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Locking to incommensurate structures—a model with three competing lengths

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Abstract. A classical pseudo-spin model in one dimension is considered, representing a variation on the Frenkel-Kontorova model to include *non-convex* interactions, resulting in *three* competing length scales. An exact algorithm is used numerically to determine the classical ground state as a function of a chemical potential. Approximate arguments suggest that only a first-order transition should occur. However, when the lengths are not rationally related, it is found that the mean lattice spacing appears to vary as a devil's staircase. The plateaux of the staircase correspond to locking to *incommensurate* structures while there is no locking to the commensurate ones. Most of the locking values observed numerically belong to a series which can be analytically calculated on the basis of simple topological hypotheses which are also consistent with numerical observations.

1. Introduction

The physical problems which have motivated the present work are those with competing interactions, which in general induce incommensurate periods. It has now become widely recognised (see, e.g., Aubry 1983a) that such problems are *prevalent* in condensed matter physics and there are numerous experimental 'observations' of incommensurate structures and commensurate-incommensurate (C-IC) transitions, e.g. in ferroelectric, magnetic, physi-absorption and charge-density-wave materials. The simplest description of incommensurate structures is based on a model in one space dimension introduced by Frenkel and Kontorova (FK) (or straightforward modifications); see equation (1.1) below. However, it is known that the FK model, treated in mean-field theory, predicts only *continuous* C-IC transformations, whereas many experimental observations suggest weakly first-order transitions.

There are a number of variations on the FK model which may be important. However, here we focus on the influence of *non-convex* interparticle interactions. The standard FK model includes only convex interactions which always lead to simple ground states, either C or IC (Aubry 1983a, b). In general there is no reason to limit ourselves to pure convexity: oscillatory interactions are quite typical as RKKY coupling in magnets; non-convex coupling will also arise through interactions between domain walls or strain-mediated interactions, etc (see, e.g., Villain and Gordon 1980).

Non-convexity *qualitatively* changes predictions of the FK model. It has been argued (e.g. Villain and Gordon 1980, Axel and Aubry 1981) that first-order transitions

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will be induced. These arguments are in a sense equivalent to replacing the periodic potential by a constant one. We have found that the situation is typically even more complicated and may include a non-trivial order which we term 'weakly periodic' (Aubry 1980, 1983a). (Such an ordering is known elsewhere in mathematical physics, e.g. the problem of tiling a two-dimensional plane (Gardner 1977, MacKay 1983). Similar orderings may be expected in the models considered by Kléman and Sadoc (1979).)

Since the general problem of competing *and* non-convex interactions will turn out to be extremely complex, it is useful to focus on a simple model which contains the essential ingredients. We have used the one-dimensional FK model with free energy

$$F = \sum_{i=1}^{N} \{V(u_i) + W(u_{i+1} - u_i) - \mu(u_N - u_0)\} \tag{1.1}$$

where W is the interaction potential, e.g. $\frac{1}{2}(u_{i+1} - u_i - a)^2$ in a convex case. In (1.1) $\{i\}$ label particles with displacements (or rotations, etc) $\{u_i\}$ and μ is a chemical potential. For the local potential V we take

$$V(u) = \cos u \tag{1.2}$$

but of course many other choices are possible. In particular we have also considered

$$V(u) = (1 - \tfrac{1}{2}\cos u)^{-1} \tag{1.3}$$

which contains higher harmonics but is otherwise similar to equation (1.2). Turning to the form of non-convex interaction which we will superimpose on (1.1), we suppose that the simplest case is that of a double well, i.e. with two potential minima and one intervening maximum: when particles visit either minimum the potential is locally convex. However, when passing between minima, non-convexity is experienced. To simplify this situation even further we have considered the limit of a very high potential barrier and idealised the interparticle interaction W in (1.1) as a pure Ising form:

$$u_{i+1} - u_i = l_1 \text{ or } l_2. \tag{1.4}$$

Here l_1 and l_2 are the locations of the consecutive minima. As remarked earlier, (1.4) might typify oscillatory interactions between domain walls (as in ANNNI models (Villain and Gordon 1980), the effect of a discrete lattice which provides a nonlinear Peierls-Nabarro pinning potential for walls (Aubry 1983a)), etc. Non-Ising interaction potentials are expected to retain the same thermodynamic phases, but walls will be less narrow, transitions may be smoother, and phases less locked.

