# Polarisation and transition by breaking of analyticity in a one-dimensional model for incommensurate structures in an electric field



1987 J. Phys. A: Math. Gen. 20 4873

(http://iopscience.iop.org/0305-4470/20/14/026)

J. Phys. A: Math. Gen. **20** (1987) 4873–4889. Printed in the UK

# Polarisation and transition by breaking of analyticity in a one-dimensional model for incommensurate structures in an electric field

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Received 28 July 1986

**Abstract.** We study the transition by breaking of analyticity on a variation of the Frenkel-Kontorova (FK) model with two sublattices, where a parameter $E$ simulates the role of the electric field in certain incommensurate structures. For the incommensurate ground states, the polarisation response $\delta(E)$ at fixed incommensurability ratio $\zeta$ and as a function of the electric field $E$ is found to be a smooth analytic curve when the parameter $K$ which characterises the coupling to the lattice is small enough, while it becomes the sum of a smooth analytic curve and a devil's staircase for larger values of $K$. The change between these two regimes corresponds to the crossing of the critical line $K_c(E, \zeta)$ of the transition by breaking of analyticity. It is shown that at fixed $\zeta$ irrational, this curve is not differentiable at an infinite set of cusps which form a Cantor set. These cusps are shown to be the terminating points of the lines corresponding to the edges of the plateaux of the devil's staircase $\delta(E)$ at fixed $\zeta$.

## 1. Introduction

A variation of the one-dimensional discrete Frenkel-Kontorova (FK) model has been recently studied (Aubry *et al* 1985). This model involves an additional term which breaks the symmetry operation that transforms the sublattice of atoms with even indices into the sublattice of atoms with odd indices. This term has been introduced in order to simulate an applied external constant electric field on thiourea which also breaks a symmetry between two equivalent sublattices (Durand *et al* 1984) (for a review, see Denoyer and Currat (1986)). The model was chosen to be one dimensional because the direction of the wavevector of the incommensurate modulation in thiourea is the simple crystallographic axis $b$. It is represented by a classical elastic chain of $N$ atoms subjected to both a periodic potential and a staggered field. The free energy of this model at 0 K is

$$\begin{aligned}\Phi(\{u_j\}) &= \sum_j [1/2(u_{j+1}-u_j)^2 - \mu(u_{j+1}-u_j) + KV(u_j) + (-1)^j E u_j] \\ &= \sum_j (u_{j+1}, u_j) \qquad (1)\end{aligned}$$

where $u_j$ is the position of the $j$th atom, $\mu$ is a tensile force, $K$ is the amplitude of the periodic potential which creates the incommensurate modulation ($2a$ is its period)

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and $E$ is the symmetry breaking term, which plays the role of the electric field in thiourea—which from now on we will call the 'electric field'. In the physical system, $u_{2j}$ and $u_{2j+1}$ represent the phase of the incommensurate modulation on the even and odd sublattices in the $j$th unit cell, respectively.

The exact phase diagram for the ground states of this model has then been calculated in the case where the potential $V$ is piecewise parabolic of the form

$$V(u_{2j}) + V(u_{2j+1} + a)$$

and the atoms of the second sublattice are subjected to the same periodic potential as the atoms of the first but shifted by half a period (figure 1($a$)).

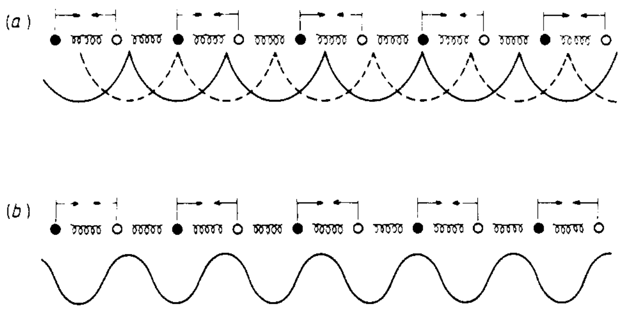

**Figure 1.** Scheme of model (1) representing a one-dimensional elastic chain of atoms subjected to a staggered electric field and ($a$) the periodic piecewise parabolic potential of Aubry *et al* (1985) or ($b$) a cosine potential.

A piecewise parabolic potential is indeed a good approximation for a smooth sinusoidal or quasi-sinusoidal periodic potential with a large amplitude $K$ because then the atoms essentially lie in the regions close to its minima, where the periodic potential is practically parabolic (figure 1($b$)). However it has been already pointed out in earlier papers that a piecewise parabolic potential is not appropriate for the description of situations where the amplitude of $V(x)$ is small. This is due to the fact that the existence of singularities where $V(x)$ is not differentiable forbids the existence of incommensurate 'analytic' ground states. The physical consequence is that the ground states of model (1) where $V(x)$ is a piecewise parabolic potential are always pinned by the lattice, while when $V(x)$ is an analytic potential which has a small amplitude, the incommensurate ground states can become unpinned and there is a gapless phason mode which is the phonon corresponding to the zero-frequency vibrations of the phase of the incommensurate structure. In addition, in the first case the devil's staircases (Mandelbrot 1977, 1982) which are found are always complete (Aubry 1978) while in the second case they may become incomplete (Aubry 1978, 1980a, b). Briefly, we recall that for a complete (incomplete) devil's staircase the total measure of the steps is (not) the full Lebesgue measure. A 'harmless' staircase has a finite number of steps (Villain and Gordon 1980, Axel and Aubry 1981).

Therefore, the analysis and the calculations of the phase diagram of model (1) with the approximation of a piecewise parabolic potential remain qualitatively valid for an analytic potential in the parameter region where the incommensurate ground states are *non-analytic*, which mathematically means that the configuration coordinates vary non-analytically with respect to the phase of the wave modulation or, physically, that the ground states are pinned by the lattice. In this paper, we study also the parameter region where the ground states are *analytic*. We find as expected that a transition by breaking of analyticity occurs for the incommensurate ground states of this model when the amplitude $K$ of the analytic periodic potential $V(x)$ increases. We also find an important qualitative change of the polarisation response to an electric field in the analytic region. Instead of a polarisation $\delta(E)$ function of the electric field $E$ which is the sum of an analytic part (more precisely a linear curve) and of a devil's staircase, this curve $\delta(E)$ simply becomes a smooth analytic curve. We analyse the transition between these two regimes. The curve $K_c(E, \zeta)$ which yields the critical value of the potential amplitude $K$ where the transition by breaking of analyticity occurs, as a function of the electric field $E$, is studied for a fixed incommensurability ratio or rotation number. We find that this curve exhibits an unusual behaviour with an infinite set of cusps where it is not differentiable. The set of points corresponding to these cusps is likely to have a Cantor set structure.

As for the FK model, our study here is done with the simple analytic periodic potential:

$$V(x) = (1 - \cos x) \tag{2}$$

where the period $2a$ is now equal to $2\pi$.

## 2. Modified standard map

The study of the transition by breaking of analyticity is done by introducing an associated map in the same way as for the FK model (Aubry 1978, 1983, 1984). The energy form (1) can be considered as the action of a dynamical system, so that each configuration $\{u_j\}$ which is a solution of the extremalisation equations of (1) can be associated with a trajectory of a map.

