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Pinning-free soliton lattices and bifurcation in a discrete double-well model: exact results

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Abstract. It is shown that the chain of coupled particles in the double-well potential introduced by H Schmidt is completely integrable in the static limit. The chaotic behaviour and the associated infinite series of bifurcations found in the related discrete φ^4 theory are absent in the model. The solutions are generally unpinned soliton lattices. The model exhibits a bifurcation where a hyperbolic fixed point becomes elliptic and splits into two hyperbolic fixed points. The bifurcation does not lead to chaos.

1. Introduction

Krumhansl and Schrieffer (1975) have studied a chain of harmonically coupled particles in the double-well φ^4 potential governed by the Hamiltonian

$$H=\sum_n p_n^2/2m+\tfrac{1}{2}(\varphi_{n+1}-\varphi_n)^2+\tfrac{1}{2}a(\varphi_n^2-1)^2. \tag{1}$$

In the *continuum* limit there are propagating soliton solutions,

$$\varphi=\tanh(\omega t-qn). \tag{2}$$

However, when the continuum approximation is not applied, the equation of motion of (1) has complicated chaotic solutions even in the static limit (Aubry 1979, Bak and Pokrovsky 1981, Bak and Høgh Jensen 1982). Some of these solutions can be characterised as irregularly pinned soliton lattices which play an important role in the theory of commensurate–incommensurate transitions (for a review, see Bak 1982). In particular the model exhibits an infinite series of period-doubling bifurcations with universal exponents leading to chaos (Bak and Høgh Jensen 1982, Janssen and Tjon 1982).

In an interesting paper H Schmidt (1979) pointed out that if the φ^4 potential is suitably modified the single soliton (2) becomes an exact solution to the *discrete* model. One might therefore wonder if it is possible in a similar way to construct a discrete model without chaotic behaviour. In this paper it will be shown that the chain of interacting particles in the potential introduced by H Schmidt is completely integrable in the static limit. The solutions are generally unpinned soliton lattices, and there are *no* chaotic stationary solutions. The model exhibits a standard bifurcation where a hyperbolic fixed point becomes elliptic and splits into two hyperbolic fixed points but there is no infinite series of bifurcations leading to chaos. Brazowskiĭ *et al* (1982a, b) have recently found that a discrete model of the Peierls transition is also completely integrable and has similar regular soliton lattice solutions. Their solutions are related to integrals of the Toda lattice. The problem studied here belongs to a larger class of problems investigated previously by McMillan (1971).

2. The model and the analytic solutions

Consider the Hamiltonian for a harmonic chain of particles in a local potential $V(\varphi_n)$, where φ_n is the position of the nth particle in the nth double-well potential

$$H=\sum_n p_n^2/2m+\tfrac{1}{2}(\varphi_n-\varphi_{n-1})^2+V(\varphi_n). \tag{3}$$

The static, stable solutions are found among the solutions to the equations

$$(\varphi_n-\varphi_{n-1})-(\varphi_{n+1}-\varphi_n)+V'(\varphi_n)=0, \tag{4}$$

which can be rewritten as an infinite series of difference equations

$$\varphi_{n+1}=V'(\varphi_n)+2\varphi_n-z_n, \qquad z_{n+1}=\varphi_n. \tag{5}$$

In the *continuum* approximation (4) takes the form

$$\mathrm{d}^2\varphi/\mathrm{d}n^2-V'(\varphi)=0. \tag{6}$$

If V is chosen as a φ^4 potential

$$V(\varphi)=\tfrac{1}{2}a(\varphi^2-1)^2 \tag{7}$$

the solutions to (6) are lattices of regularly spaced solitons

$$\varphi(n)=\varphi_0\,\mathrm{sn}[(n-x_0)/l_0], \qquad l_0=1/q \tag{8a}$$

with

$$1/l_0^2=a\varphi_0^2/k^2, \qquad |\varphi_0|\leqslant 1. \tag{8b}$$

Here sn are elliptic functions with modulus k determined by

$$k^2=\varphi_0^2/(2-\varphi_0^2). \tag{8c}$$

The single soliton solution (2) with $\omega=0$ arises from (8) in the limit $\varphi_0\to 1$ $(k\to 1)$.