We have investigated the mean-field ('ground state') properties of the problem (1.1)-(1.4) both analytically (§ 2) and numerically (§ 3). Since the results are quite complicated, we briefly summarise them here: (i) usual approaches with *constant* distances between walls predict a single first-order transition (Villain and Gordon 1980). In fact, in the present case, we have typically found many intermediate phases; (ii) the average separation between phases appears to form a 'devil's straircase' (Aubry 1980, 1983a, b); (iii) the plateaux of the staircase occur at *incommensurate* concentration values† characterised by the two lengths, l_1 and l_2, and the period of the local potential $V(u)$, i.e. *three* lengths. All of the IC configurations are locked. (The very large Peierls-Nabarro lattice pinning barrier, implied by our use of an Ising approximation

† We emphasise that this mechanism for locking is different from that described by Aubry *et al* (1984) as a 'subcommensurability' effect.

(above), implies *strong* locking of metastable states); (iv) on the basis of an empirical analysis, motivated by our numerical results, we can (§ 2) predict the locations of most of the observed plateaux. *Small* first-order transitions are not excluded (either analytically or numerically) but a single isolated first-order transition is definitely excluded in the general case; (v) a simple degenerate case is when *both* l_1 and l_2 are *rational* with respect to the period of $V(u)$. Then a finite number of transitions occur, all of which are first order.

2. Analysis

Our analysis is motivated by several assumptions which were suggested by our numerical observations (§ 3).

First, we *assume* that each ground state which corresponds to an observed plateau of the curve $l(\mu)$ is such that the set of coordinates u_i, modulo the potential period 2π, is uniformly dense on a finite set I of intervals (which we refer to as 'bands'). Second, we *assume* that the transformation

$$T(u_i) = u_{i+1} \qquad \text{mod } 2\pi, \tag{2.1}$$

which maps a dense subset of points of I onto itself, is continuous except at a finite number of points which have their images at band edges. Therefore this transformation T is uniquely defined by continuity for all points of I. It follows from the definition of the model that $T(u)$ is either a translation by $l_1 \bmod 2\pi$ or by $l_2 \bmod 2\pi$ and thus $T(u)$ is measure-preserving. Since the trajectory $u_i = T^i(u_0)$ is dense on I, this transformation does not overlap the intervals of I with each other and is invertible except at a finite number of points ('band edges'). Finally, we *assume* that it is possible to consecutively 'glue' all the left and right band edges by pairs (see figure 1), such that:

(i) the topology of the set of intervals I becomes that of a unique circle $\mathscr{C}$;

(ii) the transformation $\tilde{T}$, which corresponds to T, on this circle $\mathscr{C}$ be continuous. Since T is measure-preserving, $\tilde{T}$ is necessarily a rotation on $\mathscr{C}$. (This assumption is