The extremalisation equations of (1) are

$$\partial\Phi(\{u_j\})/\partial u_j = -u_{j+1} - u_{j-1} + 2u_j + K \sin u_j + (-1)^j E = 0. \tag{3}$$

With the angle variable modulo $2\pi$

$$\theta_j = u_j \tag{4a}$$

and its conjugate variable (action)

$$I_j = u_j - u_{j-1} \tag{4b}$$

equation (3) can be written again as

$$I_{j+1} = I_j + K \sin \theta_j + (-1)^j E \tag{5a}$$

$$\theta_{j+1} = \theta_j + I_{j+1}. \tag{5b}$$

When the electric field $E$ is zero, equations (5) yield exactly the 'standard map', i.e. the discretised Hamilton equations of the pendulum.

A solution of (3) can be obtained by alternate applications of the map $T^+$

$$(I_{2j+1}, \theta_{2j+1}) = T^+(I_{2j}, \theta_{2j}) \tag{6a}$$

defined by

$$I_{2j+1} = I_{2j} + K \sin \theta_{2j} + E \tag{6b}$$

$$\theta_{2j+1} = \theta_{2j} + I_{2j+1} \tag{6c}$$

and of the map $T^-$

$$(I_{2j}, \theta_{2j}) = T^-(I_{2j-1}, \theta_{2j-1}) \tag{7a}$$

defined by

$$I_{2j} = I_{2j-1} + K \sin \theta_{2j-1} - E \tag{7b}$$

$$\theta_{2j} = \theta_{2j-1} + I_{2j}. \tag{7c}$$

$T^+$ and $T^-$ are two dimensional, invertible, frontier and area preserving maps of the cylinder $I \times \theta$ onto itself as the standard map, which is obtained for $E = 0$. Their product $T = T^- T^+$ generates trajectories $(I_{2j}, \theta_{2j})$ which correspond to the configurations $\{u_{2j}\}$ of the even sublattice

$$I_{2j+2} = I_{2j} + K \sin \theta_{2j} - E + K \sin(\theta_{2j} + K \sin \theta_{2j} + E + I_{2j}) \tag{8a}$$

$$\theta_{2j+2} = \theta_{2j} + 2I_{2j} + 2K \sin \theta_{2j} + E + K \sin(\theta_{2j} + K \sin \theta_{2j} + E + I_{2j}). \tag{8b}$$

Let us note that the change of variables

$$I'_n = I_n + (-1)^n E/2 \tag{9a}$$

$$\theta'_n = \theta_n + (-1)^n E/4 \tag{9b}$$

which leaves the 'Laplacian' invariant transforms equations (5) into

$$I'_{j+1} = I'_j + K \sin[\theta'_j - (-1)^j E/4] \tag{10a}$$

$$\theta'_{j+1} = \theta'_j + I'_{j+1}. \tag{10b}$$

The free energy is then

$$\Phi = \sum_{j=1}^{N} \left(\tfrac{1}{2} I'^2_{j+1} - \mu I'_{j+1} - K \cos\left(\theta'_j - (-1)^j \frac{E}{4}\right)\right) \tag{11}$$

which is identical with the normal FK model with the even and odd sublattice seeing a potential shifted by $E/2$. In Aubry *et al* (1985) $E = 2\pi$.

The trajectories of transformation (10) are unchanged by changing $E$ into $E + 8\pi$. In fact, the map (10) is invariant by a change of the electric field $E$ into $E + 4\pi$ and a change of the variable $\theta'_j$ into $\theta''_j + \pi$. In addition, changing $E$ into $-E$ is equivalent to exchanging the role of the even and odd sublattices. Therefore, it is sufficient to study the transition by breaking of analyticity for an electric field $E$ in the symmetric interval $[0, 4\pi]$ only.

By definition a twist map has the property that the image of a vertical straight line $x = \theta$, where $\theta$ is an arbitrary constant, is a graph which means that the equation of this line can be put under the form $y = g(x)$. When $K < 2$ equation (8*b*) shows that $\theta_{2j+2}$ is a monotonic increasing function of $I_{2j}$. Then for fixed $\theta_{2j}$, $I_{2j}$ is a univalued function of $\theta_{2j+1}$ which implies that $I_{2j+2}$ can also be written as a univalued function for $\theta_{2j+2}$. This property proves that $T$ fulfils the twist condition for $K < 2$.

Therefore when $K < 2$, the Kolmogorov-Arnol'd-Moser (KAM) theorem (Moser 1973, Lichtenberg and Lieberman 1983) applies for the map $T$. It predicts that for most irrational $\zeta$, there exists a non-zero critical value $K_c(E, \zeta)$, such that for $K < K_c(E, \zeta)$, the dynamical system is almost integrable and there exists an invariant torus on the cylinder $I \times \theta$. Note that, strictly speaking, the KAM theorem gives an upper bound for $K$ which is very small, but in practice numerical observations indicate that it generally applies much beyond this theoretical value.

The trajectories of the associated map (6) and (7) correspond to stationary configurations of model (1) having extremal energy. The subset of these trajectories which correspond to the ground states of model (1) (which have minimum energy) can be studied using the same methods as in Aubry and André (1980), Aubry and Le Daeron (1983) and Aubry (1983, 1984, 1986) but for each sublattice separately. It suffices to note that

(i) the fundamental lemma also applies to the minimum energy configurations of model (1),

(ii) the set of minimum energy configurations $\{u_j\}$ is invariant by the Abelian group of transformations, the generators of which are

$$g_2(\{u_j\}) = \{u_{j+2}\} \tag{12a}$$

$$g_0(\{u_j\}) = \{u_j + 2\pi\}. \tag{12b}$$

Then the same theorems hold for each sublattice as in the case where there exists only one sublattice (FK model). In particular, for each irrational number $\zeta$ and electric field $E$, there exists two hull functions $f_1(x)$ and $f_2(x)$ which are monotonic increasing and either left-continuous ($f_1^-(x)$ and $f_2^-(x)$) or right-continuous ($f_1^+(x)$ and $f_2^+(x)$) and such that the functions $g_1(x) = f_1(x) - x$ and $g_2(x) = f_2(x) - x$ are $2\pi$ periodic. Then, for any incommensurate ground state with incommensurability ratio

$$2l/2\pi = (1/2\pi) \lim_{N-N' \to \infty} [(u_N - u_{N'})/(N - N')] \tag{13}$$

there exists a determination for the couple of hull functions which are both right-continuous ($f_1^+$ and $f_2^+$) or left-continuous ($f_1^-$ and $f_2^-$) and a phase $\alpha$ such that

$$u_{2j} = f_1(2jl + \alpha) \tag{14a}$$

$$u_{2j+1} = f_2((2j+1)l + \alpha) \tag{14b}$$

where $l$ is the atomic mean distance between consecutive atoms. When there exists a KAM torus for the associated map $T$ with rotation number $\zeta$, the same theorems as for the FK model (Aubry 1983, 1986) apply: they prove that the trajectories of this KAM torus correspond to the incommensurate ground states with incommensurability ratio $\zeta$ and vice versa.