In the *discrete* case the solutions can be generated numerically by iterations of the two-dimensional mapping (5) with the φ^4 potential (7) inserted. Figure 1(a) shows trajectories generated in this way for $a=0.8$. Note the regular (KAM) trajectories which are filled up ergodically as the iteration proceeds, and the chaotic, irregular trajectories outside (and between) the regular ones.

Our procedure is to look for a potential $V(\varphi_n)$ such that (8) becomes an exact solution even in the *discrete* case. Inserting (8a) into (4) we find

$$\begin{aligned}\varphi_{n+1}-2\varphi_n+\varphi_{n-1}&\\ &=\varphi_0(\mathrm{sn}(qn+n)+\mathrm{sn}(qn-n)-2\,\mathrm{sn}(qn))\\ &=2\mathrm{cn}(q)\,\mathrm{dn}(q)\{\varphi_0\,\mathrm{sn}(nq)/[1-(k^2\,\mathrm{sn}^2(q)/\varphi_0^2)\varphi_0^2\,\mathrm{sn}^2(nq)]\}-2\varphi_0\mathrm{sn}(nq)\\ &=V'(\varphi_n)\end{aligned} \tag{9}$$

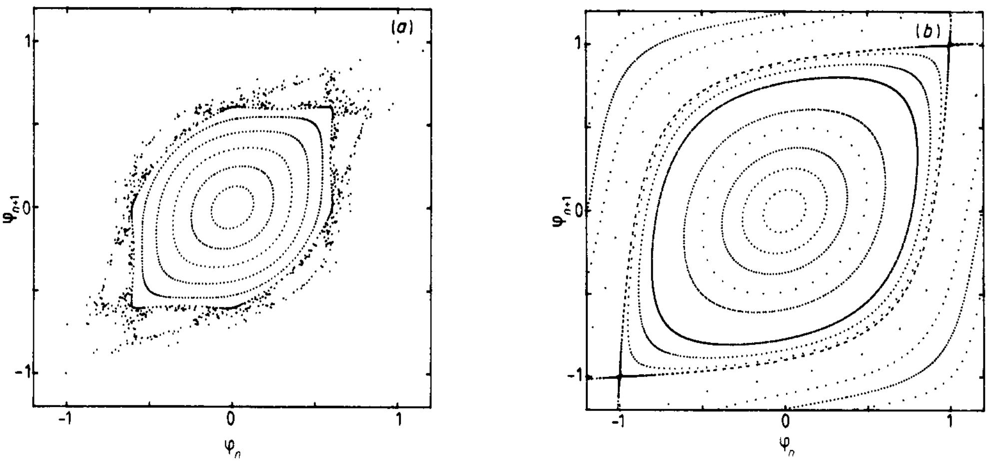

Figure 1. Plots of the numerically iterated mapping (5) for (*a*) the φ^4 potential and (*b*)
11031 the H Schmidt potential, both for $a = 0.8$. Note the absence of chaotic behaviour in the
11032 latter case. Analytic expressions for the trajectories are given in the text.

with

$$\begin{aligned} &V'(\varphi_n) = 2(1-a)\varphi_n/(1-a\varphi_n^2) - 2\varphi_n \\ &a = k^2\,\mathrm{sn}^2(q)/\varphi_0^2, \qquad 1-a = \mathrm{cn}(q)\,\mathrm{dn}(q). \end{aligned} \tag{10}$$

The elliptic functions sn, cn, dn have a modulus k determined by

$$k^2 = (\varphi_0^2 - a\varphi_0^4)/(2-a-\varphi_0^2). \tag{11}$$

The equation (10) can be integrated to yield

$$V(\varphi_n) = (1-1/a)\ln(1-a\varphi_n^2) - \varphi_n^2, \tag{12}$$

which is precisely the H Schmidt potential.

Hence the discrete system of equations (4) with the potential (12) has the same solutions as the continuous φ^4 equations.