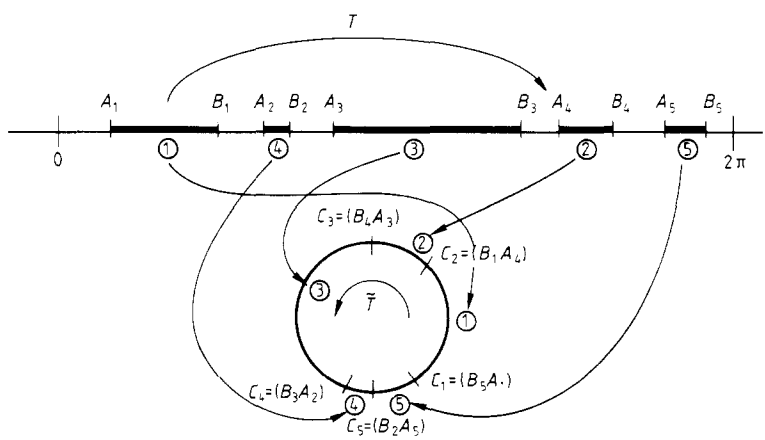

Figure 1. Schematic graph for a possible five-band structure. The five intervals are 'glued' together to form a circle. C_1 corresponds to B_5 and A_1 which are glued with each other, C_2 to B_1 and A_4, and so on. The length of the arc $\widehat{C_1C_2}$ is $\overline{A_1B_1}$, $\widehat{C_2C_3}$ is $\overline{A_4B_4}$, etc. A rotation $\tilde{T}$ on the circle corresponds to the initial map T which exchanges the intervals.

not a consequence of the previous one because there exist examples of transformations which exchange intervals and are measure-preserving but which cannot be transformed into a rotation; see, e.g., Katok and Stepin (1967).)

A set of intervals which fulfils all these conditions is called a one-circle band structure.

Typical numerical observations of band structures which suggested the above assumptions are shown in figure 4. The distribution of the sequence $\{u_i \bmod 2\pi\}$ as a function of the index i exhibits a one-band structure on the first figure and a three-band structure in the second one. These band structures are explicitly calculated in appendix 1.

The analytic justifications for our assumptions are not discussed in the present paper. At the present stage of our work, they are useful hypotheses which allow one to interpret many observed plateaux in the average distance $l(\mu) = \langle u_{i+1} - u_i \rangle$. However, it is probable that there also exist plateaux which are related to more complex band structures which cannot be reduced to a rotation on a circle but their investigation is somewhat more complex. Nevertheless, we can understand intuitively that, if band distributions for the coordinates u_i are concentrated close to the minima of the potential $V(u)$, they are quite favourable for a good minimisation of the total energy of the system.

Our assumptions must be compatible with the constraining condition, that for any x in I, we have

$$T(x) - x = l_1 \text{ or } l_2 \qquad \bmod 2\pi. \tag{2.2}$$

The analysis of this compatibility condition yields necessary and sufficient conditions for the existence of one-circle band structures. We also find that the configurations ν which correspond to these band structures are *incommensurate* with a mean distance $\langle u_{i+1} - u_i \rangle = l_\nu$ and a modulation wavevector ω_ν. In addition, the values of l_ν and ω_ν must belong to a discrete series of numbers which we explicitly calculate. It should be noted that most values of $l(\mu)$ at which a plateau is observed (particularly at the most important ones) indeed belong to this series l_ν. In addition, we will check that the corresponding configurations have the expected properties and particularly that its wavevector modulation belongs to the series of ω_ν. However our analysis, which does not involve any details about the shape of the potential $V(u)$ except the fact that it is periodic, does not prove that a possible band structure necessarily corresponds to a plateau of $l(\mu)$, and if this plateau indeed exists the width in μ is not predicted.

We now derive the topological conditions on the band structure I. To fix the idea, we assume (without any loss of generality) that

$$0 < l_1 < l_2 < 2\pi. \tag{2.3a}$$

Then we define

$$\delta = l_2 - l_1. \tag{2.3b}$$

We assume only that there exist *no* integer solutions (n_1, n_2, n) for the equation

$$n_1 l_1 + n_2 l_2 = 2n\pi \tag{2.4}$$

with n_1 and n_2 both of the same sign. Let us call $[A_1 B_1]$, $[A_2 B_2] \ldots [A_N B_N]$ the N non-overlapping consecutive intervals of the set I on $[0, 2\pi]$. By definition, the A_i are the left band edges and the B_i the right band edges of these intervals in order that the algebraic length $A_i B_i$ be always positive.