As for the FK model, let us recall and emphasise that, although the transition by breaking of analyticity of the incommensurate ground states of model (1) corresponds to the breaking of the associated torus, it *does not* imply that the incommensurate ground state becomes chaotic. In fact, it becomes *defectible*, while remaining incommensurate. The reader is referred to our previous papers or to the review paper (Aubry 1986) for more detailed explanations.

## 3. Study of the transition by breaking of analyticity as a function of the electric field

### *3.1. Method*

Our analysis is a variation of the method Greene used (Greene 1979) for the standard map. He has shown in this case that the study of the breaking of a KAM torus having an irrational rotation number $\zeta$ when the chaos constant $K$ increases can be done by analysing the behaviour of the neighbouring periodic cycles having for rotation number

$\zeta_n = r_n/s_n$, the rational truncations (or convergents) of the continued fraction expansion of $\zeta$ (see, for example, Hardy and Wright 1979)

$$\zeta = a_0 + \cfrac{1}{a_1 + \cfrac{1}{a_2 + \cfrac{1}{\dots + \cfrac{1}{a_n + \dots}}}} = \lim_{n\to\infty} r_n/s_n. \tag{15a}$$

The sequence of integers $a_n$ is unique and determines recursively the principal convergents $\zeta_n = r_n/s_n$ by the well known formula

$$\zeta_n = r_n/s_n = (a_n r_{n-1} + r_{n-2})/(a_n s_{n-1} + s_{n-2}) \tag{15b}$$

with the initial conditions $\zeta_0 = a_0/1$ and $\zeta_1 = (a_0 a_1 + 1)/a_1$.

We mostly studied in this paper the inverse golden mean $\zeta = \tau^{-1} = (\sqrt{5}-1)/2$, for which $a_0 = 0$ and $a_j = 1$ for all $j \neq 0$. This number can be considered the 'most irrational' because its continued fraction expansion converges most slowly to its limit and the problem of small denominators, with it, is minimal. It has the following principal convergents $r_n/s_n$:

$$\zeta_1 = 0 \quad \zeta_2 = \tfrac{1}{2} \quad \zeta_3 = \tfrac{2}{3} \quad \zeta_4 = \tfrac{3}{5} \quad \zeta_5 = \tfrac{5}{8} \quad \zeta_6 = \tfrac{8}{13} \qquad \dots . \tag{16}$$

For the standard map, when $K$ increases, the invariant tori are gradually destabilised and chaotic trajectories can reach increasingly large regions of phase space. There is good evidence (see, for instance, Lichtenberg and Lieberman (1983 p 217)) that the last torus to live is the 'golden' torus for which the critical value of $K$ is $K_c = 0.961\,536$ in the limit $n \to \infty$. Then 'connected stochasticity' takes place.

We use a variation of Greene's method to study its destabilisation when $K$ increases in the modified mapping (1) as a function of the electric field.

For a given $\zeta_n$ and a given electric field $E$, we find the commensurate ground state, the commensurability ratio of which is $l/2a = \zeta_n = r_n/s_n$. The associated trajectory by transformation $T$ is a periodic cycle with period $s_n$. This ground state can be found using a finite system with periodic boundary conditions

$$u_{2s_n} = u_0 + 4\pi r_n. \tag{17}$$

Then let $M$ be the product of the Jacobian matrices of $T$ along the periodic cycle of rotation number $\zeta_n = r_n/s_n$:

$$M = \prod_{j=1}^{s_n} \begin{pmatrix} 1 & K\cos\theta_j \\ 1 & 1 + K\cos\theta_j \end{pmatrix}. \tag{18a}$$

The residue $R$ of this periodic cycle is by definition

$$R = \tfrac{1}{4}(2 - \mathrm{Tr}(M)) \tag{18b}$$

and the trajectory is stable when $|R| < 0.25$ (Greene's criterion).

Periodic cycles corresponding to physically stable configurations (ground states) have been shown to be necessarily hyperbolic without reflection (Aubry 1983, 1984) (in other words, the physical system and the dynamical system have inverse stabilities), their residue is then negative or zero. For small values of $K$, $R$ is close to zero, then its modulus increases with $K$. When $s_n$ is large (and in the incommensurate limit), the breakdown of the periodic cycle occurs with a very sharp transition for $R=-0.25$. When $s_n$ is smaller the behaviour is a crossover one and the observed variation of $R$ is much smoother. For reasons of continuity the curves $K_c(E, \zeta_n)$ are calculated for this same value $R=-0.25$. When $n$ goes to $\infty$, this crossover value converges to the critical value $K_c(E, \zeta)$ at which the transition by breaking of analyticity occurs.

The determination of the commensurate ground state with the boundary condition (17) is done by a combination of the gradient method (already used in Peyrard and Aubry (1983)) and of a Newton method (Shenker and Kadanoff 1982, Coppersmith and Fisher 1983) as in de Seze and Aubry (1984).

The gradient method consists in performing the integration of the equation

$$\mathrm{d}u_j(\tau)/\mathrm{d}\tau = -\partial\Phi(\{u_j(\tau)\})/\partial u_j \tag{19}$$

where $\tau$ is a continuous variable. For $\tau$ going to infinity, $u_j(\tau)$ converges to a stationary solution which is $\tau$ independent and fulfils $\partial\Phi(\{u_j\})/\partial u_j=0$ which is equation (3). Starting from an initial configuration $\{u_j\}$ fulfilling the boundary conditions (17), the final state also fulfils the same boundary conditions and corresponds to the 'relaxed' initial state.

By contrast with the original Greene method which yields stable and unstable configurations as well, this method has the advantage that the limit configuration which is obtained is necessarily one of the *metastable configurations* of the dynamical system which are the only ones having physical interest. If the initial configuration has been well chosen, it is the physical ground state. However, the limit configuration can be also chaotic (Peyrard and Aubry 1983) when the initial state is chosen at random.

However, since the numerical convergence of the gradient method is rather slow, especially in the vicinity of the crossover, it is more efficient to only start the numerical procedure with this method in order to get a rough but reasonable approximation of the solution of (3), and to terminate the convergence with a Newton method consisting in solving recursively the system of linearised equations

$$\frac{\partial\Phi(\{u_j^{(n)}\})}{\partial u_j}+\frac{\partial^2\Phi(\{u_j^{(n)}\})}{\partial u_j\,\partial u_i}(u_j^{(n+1)}-u_j^{(n)})=0. \tag{20}$$

This second method does not necessarily converge to a metastable configuration but since it is started on an initial state which is rather close to a metastable configuration, it will converge accurately to this configuration. In practice, after a few iterations, the sequence of configurations $\{u_j^{(n)}\}$ converges to a solution of (3) with an accuracy of $10^{-9}$ at least.