The functions $\varphi_n = \varphi_0\,\mathrm{sn}[(n-x_0)/l_0]$ describe lattices of solitons with widths l_0. By adding a phase constant to this solution or changing the modulus we can construct other solutions to (5) expressed in terms of elliptic functions (see for instance Abramowitz and Stegun 1964):

$$\bar{\varphi}_n = \varphi_0\,\mathrm{sn}[(n-x_0)/l_0 + \mathrm{i}K'] = (\varphi_0/k)\mathrm{ns}[(n-x_0)/l_0] \tag{13}$$

where $\mathrm{i}K'$ is the imaginary half-period for the sn function;

$$\begin{aligned} \hat{\varphi}_n &= (\varphi_{01} + \mathrm{i}\varphi_{02})\,\mathrm{sn}\{(k+\mathrm{i}k')[(n-x_0)/l_0], (k-\mathrm{i}k')/(k+\mathrm{i}k')\} \\ &= \frac{\varphi_{01}}{k}\,\frac{\mathrm{sn}((n-x_0)/l_0, k)\,\mathrm{dn}((n-x_0)/l_0, k)}{\mathrm{cn}((n-x_0)/l_0, k)} \end{aligned} \tag{14a}$$

where $k^2 + k'^2 = 1$ and the parameters fulfil the rather complicated equation

$$(k^4/\varphi_{01}^4)(\varphi_{01} + \mathrm{i}\varphi_{02})^2 = [1 - a(\varphi_{01} + \mathrm{i}\varphi_{02})^2]/[2 - a - (\varphi_{01} + \mathrm{i}\varphi_{02})^2]. \tag{14b}$$

Altogether the solutions (8), (13) and (14) fill up the whole (φ, z) space of the mapping

(5) for $0 < a < 2$, so the integration is complete. For $a > 2$ there are solutions of the form

$$\tilde{\varphi}_n = -\mathrm{i}\varphi_0 \operatorname{sn}(\mathrm{i}(n-x_0)/l_0, k) = \varphi_0 \operatorname{sc}((n-x_0)/l_0, k') \qquad (15a)$$

with

$$k^2 = (\varphi_0^2 + a\varphi_0^4)/(a - 2 - \varphi_0^2). \qquad (15b)$$

The functions (13), (14a) and (15a) assume values $|\varphi_n| > 1/\sqrt{a}$ such that (12) becomes imaginary. However, when the equation for stability (4) is constructed, an imaginary part is differentiated out and the mapping remains unchanged. Because of discreteness, trajectories in the (φ, z) space can jump across the singularity.

Of course we can also generate the *same* trajectories numerically by iterating (5) with the potential (12) inserted. Figure 1(b) shows the results for $a = 0.8$. Compare with figure 1(a) and note that the complicated chaotic trajectories found for the φ^4 potential have disappeared. In fact almost all the features found by Bak and Høgh Jensen for the φ^4 theory have vanished, including the infinite series of bifurcations. We have thus established that (5) constitutes an area-preserving two-dimensional mapping with regular periodic trajectories only. Besides the regular KAM trajectories which are filled up ergodically there are also trajectories with finite period (limit cycle points) corresponding to solutions with rational values of $l_0 K$, where K is the quarter period of the sn function (see Abramowitz and Stegun 1964).

A shift of the parameter x_0 does not affect the solutions (8), (13), (14), (15). *All* the solutions are thus 'unpinned' i.e. there is a Goldstone sliding mode associated with x_0 even for the commensurate orbits, in contrast to the discrete φ^4 theory. Note in figure 1(b) the regular orbits with $\varphi_n > 1$. In this regime the corresponding φ^4 trajectories are chaotic.

Figure 2 shows the H Schmidt potential (12) compared with the φ^4 potential. For small values of a, where discreteness effects are small, the potentials must necessarily be very similar. When the parameter a exceeds 1 the potential loses its double-well nature.

