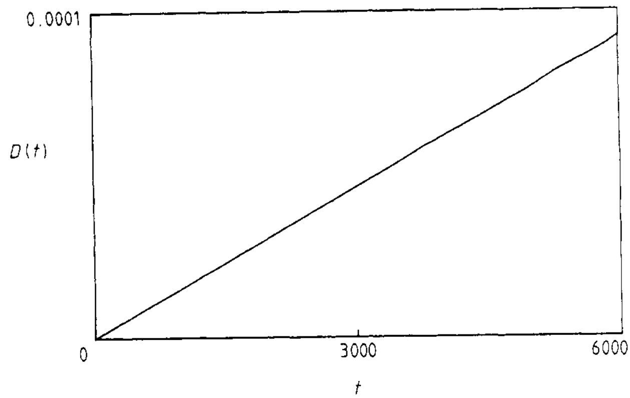


Figure 9. Poincaré surface of a section of a trajectory of the Hénon-Heiles system, where $E = 0.155$. The initial conditions are $q_1 = 0$, $p_1 = 0.291\,65$, $q_2 = 0.6143$, $p_2 = -0.046$. This trajectory produces 67 points near the central island of regular motion (a), before it fills the whole chaotic regime (b).

result of a mutual exchange of energy between the soliton and some of the linear normal modes of the lattice. More specifically, the time period between two successive collisions of the soliton with the impurity defines a frequency ω_s. If this frequency is close to the frequencies of some normal modes, these are excited. In § 3, using a simple model, we have shown that the interaction between the soliton and the normal modes results to a periodic behaviour of the energy of the soliton. A perturbation method was also developed, which predicts these resonances for a given set of parameters E_s, N and m_{imp}. If a resonance is very good, in other words, if a multiple of ω_s is very close to an eigenfrequency, the soliton decays.

Finally, in § 4 we discussed an intermediate case, where the energy of the soliton exhibits a recurrence for a long period of time before it decreases rapidly. We explained that this is a result of the non-linear interaction between the normal modes, which was not considered in the perturbation scheme of § 3. This 'metastable' behaviour is generic in all nearly integrable systems. The persistent regular motion appears when the corresponding trajectory initiates in a few special regions of the chaotic part of the phase space of the system. Nevertheless, any chaotic trajectory will visit these regions because of ergodicity. Therefore any chaotic trajectory of a nearly integrable system behaves almost regularly for certain periods of time of a long but finite duration.



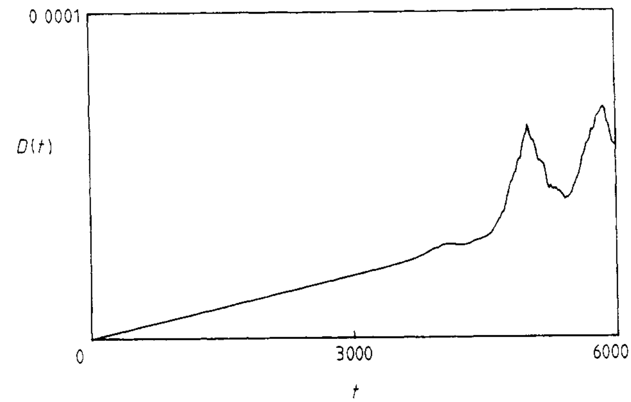


Figure 10. Divergence of trajectories in the phase space of a Morse lattice where $E_s = 3.014$, $N = 40$ and $m_{imp} = 1.13$. As starting points the states of the system were used at (*a*) $t_{I'} = 10^4$ and (*b*) $t_I = 2 \times 10^4$ (see figure 7) respectively.

Hence, this approximate regularity should be carefully considered when statistical or transport properties (i.e. thermal conductivity, diffusion or chemical behaviour) of nearly integrable systems are examined.

Our results illustrate the possibility of coexistence of a coherent (soliton) and an incoherent (chaotic) dynamical behaviour in large non-linear Hamiltonian systems, namely Morse or Toda chains with one impurity. We expect that this behaviour can also be detected in other non-linear systems.

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