A good choice of the initial configuration $\{u_j^{(0)}\}$ for finding the ground state of the FK model is $u_j^{(0)}=jl+\alpha$ which corresponds to the unmodulated chain. In model (1) where there exists two different sublattices, the existence of two different hull functions $f_1$ and $f_2$ allows one to show that an appropriate initial configuration $\{u_j^{(0)}\}$ is given by

$$u_j^{(0)}=jl+\alpha+(-1)^j\delta^{(0)}/2 \tag{21}$$

where $\delta^{(0)}$ is some unknown initial relative phase shift between the even and odd sublattices.

The limit configuration may depend on this phase shift $\delta^{(0)}$. This result is easily understood because the initial phase shift $\delta^{(0)}$ determines the wells of the periodic potential $V(x)$ above which the atoms are initially located. If the amplitude of $V(x)$ is large enough, the atoms may always stay in their initial well. However, when $\zeta$ is close to an irrational number and $K$ small enough, the limit is unique (apart from a global translation of the chain). For the FK model, we proved that this situation occurs for the analytic incommensurate structures. This proof extends to the present model (1). This property has been called 'undefectibility' (Aubry 1978).

In our numerical calculations, we vary the initial phase shift. When we find several limit configurations, the minimisation of the energy (1) allows one to determine the ground state. This situation corresponds to first-order transitions in the commensurate cases as are shown below.

### *3.2. Results*

We study the generation of $K_c(E, \zeta)$.

(i) For the first convergents of $\tau^{-1} = (\sqrt{5}-1)/2$

$$\zeta_0 = \tfrac{0}{1} \quad \zeta_1 = \tfrac{1}{1} \quad \zeta_2 = \tfrac{1}{2} \quad \zeta_3 = \tfrac{2}{3} \quad \zeta_4 = \tfrac{3}{5} \quad \zeta_5 = \tfrac{5}{8} \quad \zeta_6 = \tfrac{8}{13}$$

for which the results of the numerical calculations are shown in figures 2-7.

(ii) For an irrational number $\zeta'$ with a continued fraction expansion beginning with $a'_0 = 0$, $a'_1 = 1$, $a'_2 = 2$, $a'_3 = 1$, $a'_4 = 3$ and convergents

$$\zeta'_0 = \tfrac{0}{1} \quad \zeta'_1 = \tfrac{1}{1} \quad \zeta'_2 = \tfrac{2}{3} \quad \zeta'_3 = \tfrac{3}{4} \quad \zeta'_4 = \tfrac{11}{15}$$

for which the results are in figures 3 and 4 and also figures 8 and 9.

The results clearly show the following.

(i) $K_c(E, r_n/s_n)$ defined by $R = -0.25$ is a continuous curve having $s_n$ discontinuities of its derivative for $E$ in the interval $[0, 4\pi[$. At these cusps the two parts of the curve

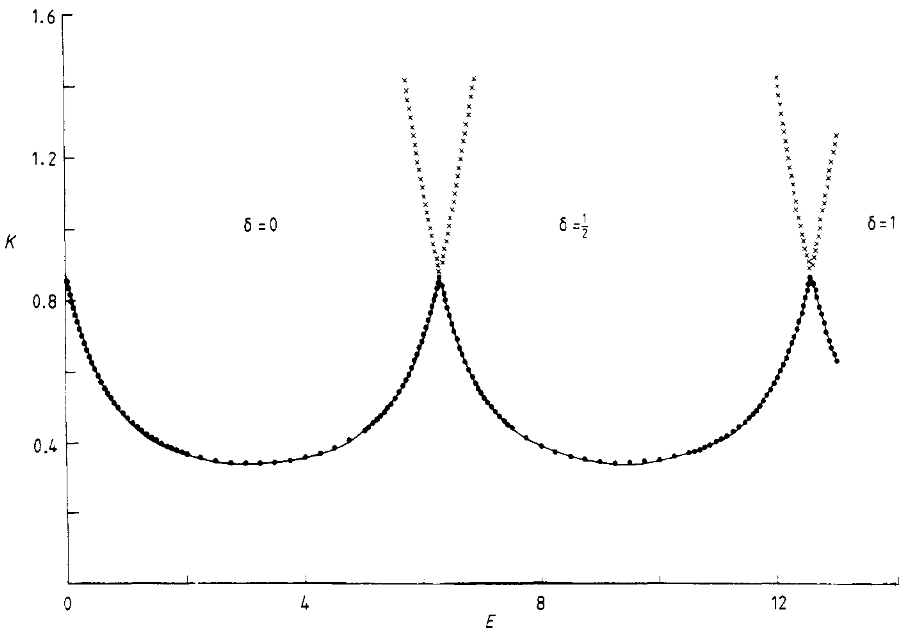


**Figure 2.** $K_c(E)$ (defined by $R = -0.25$), see text) for $\zeta_2 = \frac{1}{2}$. ●, Ground states of the physical system; ×, metastable states of the physical system.

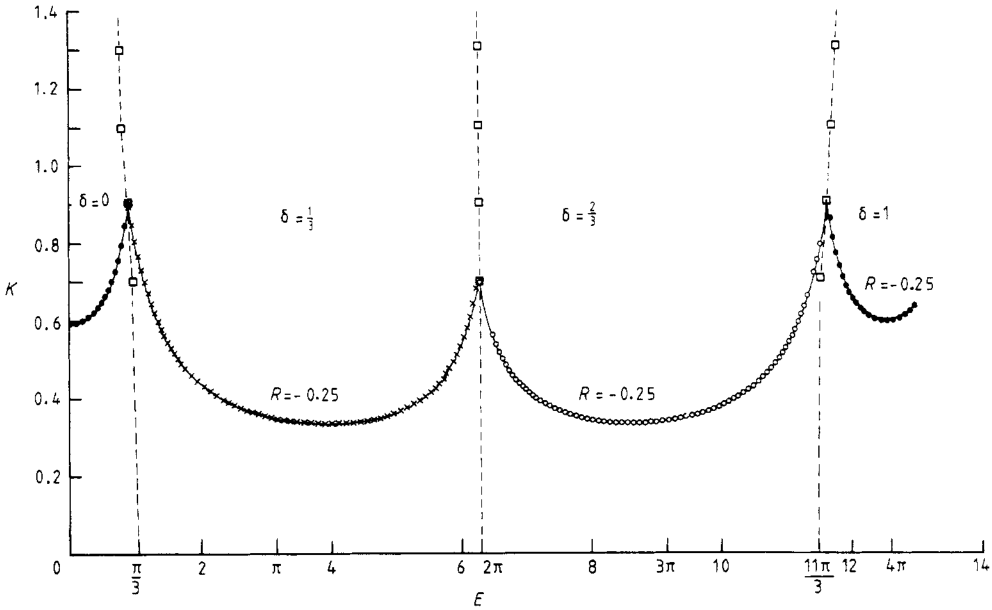


**Figure 3.** As figure 2 for $\zeta_3 = \frac{2}{3}$. The drawing explains the mechanism of generation of the curve $K_c(E)$, ○, states having $\delta = 0$ or 1; ×, $\delta = \frac{1}{3}$; ○, $\delta = \frac{2}{3}$ ($\delta$ is defined in (26), see text). □ indicate the first-order transitions between ground states of different polarisation $\delta$ for values of $R$ different from $-0.25$.