Figure 3 shows φ_n calculated with $a = 0.5$ for the two different potentials. The starting point is the same in both cases. In (a) we recognise the regular soliton lattice with a soliton for approximately every 5th lattice point (solitons marked by arrows). The corresponding solution for the φ^4 model is *chaotic* (figure 3(b)). The solitons are pinned randomly and the iteration can proceed only a finite number of steps before divergence.

Bak and Pokrovsky (1981) found that the φ^4 solitons will be pinned and the KAM trajectories disappear when the distance between the solitons exceeds a critical value $l_c \sim -\log E_{\mathrm{pin}}$ where E_{pin} is the single soliton pinning energy. In order to investigate the pinning effects we add a perturbation term to the pinning-free potential (12)

$$V^*(\varphi_n) = V(\varphi_n) + \tfrac{1}{2}\lambda a^2 \varphi_n^4. \qquad (16)$$

For $\lambda = 1$ (16) coincides with (7) up to the fourth-order term. The pinning energy becomes

$$E_{\mathrm{pin}} = \tfrac{1}{2}\lambda a^2 \sum_n [\tanh^4(n/l_0) - \tanh^4((n+\tfrac{1}{2})/l_0)] \qquad (17)$$

which is necessarily proportional to λ; hence $l_c \sim -\log \lambda$. The chaotic regime of the mapping (5) with V defined in (16) therefore increases as $\sim \log \lambda$, which agrees with our numerical studies. Also we have confirmed the logarithmic variation of l_c with λ numerically.

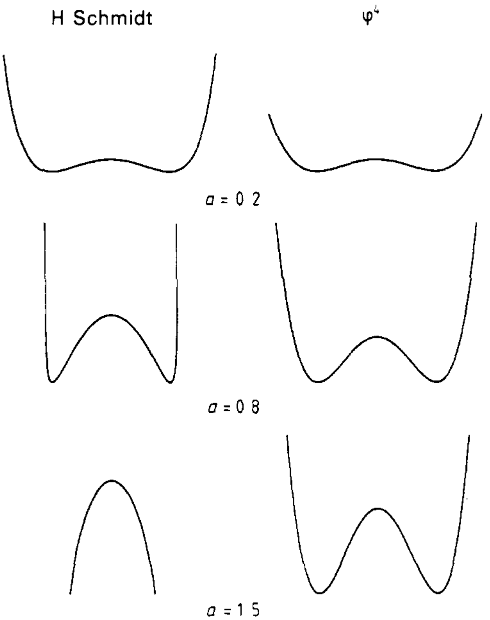

Figure 2. The potential (12) and the ϕ^4 potential for various values of a.

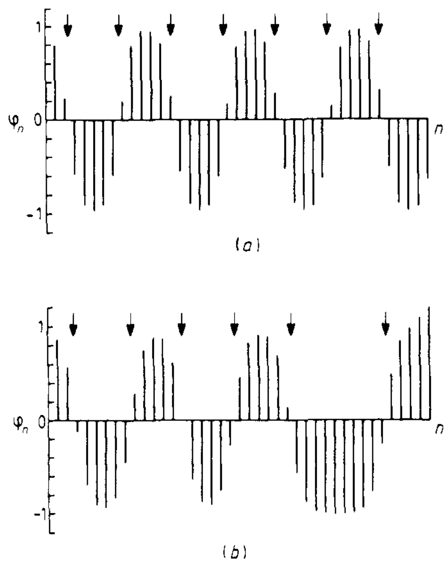

Figure 3. Soliton-array solution for $a = 0.5$. The solitons are marked by arrows. (a) Integrable model: regular soliton lattice. (b) ϕ^4 model: randomly pinned solitons (chaotic behaviour).

