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Bifurcations and chaos in the ϕ^4 theory on a lattice

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Abstract. We have studied numerically and analytically the discrete ϕ^4 model defined by Bak and Pokrovsky. The model may describe Peierls systems, structural instabilities, metal-insulator transitions, etc in solid state physics. The ϕ^4 theory can be formulated as an area-preserving two-dimensional mapping. This mapping exhibits infinite series of period-doubling bifurcations leading to chaos. The bifurcations are characterised by universal numbers $\delta = 8.721\ 09\ldots$ and $\alpha = 4.0180\ldots$, which appear to be identical to those found by Bountis for the Hénon mapping, but different from the Feigenbaum numbers for dissipative systems. In addition, novel features arise because of marginally stable fixed points and the splitting of one 2-cycle orbit into two 2-cycle orbits.

1. Introduction

Recently Bak and Pokrovsky (1981) studied the one-dimensional discrete ϕ^4 theory defined by the Hamiltonian

$$\mathcal{H} = \frac{1}{2}\lambda \left(\sum_{n} \frac{1}{2} (\phi_n - \phi_{n-1})^2 + \frac{1}{4} a (\phi_n^2 - 1)^2 \right)$$
(1.1)

where \mathcal{H} might be thought of as the energy of an array of atoms, connected with harmonic springs, in the double-well ϕ^4 potential (figure 1). λ is the spring constant and $a\lambda$ the strength of the potential. The configurations which satisfy an energy extremum condition are found by differentiating (1.1) with respect to ϕ_n :

$$W_{n+1} = W_n + a\phi_n(\phi_n^2 - 1) \qquad \phi_{n+1} = \phi_n + W_{n+1}$$
(1.2)

with W_n defined by the latter equation. It was found that, in addition to regular commensurate and incommensurate solutions, these equations have *chaotic* solutions. The model was used to generate a theory of metal-insulator transitions in Peierls systems, such as polyacetylene (Chiang *et al* 1977, Rice 1979, Su *et al* 1979), but the lattice ϕ^4 theory probably applies to a large class of problems in condensed matter physics (structural transitions, magnetic transitions, etc).



Figure 1. Array of classical particles connected with springs in the double-well ϕ^4 potential.

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In this paper the discrete ϕ^4 theory will be studied in detail for potentials stronger than those considered by Bak and Pokrovsky. We find infinite series of bifurcations described by universal numbers, as the strength of the potential is increased.

In the last few years there has been considerable interest in deterministic systems exhibiting chaotic behaviour. In particular, it was shown by Feigenbaum (1978, 1979) that the sequences of bifurcations in the simple one-dimensional logistic mapping

$$x_{n+1} = bx_n(1-x_n)$$

are characterised by universal numbers and lead to chaos. This may provide a description of the onset of turbulence in dissipative systems. Universal behaviour has also been found in two-dimensional area-preserving or 'conservative' systems (see e.g. Benettin *et al* 1980a, b, Derrida and Pomeau 1980, Bountis 1981, Collet *et al* 1981, Greene *et al* 1981). The expression (1.2) is an example of a two-dimensional mapping. Generally, the universal constants are different from those found in dissipative systems.

The discrete one- and two-dimensional mappings define the solutions to an infinity of difference equations. In classical mechanics and hydrodynamics the systems are governed by differential equations. The connection between the well-understood chaotic behaviour in the discrete models and the chaotic behaviour in realistic continuous systems is far from trivial. In condensed matter physics, however, the physical quantities or fields are defined on a *discrete* lattice. The discrete mathematical models therefore apply more directly to problems related to solids.

The properties of structurally and magnetically modulated systems have been analysed numerically and analytically by studying the appropriate two-dimensional mappings (Aubry 1979, 1980, Bak 1981, Pokrovsky 1981, Bak and Pokrovsky 1981, Fradkin and Huberman 1981). It was found that chaotic structures (i.e. structures with randomly pinned defects) are at least metastable. This result may be relevant in understanding commensurate-incommensurate transitions, spin glasses, metalinsulator transitions in Peierls systems and superionic conductors. No systematic study of the onset of chaotic behaviour through bifurcations has been reported so far for these models.