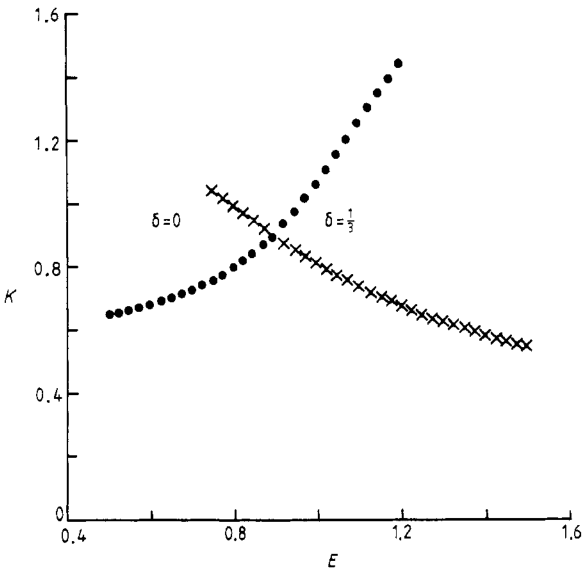


**Figure 4.** Detail of figure 3: $K_c(E)$ is composed of the points corresponding to the states of minimum energy: it has a 'cusp' at the intersection of the $\delta = 0$ and $\delta = \frac{1}{3}$ curve.

intersect at an angle which is finite when $s_n$ is small and goes to zero when $n$ goes to infinity. The cusps are concentrated in two regions: around $E = 0$ (or $4\pi$) and $E = 2\pi$ and there is a numerical indication that they remain there when $n$ increases since the width of the large gap between these regions tends rapidly to a finite value.