According to the above assumptions, it is possible to 'glue' the intervals $[A_iB_i]$ to form a circle with length Φ which is the total of the interval width $\Sigma_{i=1}^{N} \overline{A_iB_i}$. Figure 1 illustrates, through an example with five intervals, how these intervals could be glued in order to form the circle $\mathscr{C}$. The initial order of these intervals in I is generally interchanged and becomes

$$\ldots[A_{k_1}B_{k_1}][A_{k_2}B_{k_2}][A_{k_3}B_{k_3}]\ldots[A_{k_n}B_{k_n}][A_{k_1}B_{k_1}]\ldots$$

where $\{k_i\}$ is a permutation on the integers $1 \leqslant i \leqslant n$. By definition, $(B_{k_1}A_{k_2})(B_{k_2}A_{k_3})$ $\ldots$ $(B_{k_{N-1}}A_{k_N})(B_{k_N}A_{k_1})$ are the pairs of band edges which are 'glued'. Their images are called $C_1, C_2, \ldots, C_N$, respectively, on the circle $\mathscr{C}$.

Let us now consider a point C_i on the circle $\mathscr{C}$. There necessarily exist some integer m such that

$$\tilde{T}_m(C_i) \neq C_j \qquad \text{for all } j. \tag{2.5}$$

Indeed, if for all m there existed $1 \leqslant j_m \leqslant N$ such that $\tilde{T}^m(C_i) = C_{j_m}$, there would also exist a periodic cycle for $\tilde{T}$ because the set of C_j is finite. Consequently T would also have periodic cycles but this is impossible because (2.4) has no integer solutions. Therefore, for the initial transformation T, we necessarily have some point P which is not a band edge and such that

$$T^m(A_{k_i}) = T^m(B_{k_{i-1}}) = P \qquad \mod 2\pi. \tag{2.6}$$

Because of (2.2), there exist two positive integers n_A and n_B, both smaller than m, such that

$$\overline{A_{k_i}P} = [n_A l_1 + (m - n_A) l_2] \qquad \mod 2\pi \tag{2.7a}$$

and

$$\overline{B_{k_i}P} = [n_B l_1 + (m - n_B) l_2] \qquad \mod 2\pi \tag{2.7b}$$

which implies that there exists an integer $n_i = n_A - n_B$ with

$$\overline{B_{k_{i-1}}A_{k_i}} \qquad \mod 2\pi = n_i\delta \qquad \mod 2\pi. \tag{2.8}$$

For each C_i, this associated integer n_i gives the width of the gap which has been shrunk in order to glue the corresponding points $B_{k_{i-1}}$ and A_{k_i} of I. It is now more convenient to consider, instead of the set of intervals $[A_iB_i]$, an infinite set I' of intervals $[A'_iB'_i]$ which is equivalent modulo 2π to I but which is also periodic, and for which the intervals are in the same order as on the circle $\mathscr{C}$. These intervals are defined for $1 \leqslant i < N$ by

$$\overline{A'_iB'_i} = \overline{A_{k_i}B_{k_i}} \tag{2.9a}$$

$$\overline{B'_{i-1}A'_i} = n_i\delta. \tag{2.9b}$$

This definition implies, by using (2.8), that for $i = N+1$ there necessarily exists an integer q such that

$$\overline{B'_NA'_1} = n_1\delta - 2\pi q. \tag{2.9c}$$

Then the sequence of intervals $[A'_iB'_i]$ can be defined for all i. The initial sequence is repeated periodically with the definition:

$$\overline{A'_iA'_{i+N}} = \overline{B'_iB'_{i+N}} = 2\pi q \tag{2.9b}$$

in order that (2.9b) is true for all i. By definition, on the circle $\mathscr{C}$, the sequence of

points C_i which correspond to (B'_{i-1}, A'_i) is periodic with period N as well as the associated sequence of integers n_i:

$$C_{i+N} = C_i \tag{2.10a}$$

$$n_{i+N} = n_i. \tag{2.10}$$

With this definition, the coordinate of a point X on the real axis belonging to this set I' is easily related to the angular coordinate of its image x on the circle $\mathscr{C}$. Let O and Ω be the corresponding origins on the real axis and on the circle $\mathscr{C}$. To fix ideas we suppose that O belongs to the interval $[A'_n B'_n]$ and that $0 < \overline{OX} < 2\pi q$. Then X belongs to an interval $[A'_m B'_m]$ such that $n \leqslant m \leqslant N$. We write

$$\overline{OX} = \overline{OB'_n} + \overline{B'_n A'_{n+1}} + \overline{A'_{n+1} B'_{n+1}} + \ldots + \overline{A'_{m-1} B'_{m-1}} + \overline{B'_{m-1} A'_m} + \overline{A'_m X} \tag{2.11a}$$

which becomes, by using (2.9*b*),

$$\overline{OX} = \widehat{\Omega x} + \sum_{C_i \in \widehat{\Omega x}} n_i \delta. \tag{2.11b}$$

The sum

$$S(\Omega, x) = \sum_{C_i \in \widehat{\Omega x}} n_i$$

is made with all the points C_i in the arc $\widehat{\Omega x}$. This formula readily extends to situations where $\overline{OX}$ is negative or where $\overline{OX}$ is larger than $2\pi q$. Then the arc $\widehat{\Omega x}$ which could be longer than the length of the circle has to be considered as algebraic. In addition, the indices n_i have to be counted with their order of multiplicity (the number of times the arc $\widehat{\Omega x}$ passes over the point C_i) and a sign which corresponds to the direction of the arc $\widehat{\Omega x}$ on the circle $\mathscr{C}$.

The net result is that the algebraic distance between two points O and X on the real axis is just equal to their angular distance on the circle $\mathscr{C}$ plus the gap widths which are passed through in going from O to X. Formula (2.11*b*) is the basic relationship from which we determine: (i) the length of the circle $\mathscr{C}$; (ii) the rotation length θ of $\tilde{T}$; and (iii) the concentration c of bounds l_2 in the corresponding configuration which yield the mean distance

$$\langle u_{i+1} - u_i \rangle = (1-c) l_1 + c l_2. \tag{2.12}$$

We next obtain necessary conditions expressing the compatibility between the initial assumptions by showing: (*a*) that the length Φ of the circle which is the total bandwidth of I is necessarily between 0 and 2π; (*b*) that the rotation length θ of $\tilde{T}$ corresponds to a translation on the real axis by only two possible lengths, l_1 or l_2; and (*c*) that the concentration c of bounds l_2 is between 0 and 1. These conditions force the set of possible values for Φ, and θ and c to be discrete. Reciprocally, it is shown next that when these conditions are fulfilled, there exists a band structure I with a map T' which satisfies condition (2.2).

2.1. Total bandwidth Φ

We consider two points A and A' in the set I' which are separated by $2\pi q$. They are represented by the same point on the circle but the corresponding arc $\widehat{\alpha\alpha'}$ is just equal to the total circle length Φ. Formula (2.11) yields

$$\Phi = 2\pi q - p\delta \tag{2.13a}$$

where the algebraic integer p is defined by

$$p = \sum_{i=1}^{N} n_i. \tag{2.13b}$$

Since the intervals in the initial interval do not overlap, we necessarily have $0 < \phi < 2\pi$, which implies

$$q = \mathrm{Int}\left(\frac{p\delta}{2\pi}\right) + 1. \tag{2.13c}$$

(Int(x) is the integer part of x, i.e. the largest integer smaller than or equal to n.) The possible lengths of the circle are determined by a unique integer p.