To see that (1.2) indeed is a two-dimensional area-preserving mapping, let us introduce new variables x_n and y_n defined by

$$x_n = \phi_n \qquad \qquad y_n = \phi_{n-1}. \tag{1.3}$$

The transformation now takes the form

$$T: \quad \frac{x_{n+1} = -y_n + x_n (ax_n^2 + 2 - a)}{y_{n+1} = x_n}.$$
(1.4)

The transformation T maps one point in the (x, y) space onto another point in (x, y) space. The mapping is area-preserving, since its Jacobian is equal to -1. In the paper by Bak and Pokrovsky the recursion relation (1.4) was studied for $a = \frac{8}{9}$ and $a = \frac{1}{8}$. For these values (see figure 2, where $a = \frac{8}{9}$) the mapping includes one-dimensional orbits (KAM surfaces, see Arnold and Avez 1978), defining incommensurate structures, which surround the fixed point at (x, y) = (0, 0).

We find that for larger values of a the fixed point at (0, 0) bifurcates into a 2-cycle orbit. Two iterations of (1.4) bring the 2-cycle fixed points (FP) back to their original values. At the bifurcation point, the fixed point (0, 0) goes from being stable (elliptic)

to being unstable (hyperbolic). When a is further increased, the system undergoes an infinite series of bifurcations. This behaviour is very similar to that discovered by Bountis (1981) for the Hénon mapping (Hénon 1969, 1976, Hénon and Heiles 1964). In fact, we found two series of bifurcations, and probably there is an infinity of infinite series of bifurcations (as also found by Greene *et al* 1981). In studying the stability of FP and limit cycle sequences we follow a method introduced by Greene (1979), who found that, for a large class of 2N-cycles, two of the limit cycle points lie on a simple one-dimensional curve (the symmetry curve). This facilitates the search in the two-dimensional (x, y) space.

At this point a word of caution is important. The fixed points or limit cycle series, which undergo bifurcations, are always elliptic and 'mathematically' stable. However, the corresponding physical configurations are usually mechanically unstable. Although they are extrema of the energy, they do not minimise it. On the other hand, the mathematically unstable hyperbolic limit cycle sequences may define mechanically stable configurations, but they never bifurcate. Thus, at present, no direct application of the theory developed here is obvious.

In addition to the infinite series of bifurcations we find new features not seen in the Hénon mapping. For instance, we find a situation where the fixed point, for increasing a, becomes marginally unstable and then becomes stable again. The structure of nearby orbits is influenced by this behaviour. Also, at one of the instabilities a 2-cycle splits into two 2-cycles and not into one 4-cycle as one would expect at a regular bifurcation.

On the basis of the numerical calculations we determine the 'Feigenbaum' convergence number.

$$\delta = \lim_{k \to \infty} \frac{a_{k-2} - a_{k-1}}{a_{k-1} - a_k} \tag{1.5}$$

where a_k is the value of a for which the bifurcation from period 2^k to period 2^{k+1} takes place. We find $\delta = 8.721\,096\ldots$ We also calculate the number

$$\alpha = \lim_{k \to \infty} \frac{d_{k-1}}{d_k} \tag{1.6}$$

where d_k is the distance between the two points on the symmetry curve at the bifurcation. α determines the scaling of orbits around the limit cycle points as one goes from one bifucation to the next. We find $\alpha = 4.0180...$

These values are, up to the numerical accuracy, the same as for other twodimensional area-preserving mappings (Benettin *et al* 1980a, b, Bountis 1981, Greene *et al* 1981). This supports the hypothesis that α and δ are universal constants for conservative systems.

2. Orbits and bifurcations

2.1. The first bifurcation

The mapping defined by (1.4) has fixed points at $(x, y) = \pm (1, 1)$ and (0, 0). For small values of a the fixed point at (0, 0) is 'elliptic' or stable. Figure 2 shows orbits calculated for $a = \frac{8}{9}$. Apart from a change in variables, this figure corresponds to figure 1(a) of Bak and Pokrovsky. The elliptic fixed points are always surrounded by closed KAM



Figure 2. Orbits of the discrete ϕ^4 mapping defined by (1.4) calculated for $a = \frac{8}{9}$. The elliptic (stable) fixed point at (x, y) = (0, 0) is surrounded by one-dimensional invariant KAM surfaces. For a discussion of the various types of orbits, see Bak and Pokrovsky (1981).