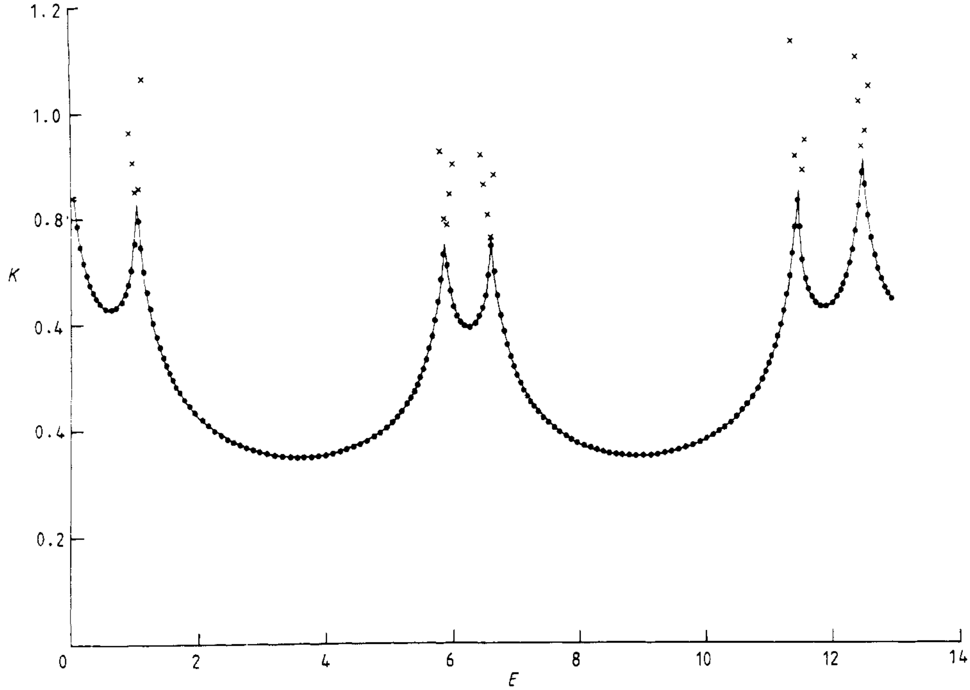


**Figure 5.** $K_c(E)$ for $\zeta_4 = \frac{3}{5}$: ●, states of minimum energy; ×, metastable states.

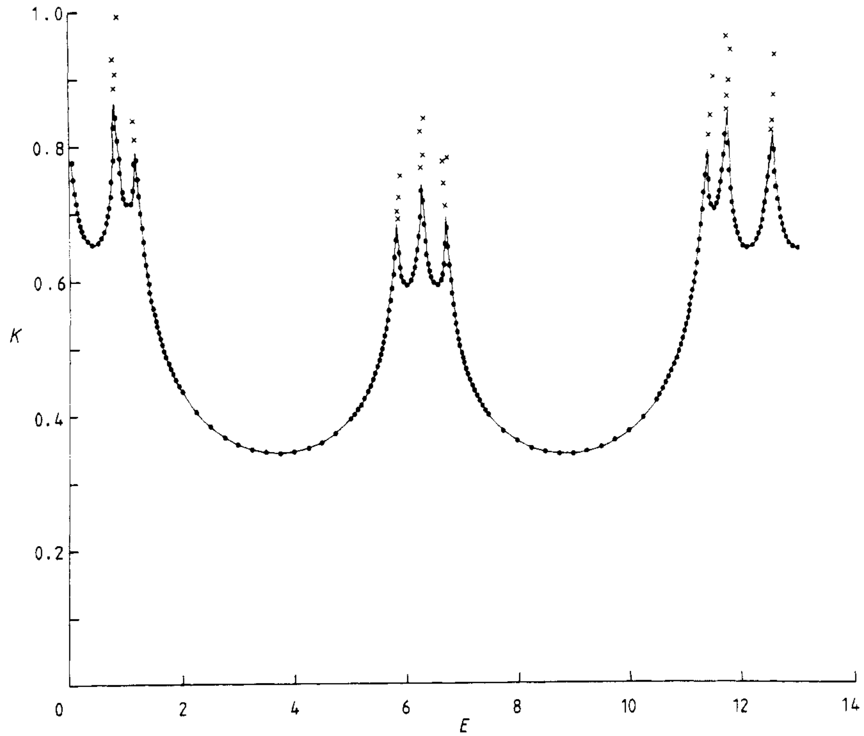


**Figure 6.** As figure 5 for $\zeta_5 = \frac{5}{8}$.

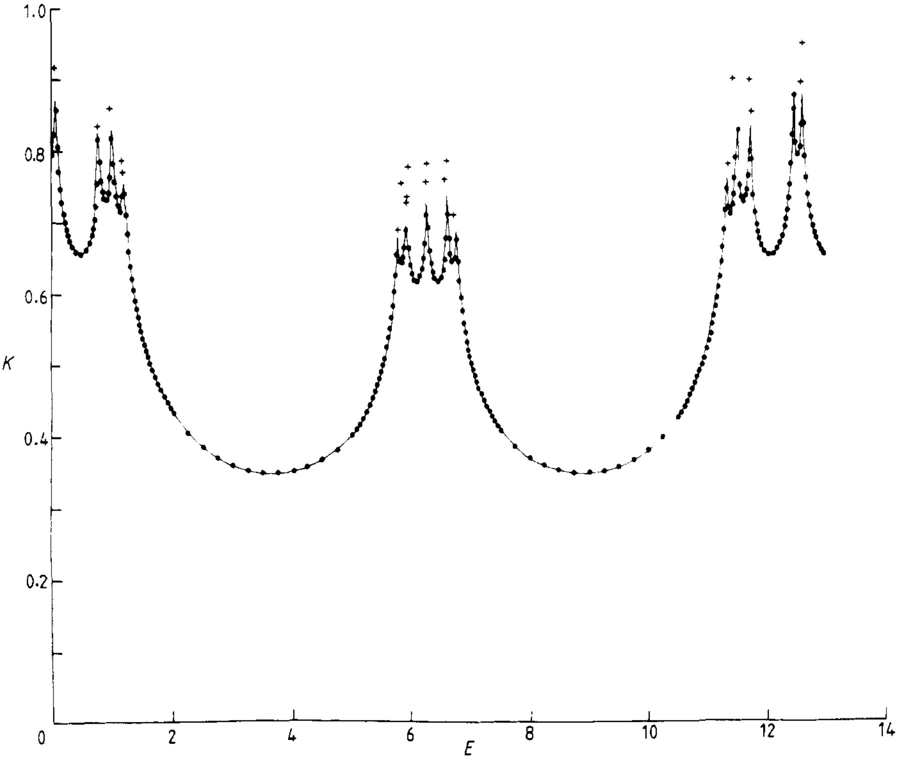


**Figure 7.** As figure 5 for $\zeta_6 = \frac{8}{13}$.

(ii) The 'budding' of the cusps is completely determined by the continued fraction expansion sequence $\{a_j\}$. The recurrence relation (15*b*) $s_n = a_n s_{n-1} + s_{n-2}$ with $s_0 = 1$ and $s_1 = a_1$ describes in a natural fashion the transformation which maps $K_c(E, r_n/s_n)$ into $K_c(E, r_{n+1}/s_{n+1})$ for the two groups of cusps around $E = 0$ and $E = 2\pi$. Figure 8, for example, has $s'_3 = 4$ cusps, of which $r'_3 = 3$ around $E = 0$. Then figure 9 shows $s'_4 = 15$ cusps of which $r'_4 = 11$ around $E = 0$. In the case of the golden sequence, $r_n$ and $s_n$ are among the Fibonacci numbers.

(iii) The calculations described in figures 2-9 give good evidence for the mechanism of formation and the properties of $K_c(E, \zeta)$. (They were not carried out for higher values of $n$ which would have required very large amounts of CPU time.) Hence in the limit $n \to \infty$, $K_c(E, \zeta)$ has a countable number of cusps which become dense on a Cantor set.

## 4. Polarisation and phase diagram

The presence of the $(-1)^j E u_j$ term in (1) results in the differentiation of the odd and even sublattice of the chain. The first length which is characteristic of model (1) is the average distance between atoms $l$ which is the conjugate variable to the tensile force $\mu$ and yields the rotation number $\zeta$:

$$\zeta = \frac{l}{2\pi} = \frac{1}{2\pi}\frac{1}{N}\sum_j (\theta_{j+1} - \theta_j). \tag{22}$$

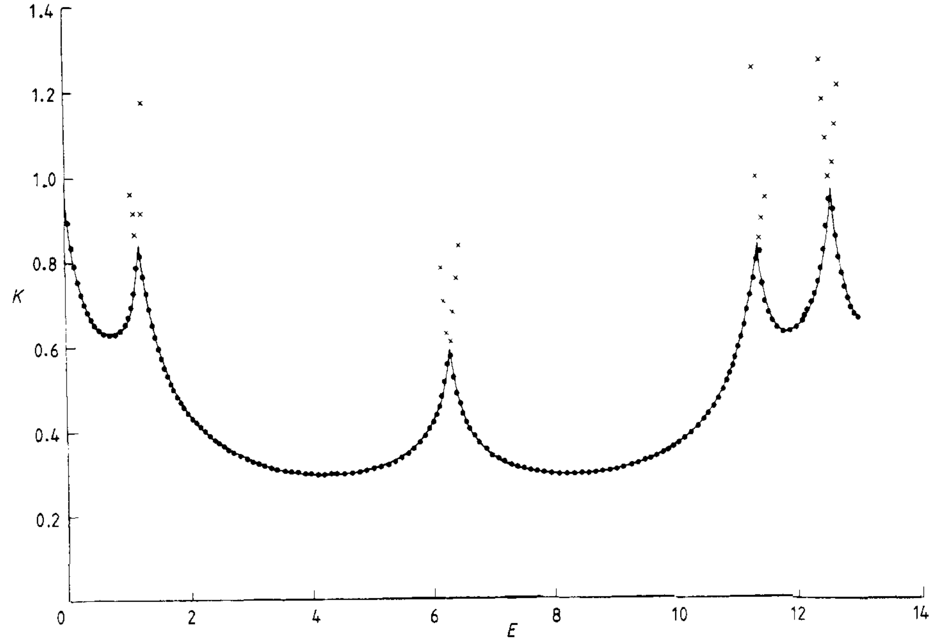


**Figure 8.** As figure 5 for $\zeta_3' = \frac{3}{4}$.

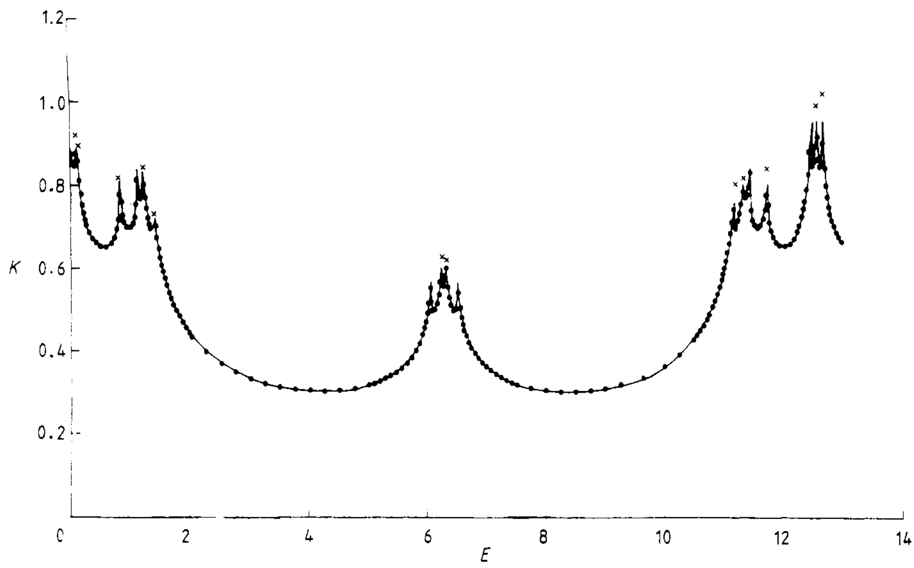


**Figure 9.** As figure 5 for $\zeta_4' = \frac{11}{15}$.

The response per atom to the electric field at fixed $\zeta$ is the conjugate variable to $E$ and the second characteristic length of the model or, in convenient units, the phase difference $\delta'$ between the two sublattice modulations

$$\delta'(E) = -\frac{1}{N}\frac{\partial \Phi}{\partial E} = \frac{1}{2\pi}\frac{1}{N}\sum_{j=1}^{N/2}(u_{2j+1} + u_{2j-1} - 2u_{2j}). \tag{23}$$