2.2. *Rotation length* θ

We now consider a point A in I' and its image $T(A)$ in I' which is at a distance l_1 or l_2, mod 2π. On the circle, the corresponding points α and $\alpha' \equiv \tilde{T}(\alpha)$ are separated by θ which we call the rotation length of $\tilde{T}$. Formula (2.11b) yields

$$\theta + \left(\sum_{C_i \in \widehat{\alpha,\alpha}+\theta} n_i\right)\delta = l_1 \text{ or } l_2 \qquad \mod 2\pi. \tag{2.14a}$$

Since $\delta/2\pi$ is irrational, there exists a unique pair of integers r and s such that

$$\theta + s\delta = l_1 + 2r\pi \tag{2.14b}$$

and another unique pair, r' and s', such that

$$\theta + s'\delta = l_2 + 2r'\pi. \tag{2.14c}$$

(Since $\delta = (l_2 - l_1)$, (2.14a) and (2.14b) are compatible, with $s' = s+1$ and $r = r'$.) Consequently (2.14) implies that for any point α on $\mathscr{C}$

$$\sum_{C_i \in \widehat{\alpha,\alpha}+\theta} n_i = s \text{ or } (s+1) \tag{2.15}$$

and then the rotation length θ necessarily has the form

$$\theta = l_1 + 2r\pi - s\delta \tag{2.16}$$

where r and s are integers,

2.3. *Configuration hull functions*

We now define a function h that will allow us to describe the initial configuration $\{u_i\}$ which was supposed to be dense mod 2π on the set I. This function $h(x)$ is defined by the equality

$$h\left(\frac{2\pi}{\Phi}\alpha\right) = \sum_{C_i \in \widehat{\Omega\alpha}} n_i. \tag{2.17a}$$

It is the sum of the indices of the points C_i which belong to the arc $\widehat{\Omega\alpha}$. It is readily established from (2.11) that $h(x)$ has the property

$$h(x + 2\pi) = h(x) + p. \tag{2.17b}$$

It is thus convenient to also define the periodic function g with period 2π,

$$g(x) = \left(h(x) - \frac{p}{2\pi} x \right) \delta \tag{2.17c}$$

and the function

$$\sigma(x) = h(x+\omega) - h(x) - s. \tag{2.18a}$$

Earlier we defined

$$\omega = 2\pi\theta/\Phi \tag{2.18b}$$

as the rotation number of $\tilde{T}$. It can be shown from (2.17a) that

$$\sum_{C_i \in \widehat{\alpha,\alpha+\theta}} n_i = \sigma\left(\frac{2\pi}{\Phi} \alpha \right) + s \tag{2.19}$$

which, when compared with (2.15), implies that $\sigma(x)$ can take only two values, 0 or 1. In addition, because of (2.17b), $\sigma(x)$ is periodic with period 2π.

The coordinates of the initial configuration $\{u_i\}$ are represented by a sequence of coordinates $\alpha_i = \alpha_0 + i\theta$ on the circle $\mathscr{C}$. Using equalities (2.19) and (2.14b), we find

$$u_{i+1} - u_i = l_1 + \sigma(i\omega + \beta)\delta \tag{2.20}$$

where $\beta = 2\pi\alpha_0/\Phi$. Because of (2.18$a$), the configuration $\{u_i\}$ is described by the function h:

$$u_i = i(l_1 - s\delta) + [h(i\omega + \beta) - h(\beta)]\delta + u_0 \tag{2.21a}$$

or equivalently

$$u_i - u_0 = f(i\omega + \beta) - f(\beta) \tag{2.21b}$$

where $f(x)$ is the 'hull' function of the configuration $\{u_i\}$ defined as

$$\begin{aligned} f(x) &= x\left(\frac{l_1 - s\delta}{\omega} \right) + h(x)\delta \\ &= x\left(\frac{l_1 - s\delta}{\omega} + \frac{p\delta}{2\pi} \right) + g(x). \end{aligned} \tag{2.21c}$$

The forms (2.21b) and (2.21c) show that the configuration $\{u_i\}$ is modulated by the periodic function $g(x)$ and is an incommensurate structure. The average distance between consecutive coordinates,

$$l = \langle u_{i+1} - u_i \rangle = l_1 - s\delta + p\omega\delta/2\pi, \tag{2.22a}$$

corresponds to the concentration of bounds l_2:

$$c = (p\omega/2\pi) - s. \tag{2.22b}$$

The wavevector of the modulation is the rotation angle of $\tilde{T}$ given by (2.18b).