surfaces. As the iteration proceeds, the surfaces are filled up ergodically. Some of the orbits appear to be broken curves, because the iterations were stopped before the curve was 'filled up'. The fixed points at $\pm (1, 1)$ are always hyperbolic and unstable. In addition to the KAM curves there are chaotic orbits and Birkhoff (1917) islands, as is quite usual for two-dimensional mappings. If the iteration is started near an elliptic fixed point, the orbit will remain near the FP on a KAM surface. If the iteration is started near a hyperbolic FP, the procedure will eventually carry the orbit away from the FP.

The stability of FP can be investigated by studying the tangent space orbits $(\delta x_n, \delta y_n)$ (Greene 1979). The tangent space orbits at the points (x_n, y_n) and (x_{n+1}, y_{n+1}) are related through a matrix M_n :

$$(\delta x_{n+1}, \delta y_{n+1}) = M_n(\delta x_n, \delta y_n)$$

$$M_n = \begin{pmatrix} 3ax_n^2 + 2 - a & -1 \\ 1 & 0 \end{pmatrix}$$
(2.1)

det M_n is the Jacobian of the transformation. We note that det M_n is -1, so the transformation is indeed area-preserving. The fixed point at (0, 0) is stable as long as

$$|\mathrm{Tr}\,M_n| < 2 \tag{2.2}$$

at this point (Greene 1979). We see that the fixed point becomes unstable for a = 4. Figure 3 shows orbits calculated for a = 3.98 and a = 4.02. Note that the KAM surfaces have rotated 90° compared with figure 2. The fixed point bifurcates into a 2-cycle. It is not difficult to find the 2-cycle FP analytically from (1.4). The equation

$$(x, y) = T^{2}(x, y)$$
 (2.3)



Figure 3. (a) Orbits calculated for a = 3.98. This value is slightly below the first bifurcation point, a = 4. (b) Orbits calculated for a = 4.02. The fixed point has bifurcated into a 2-cycle. The original fixed point at (0, 0) has become unstable (hyperbolic).

has the solutions

$$(x, y) = \pm(\sqrt{1-4/a}, -\sqrt{1-4/a}).$$
 (2.4)

In general, the equations for higher-order limit cycle fixed points cannot be found analytically. After the bifurcation the original fixed point is hyperbolic. The new elliptic fixed points are surrounded by closed orbits of their own, forming two 'islands'. As the iteration proceeds, these islands are visited successively. At a = 4.02 there

are still KAM orbits encircling both FP. At larger values of a these orbits will eventually disappear. This process has been studied in detail by Greene (1979) and by Shenker and Kandanoff (1981).

2.2. The 'starfish'

The stability of an N-cycle orbit x_1, x_2, \ldots, x_N depends on the matrix \mathcal{M} :

$$(\delta x_N, \delta y_N) = \mathcal{M}(\delta x_0, \delta y_0)$$

$$\mathcal{M} = \prod_{n=1}^N M_n = \prod_{n=1}^N \binom{3ax_n^2 + 2 - a \quad -1}{1 \quad 0}.$$
 (2.5)

The *N*-cycle is stable if $|\text{Tr }\mathcal{M}| < 2$. For the 2-cycle with x_n given by (2.4),

$$Tr \mathcal{M} = 4a^2 - 40a + 98. \tag{2.6}$$

The 2-cycle becomes marginally unstable at a = 5, since (2.6) has a minimum with Tr $\mathcal{M} = -2$ for this value of a. We do not expect bifurcation at a = 5, since the 2-cycle is stable also for a > 5.

Figure 4 shows the orbits for a = 4.995 and a = 5.005. Only half the points are shown (those with x > 0, y < 0). For each point (x, y) plotted there is a symmetric point at (y, x) not shown. As a increases beyond 4.02 (figure 3), the two fixed points move away from each other, and the surrounding KAM orbits become more and more deformed. For instance, it seems that one of the orbits is almost quadratic. As the marginally stable value of a is approached, the square orbit seems to get closer and closer to the FP, and at a = 5 it rotates 45° (compare 4(a) and 4(b)). A little further away there is a series of four islands. The islands belong pairwise to two 4-cycles. We have not investigated the history of these islands and the 4-cycle points inside them for smaller values of a.