Because of equation (3), this polarisation is equal to

$$\delta'(E) = -\frac{E}{2} + \frac{K}{2N} \sum_{j=1}^{N/2} \sin u_{2j}. \tag{24}$$

In formula (26$a$) of Aubry *et al* (1985), it was shown for model (1) with a piecewise parabolic potential having a phase difference of $\pi$ for the odd and even sublattice that the polarisation $P$ is the sum of a linear part

$$P_{\text{lin}} = \frac{E}{(4+\lambda)} \tag{25a}$$

and of a non-linear part

$$P_{\text{nlin}} = \frac{a}{4+\lambda}\,\delta \tag{25b}$$

where

$$\delta = \frac{1}{2\pi}\frac{1}{N} \sum_{j=1}^{N/2} (m_{2j+1} + m_{2j-1} - 2m_{2j}) \tag{26a}$$

and

$$m_j = \text{Int}(u_j/2\pi). \tag{26b}$$

$\delta$ shows locking to the lattice after a 'subcommensurability' condition and, when $\zeta$ is irrational, is a devil's staircase (formula (45) in Aubry *et al* (1985)). This condition, in our model, for a piecewise parabolic potential or a cosine potential at high $K$ would be

$$p - \frac{2q+1}{2} = \delta \tag{27}$$

with $p$ and $q$ some integers.

The configuration of each phase is then characterised by the distribution of the integers $m_j$ which label the wells where the atoms are located. It has been shown that these integers are given by the formula

$$m_j = \text{Int}(jl/2 + \gamma + (-1)^j\delta/2) \tag{28}$$

where $\gamma$ corresponds to the average phase of the modulation and where $\delta$ describes the relative phase shift of the modulations of the even sublattice and of the odd sublattice. Since the energy of the chain is independent of $\gamma$, it is arbitrary and, for convenience, it can be chosen equal to $-\delta/2$. This sequence $\{m_j\}$ discontinuously changes when $jl/2 + (-1+(-1)^j)\delta/2$ becomes an integer $q$ for some value of $j = p$ which is the subcommensurability condition (27). Then, the corresponding configuration $\{u_j\}$ also undergoes a discontinuous variation.

When $\zeta = r/s$ is rational (with $r$ and $s$ two irreducible integers), the devil's staircase $\delta(E)$ becomes a harmless staircase. The discontinuities of the sequence $\{m_j\}$ are obtained for $\delta$ given by (27) for some integers $p$ and $q$. This sequence is given by $\delta = m/s$ when $r$ is even and by $\delta = (2m+1)/(2s)$ when $r$ is odd ($m$ is an arbitrary integer).

To substantiate the analogy, between the high $K$ cosine potential and the piecewise parabola potential situations, we calculated for $K = 1.9$ and $\zeta_3 = \frac{2}{3}$, $\delta(E)$ as defined here by (26) and the energies of the possible configurations of the chain. The results are shown in figures 10 and 11. They show the following.

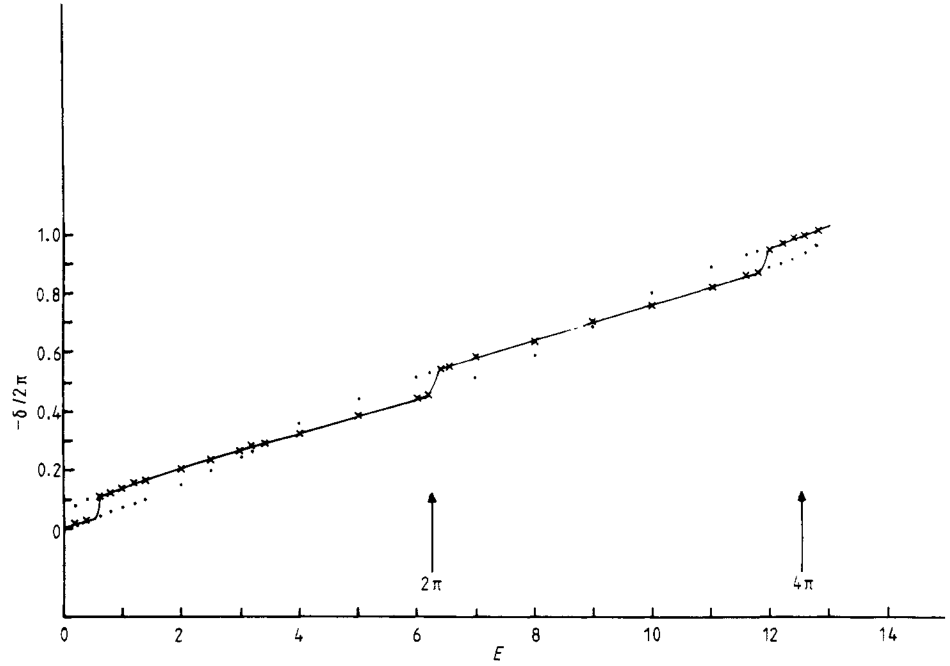


**Figure 10.** $\delta(E)$ for $\zeta_3 = \frac{2}{3}$ and $K = 1.9$. The crosses indicate the polarisation of the ground state. The curve is a 'harmless' staircase.

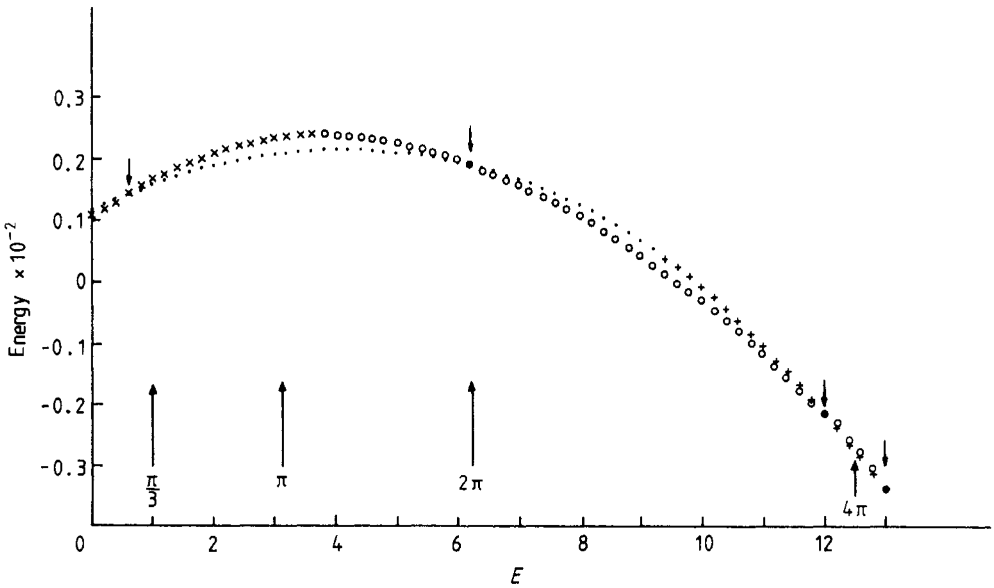


**Figure 11.** The free energy of model (1) with a cosine potential as a function of $E$ for $\zeta_3 = \frac{2}{3}$ and $K = 1.9$. The downward arrows indicate the first-order transitions (compare with figures 10 and 12). The following describe the cosine potential wells to specify the chain configuration $\{m_j\}$: ×, 000111; ●, 001111; ○, 001011; +, 001021.