3. Bifurcation

The discrete φ^4 model exhibits a bifurcation of the point $(0, 0)$ at $a = 2$. To investigate if a similar bifurcation occurs in the integrable model we consider the linearised version of the mapping (5) defined by the Jacobian matrix:

$$D\hat{T} = \begin{pmatrix} -2(a-1)\dfrac{1+a\varphi_n^2}{1-a\varphi_n^2} & -1 \\ 1 & 0 \end{pmatrix}. \qquad (18)$$

Note $\det D\hat{T} = 1$, confirming that the mapping is area preserving. A bifurcation might take place when $\mathrm{Tr}\, D\hat{T} = -2$, which happens for $a = 2$ (when the potential has lost its double-well nature). When $0 < a < 2$ the eigenvalues of (18) are on the complex unit circle and the point $(0, 0)$ is an elliptic fixed point. When $a = 2$ the eigenvalues collide at $\lambda = -1$ and for $a > 2$ they are confined to the real axis so the fixed point indeed becomes hyperbolic. However, there is *not* a bifurcation like the one for the φ^4 theory. Let us find analytically the possible period-two solutions. Inserting $\varphi_{n+1} = \varphi_{n-1}$ in (5) we find

$$\varphi_n = (1-a)z_n/(1-az_n^2). \qquad (19a)$$

If (φ_n, z_n) belongs to the two-cycle, (φ_{n+1}, z_{n+1}) must be the other point of the cycle:

$$z_n = (1-a)\varphi_n/(1-a\varphi_n^2). \qquad (19b)$$

The equations (19*a*, *b*) have the solution

$$(\varphi, z) = \pm[(2/a-1)^{1/2}, -(2/a-1)^{1/2}] \tag{20}$$

defining the two-cycle. This solution exists for *a less* than 2, not for *a* greater than 2. The points (20) collapse at (0, 0) for $a = 2$ and move to complex space. Hence a bifurcation occurs for decreasing *a*. To illustrate this situation figures 4(*a*) and (*b*) show iterated trajectories for values of *a* slightly less than and slightly larger than 2. For $a > 2$ (4*b*) the fixed point is hyperbolic, and there is no evidence of a two-cycle; for $a < 2$ (4*a*) the fixed point (0, 0) is elliptic. The limit cycle points (20) are indicated by dots; their surroundings are hyperbolic. We have thus established that as *a* passes through 2 from above, a *hyperbolic* fixed point bifurcates into a *hyperbolic* two-cycle and becomes *elliptic.*

Apparently, the mapping, although discrete and nonlinear, cannot produce infinite series of bifurcations or chaos. However, a single bifurcation occurs. All this is contained in the analytic solutions (8), (13), (14) and (15).

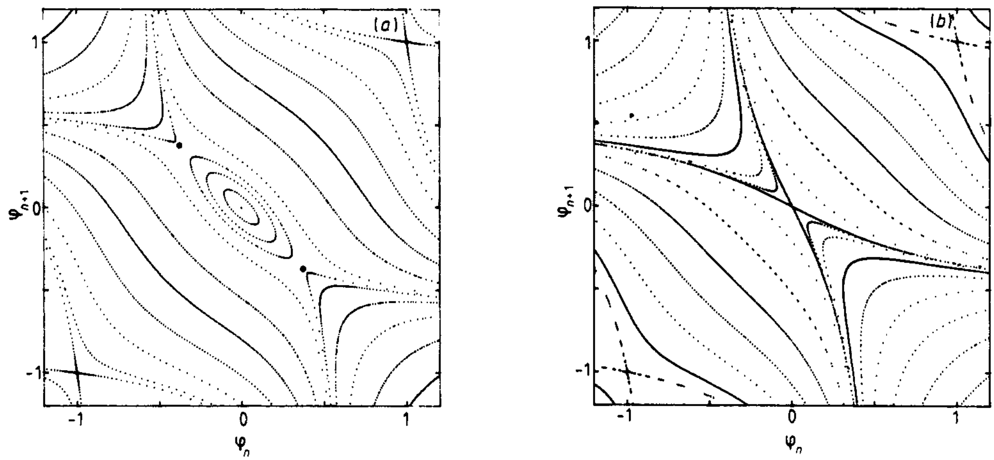

Figure 4. Plots of trajectories for (*a*) $a = 1.75$ and (*b*) $a = 2.25$. The large dots on (*a*) mark the two-cycle found analytically in the text. The fixed point (0, 0) is hyperbolic on (*b*) and elliptic on (*a*). A bifurcation has taken place at $a = 2$.

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