All of these fixed points are surrounded by a chaotic orbit. For a = 4.995 the orbits shown are one-dimensional KAM surfaces surrounded by a chaotic orbit (the scattered points). For a = 5.005 we found a 'starfish' formed by a very irregular chaotic orbit. The scattered points outside this orbit belong to a separate chaotic orbit. Presumably there are regular and irregular 'starfish' orbits both for a < 5 and a > 5.

We have followed the 4-cycle fixed points numerically for larger values of a. It turns out that these cycles bifurcate *ad infinitum* in a way characterised by universal numbers. The first bifurcation (from 4-cycle to 8-cycle) takes place at a = 5.07575... and the last at a = 5.084593... Since this series of bifurcations is structurally identical to the one which will be described in the remaining part of this section, we shall not discuss it further here.

2.3. The 'banana split'

Let us return to the original 2-cycle. Nothing dramatic happend to it at a = 5. By inspection of (2.6) we see that Tr $\mathcal{M} = +2$ for a = 6, so the 2-cycle becomes unstable at this point. Does the 2-cycle bifurcate into a 4-cycle? Figure 5 shows orbits calculated for a = 5.98 and a = 6.02; again, only half the points are shown. For a = 5.98 the fixed point is surrounded by stable KAM surfaces, by higher-order islands and by chaotic orbits in the usual way. The orbits are stretched in one direction, indicating



Figure 4. (a) The 'starfish' (a = 4.995). The fixed point in the middle is stable, but a is approaching the value a = 5, where it becomes *marginally* unstable. (b) The 'starfish' (a = 5.005). The fixed point has passed through the metastable point. Note that the square orbit in the middle has rotated 45° compared with figure 4(a). Note also the irregular orbit forming the arms of the 'starfish'. The scattered points outside this orbit belong to a separate chaotic orbit.

that a bifurcation is about to take place. The figure has a clear resemblance to a banana. Indeed, the fixed points splits (figure 5(b)) into *two* elliptic fixed points, surrounded by KAM orbits with a hyperbolic FP in between. However, the new fixed points belong to two different, but symmetric, 2-cycles and not to the same 4-cycle.



Figure 5. (a) The 'banana' (a = 5.98). The 2-cycle is approaching instability (a = 6). (b) The 'banana split' (a = 6.02). The 2-cycle has not bifurcated, but has split into two 2-cycles.

We call this unusual behaviour, which is distinctly different from a bifurcation, the 'banana split'.

2.4. The symmetry curve

The fixed points belonging to higher-order cycles cannot be found analytically. A method developed by Greene (1979) makes the numerical search easier. It might seem that to find fixed points one should search the full (x, y) space. However,

Greene's method shows that *two* of the fixed points, belonging to a 2N-cycle, are on a simple one-dimensional curve in (x, y) space (see also Bountis 1981). The remaining points follow automatically by iteration.



Figure 6. The 'dominant' symmetry curve $y = \frac{1}{2}ax(x^2-1)+x$ for three different values of a ($a = \frac{8}{5}$, a = 4 and a = 6.02, related to figures 2, 3 and 5(b) respectively). The dots on the curve with a = 6.02 show the fixed points of the 'banana split'. Points marked ' α ' form a 2-cycle, whereas points marked ' β ' are fixed points of another 2-cycle.



Figure 7. Bifurcation of the 2-cycle into a 4-cycle orbit: (a) a = 6.24; (b) a = 6.245.



Figure 8. Period-doubling bifurcation of the 4-cycle into an 8-cycle. (a), (b) a = 6.27. The bifurcation has not yet taken place. Note the very different shapes of orbits around the two points belonging to the 4-cycle. As usual the limit cycle points are surrounded by KAM orbits, Birkhoff islands and chaotic orbits.