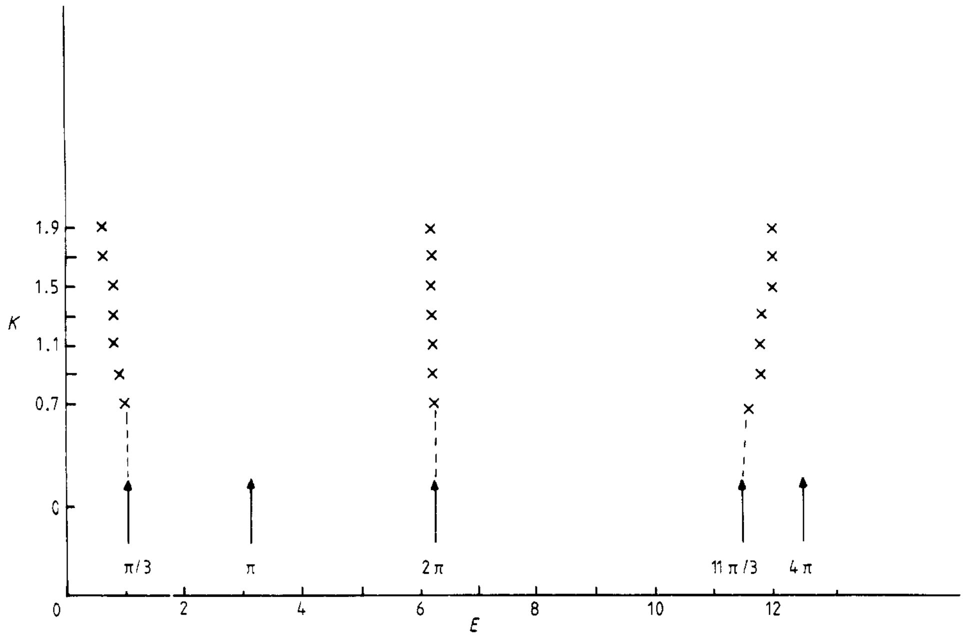


**Figure 12.** The phase diagram of model (1) with a cosine potential for $\zeta_3 = \frac{2}{3}$ (see text). The first-order transition lines extend down to the $K = 0$ axis. Compare with figure 3.

(i) The same 'harmless' staircase behaviour is found in the rational case for $\delta(E)$ in model (1) in the high $K$ limit.

(ii) There are first-order transitions between states of different polarisations at constant $K$ since the free energy curve has a discontinuity in its slope just at the value of $E$ at which the stair in $\delta(E)$ happens (compare figures 10 and 11). Let us now go back to figures 2 and 3 which show how $K_c(E)$ for $\zeta_3 = \frac{2}{3}$ (and more generally $\zeta = r/s$) is generated by $s$ parabolic-like curves having constant polarisation (defined after (26)) which intersect at an angle. Calculation of the free energy shows that the ground states lie on the lower part of the curve, indicated by a continuous line. The 'cusps' in $K_c(E)$ (for $R = -0.25$) on figure 3 will line up on the three curves of figure 12 when $R$ is varied. They correspond to the $s$ discontinuities in $\delta(E)$ of figure 10 (the plateau edges) and to changes of slope of the free energy on figure 11, indicating first-order transition lines which extend down to the $K = 0$ axis in the rational case.

When the order $s$ of the rational $\zeta = r/s$ increases the number $s$ of first-order lines also increases, and in the limit $s \to \infty$ and $\zeta$ irrational, $K_c(E, \zeta)$ as shown above is composed of a countable number of cusps. When $K < K_c(E, \zeta)$, the limit configuration is an incommensurate 'sliding' ground state which can be described with an analytic hull function. Therefore, in the region $R$ of the parameter space $(E, K)$ which is determined by the condition $K < K_c(E, \zeta)$, it can be easily proven that the physical ground state is *unique*. As a result, no line corresponding to a discontinuity of the ground state configuration can exist in this analytic region $R$. The polarisation $\delta(E, \zeta)$ is then necessarily a smooth function of the electric field while $E$ remains in this region.

On the contrary, outside $R$, in the region determined by $K > K_c(E, \zeta)$, there exist many metastable configurations besides the ground state and the first-order transition lines which die out at the cusps separating regions of constant polarisation

$\delta$ where the chain is locked to the lattice. It has been shown in Aubry *et al* (1985) that, for a piecewise parabolic potential, the polarisation curve is the sum of a smooth analytic part and a devil's staircase. This devil's staircase component still exists in the region $K > K_c(E, \zeta)$ for the cosine potential model we study here.

Indeed, the limit of the set of $s$ first-order lines observed in the commensurate case is superior to a set which has the topology of the product of a one-dimensional Cantor set and of a continuous line. It corresponds to the edges of the plateaux of the devil's staircase components of $\delta(E)$ at fixed $\zeta$. In the non-analytic region, for the incommensurate ground states with incommensurability ratio $\zeta$, there exists infinitely many such critical quasi-first-order lines which terminate at the critical curve corresponding to the curve $K = K_c(E, \zeta)$ and each terminating point of a critical line is a cusp of the curve $K = K_c(E, \zeta)$.

## 5. Conclusion

When the incommensurability ratio $\zeta$ is fixed at an irrational number, our model exhibits a phase diagram in the parameter space formed by the electric field $E$ and the coupling constant $K$ to the lattice that has infinitely many phases. These phases are separated by infinitely many transition lines which can be interpreted as first-order lines with a discontinuity of the physical quantities which is infinitely small at the macroscopic scale but does exist for the microscopic configuration.

The new interesting feature which is observed here is that this phase diagram also exhibits an infinite number of critical points. These critical points are the terminating points of the quasi-first-order lines at the second-order critical line $K_c(E, \zeta)$ of the transition by breaking of analyticity of this model. This critical line exhibits infinitely many cusps at each of these critical points. So this model provides the first example which generalises the concept of critical point of the standard theory of phase transitions to a situation where the phase diagram exhibits devil's staircases.

## Acknowledgments

FA gratefully thanks Professor J Friedel for his interest and for stimulating discussions during the course of this work and acknowledges partial support for this work from Centre National de la Recherche Scientifique (CNRS) under Action Thématique Programmee (ATP) 'Application des Mathématiques Pures'.

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