We note that the transformation T (equation (1.4)) can be split into the product of two involutions:

$$T = I_2 I_1$$

$$I_1: \begin{pmatrix} x_n \\ y_n \end{pmatrix} \rightarrow \begin{pmatrix} x_n \\ -y_n + a x_n (x_n^2 - 1) + 2 x_n \end{pmatrix}$$

$$I_2: \begin{pmatrix} x_n \\ y_n \end{pmatrix} \rightarrow \begin{pmatrix} y_n \\ x_n \end{pmatrix}$$
(2.7)

where

$$I_1^2 = I_2^2 = 1.$$

Periodic orbits of T can be found by choosing initial conditions (x_1, y_1) which are



Figure 8. Period-doubling bifurcation of the 4-cycle into an 8-cycle. (c), (d) a = 6.2716. The 4-cycle has bifurcated into an 8-cycle. The two limit cycle points surrounded by 'two-dimensional' orbits are no longer on the symmetry curve, whereas the limit cycle points surrounded by 'one-dimensional' orbits are on the symmetry curve.

fixed points of I_1 :

$$(x_1, y_1) = I_1(x_1, y_1) \tag{2.8a}$$

or

$$2y_1 = ax_1(x_1^2 - 1) + 2x_1. (2.8b)$$

This curve contains either two or no points of any 2N-cycle orbit. If it contains the point (x_1, y_1) , it also contains the point (x_{N+1}, y_{N+1}) . Following Bountis and Greene *et al* we call the curve (2.8) the 'dominant' symmetry curve.

It should be noted that a curve of the form (2.8) with x and y interchanged also describes the symmetry of the mapping. This is seen by rewriting $T = I_2I_1 = (I_2I_1I_2)I_2$ where the fixed point line of the involution $I'_1 = I_2I_1I_2$ is the curve (2.8) reflected in the y = x line. It indicates that all 2N-periodic orbits with pairs of points on the symmetry curves are symmetric about the 45° line in the plane. For a further discussion

of symmetry properties of Hamiltonian maps, see Greene *et al* (1981). In figure 6 the symmetry curve (2.8) is shown for different values of the parameter *a*. The dots on the curve with a = 6.02 are fixed points of the mapping, as shown in figure 5(b) ('banana split'). Points marked ' α ' form one 2-cycle and points marked ' β ' another 2-cycle. Curves for values of *a* slightly higher than a = 6.02 (related to further bifurcations) are very close to this curve.

2.5. Further bifurcations

Higher-order limit cycles and their bifurcations are found by the following procedure. Suppose we have found an N-cycle for a given value of a and wish to find the N-cycle for a slightly different value of a. A point (x_1, y_1) on the symmetry curve near the previous fixed point is chosen and iterated N times, ending up at a point (x_{1+N}, y_{1+N}) which is different from (x_1, y_1) . A new point (x'_1, y'_1) on the symmetry curve is chosen, and the procedure is iterated until convergence using a Newton iteration technique.

If we want to find the bifurcation point, the trace of \mathcal{M} (equation (2.5)) is calculated. If $|\operatorname{Tr} \mathcal{M}| < 2$ the limit cycle is stable. If $|\operatorname{Tr} \mathcal{M}| > 2$ it is unstable. If $|\operatorname{Tr} \mathcal{M}| < 2$ we choose a larger value of a and find a new N-cycle following the procedure above, and $\operatorname{Tr} \mathcal{M}$ is calculated again. The double iteration process is continued until a limit cycle with $|\operatorname{Tr} \mathcal{M}| = 2$ has been found. This defines the bifurcation point. The point must be determined with high precision in order to obtain a good estimate of the universal constants. We found this bifurcation series to an accuracy of 16 digits. The procedure seems complicated, but can actually be performed in a few minutes on a desk computer.

The bifurcation of the 2-cycle is found to take place at $a_1 = 6.24264...$ This time it is a real bifurcation leading to a 4-cycle. Figure 7(a) shows the neighbourhood of one of the 2-cycle fixed points before the bifurcation (a = 6.24), with the usual KAM orbits and Birkhoff islands. Figure 7(b) shows the situation after the bifurcation (a = 6.245).

The next bifurcation occurs at $a_2 = 6.270\ 85...$ Figures 8(a) and 8(b) show the behaviour of the orbits around the two 4-cycle points, which bifurcated out of the 2-cycle in figure 7(b). Both points are on the symmetry curve. Note that the orbits around one of the 4-cycle points are stretched, while the orbits around the other point retain their two-dimensional character. The orbits of figures 8(a) and 8(b) were calculated for a value of a slightly below the bifurcation point a_2 . The scale of figure 8 is much smaller than those in the previous figures. After the bifurcation, both the 'flat' fixed points are on the symmetry curve for the 8-cycle (figure 8(c)). The two elliptic fixed points within the two-dimensional orbits lose their symmetry and bifurcate away from the symmetry curve (figure 8(d)). Note that this bifurcation takes place along the y axis.

The story now repeats itself again and again on a smaller and smaller scale. The two symmetry points on the 8-cycle behave differently: the surroundings of the points become one- and two-dimensional, respectively. The two-dimensional point loses its symmetry; the one-dimensional fixed point splits into two fixed points on the symmetry curve of the bifurcated orbit.

Figure 9 shows the *N*-cycle fixed points as a function of *a*. The bifurcations of cycles 2^{0} to 2^{1} , 2^{1} to 2^{2} are shown in figure 9(*a*) and 2^{2} to 2^{3} , 2^{3} to 2^{4} , 2^{4} to 2^{5} in figure 9(*b*). The marginal stability of the 2-cycle at a = 5 causes no irregularity, because this cycle is also stable for a > 5. At a = 6 the 'banana split' occurs, and we



Figure 9. Positions of the fixed points (x values) as a function of a. The observable bifurcations are in (a) from period 1 to 2, 2 to 4 and in (b) from period 4 to 8, 8 to 16, 16 to 32. At a = 6 the 2-cycle splits into two 2-cycles (the 'banana split', figure 5). The full curve shows the symmetry road, which always leads to wide fork bifurcations.

follow only one branch of this splitting. The bifurcation of fixed points away from the symmetry curve takes place along the y axis and does not cause a fork in the diagram. The bifurcation of the one-dimensional points, on the other hand, leads to wide forks defining a symmetry road (cf Bountis 1981), marked by the full curve.

Table 1 shows the values as a_k as a function of k. The distance between the symmetry points, d_k , at the bifurcation point is also shown.

We find that the Feigenbaum ratio

$$\delta_k = \frac{a_{k-2} - a_{k-1}}{a_{k-1} - a_k}$$

approaches the value $\delta = 8.721\ 09\ldots$ for large numbers k. This value is the same as found for other two-dimensional conservative mappings, such as the Hénon mapping. The quantity

Table 1. a_k are the values of a, where the 2^k -cycles bifurcate into 2^{k+1} -cycles; d_k is the distance between the two points x_0 and $x_{N/2}$ on the *N*-cycle at the bifurcation point. δ_k and α_k are the 'Feigenbaum ratios', which approach the universal values $\delta = 8.721\,096\ldots \alpha = 4.018\ldots$

Period 2^k	a_k	d_k	δ_k	α_k
$2^1 = 2$	6.242 640 687 119 285	1.625 039 840 13		
$2^2 = 4$	6.270 857 564 384 179	$5.08756157266 \times 10^{-2}$		
$2^3 = 8$	6.274 095 612 259 405	$1.287\ 251\ 652\ 77 \times 10^{-2}$	8.714 160 3	3.952 26
$2^4 = 16$	6,274 466 973 111 542	$3.17415687178 \times 10^{-3}$	8.719 413 3	4.055 41
$2^5 = 32$	6.274 509 555 467 522	$7.915\ 472\ 012\ 88 imes 10^{-4}$	8.721 009 2	4.010 06
$2^6 = 64$	6.274 514 438 163 561	$1.96894475993 imes 10^{-4}$	8.721 074 5	4.020 15
$2^7 = 128$	6.274 514 998 035 401	$4.90084310049 \times 10^{-5}$	8.721 095 9	4.017 56
$2^8 = 256$	6.274 515 062 232 811	$1.21965982463 \times 10^{-5}$	8.721 096 9	4.018 20
$2^9 = 512$	6.274 515 069 593 974	$3.03545604373 \times 10^{-6}$	8.721 096 5	4.018 04

gives the reduction of scale from the (k-1)th bifurcation to the kth bifurcation. We find $\alpha_k \rightarrow \alpha = 4.0180...$ as $k \rightarrow \infty$. Both values are different from the Feigenbaum numbers for one-dimensional mappings or two-dimensional dissipative mappings ($\delta = 4.669\ 21..., \alpha = 2.502\ 90...$).

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