Now, we have to check that this concentration of bounds l_2 lies between 0 and 1. This condition expresses the fact that it is possible to find θ, i.e. two integers r and s such that (2.14a) is fulfilled for any α. The inequalities $0 < c < 1$ become, with (2.18b)

and (2.22*b*),

$$\frac{pl_1}{2\pi}-\left(q-\frac{p\delta}{2\pi}\right)<qs-pr<\frac{pl_1}{2\pi}. \tag{2.23}$$

We note that the difference between the left and right numbers in (2.23), $q-p\delta/2\pi$, is smaller than 1 because of (2.13*c*). Then, since $(qs-pr)$ is an integer, we must satisfy both equalities

$$qs-pr=\mathrm{Int}(pl_1/2\pi) \tag{2.24a}$$

and

$$qs-pr=\mathrm{Int}(pl_2/2\pi)-\mathrm{Int}(p\delta/2\pi). \tag{2.24b}$$

The set of equalities (2.24*a*) and (2.24*b*) is equivalent to (2.24*a*) and (2.24*c*):

$$\mathrm{Int}(pl_2/2\pi)-\mathrm{Int}(pl_1/2\pi)=\mathrm{Int}(p(l_2-l_1)/2\pi). \tag{2.24c}$$

Therefore, a necessary condition to have a N-band structure with $\Sigma_{i=1}^{N} n_i=p$ is that two out of the three conditions (2.24) are fulfilled with q given by (2.13*c*).

The conditions (2.24) are also sufficient to build a one-circle band structure with $\Sigma_{i=1}^{N} n_i=p$. The proof of the existence of such a band structure is straightforward. Suppose that we have four integers p, q, r, s which fulfil the above conditions. Then Φ and θ are determined by (2.13*a*) and (2.16). We define a set of intervals I with $|p|$ equal and equidistant intervals. Each interval has the length $\phi/|p|$ and the gap between two consecutive intervals is $2\pi-\phi/|p|$. On the associated circle, which corresponds to these intervals, the $|p|$ points C_i are equidistant with a constant index, namely $n_i=\mathrm{sgn}\,p=\pm 1$. With the angle θ defined by (2.16), an arc of length θ contains either s or $(s+1)$ points C_i since $\mathrm{Int}(\theta/|p|))=s$, using the definitions of p, q, r, s. Therefore equation (2.15) is fulfilled. Considering the non-overlapping intervals $[A_i, B_i]$ on the real axis with $A_i=i(\phi/|p|+\delta)$, $B_i=i(\phi/|p|+\delta)+(\phi/|p|)\ (\mathrm{mod}\ 2\pi)$, the transformation T', corresponding to the rotation on the circle $\mathscr{C}$, is then given by a translation by either l_1 or l_2 (see equation (2.2)). It is also clear that this construction is not unique since it is possible to move the points C_i on the circle in some neighbourhood of the initial positions and still satisfy condition (2.15). The potential $V(x)$ will determine a band structure among the possible ones, minimising the total energy of the chain.

In conclusion, we have shown that for each set of integers p, q, r, s fulfilling (2.13*c*) and (2.24), there exists one-circle band structures and vice versa: each one-circle band structure is associated with such a set of number p, q, r, s. Then the corresponding configurations are incommensurate and describe by a hull function $f(x)$, (2.21*b*), which is piecewise constant with $g(x)$, (2.21*c*), periodic with period 2π.

Because of condition (2.24*a*), the concentration of bounds l_2 can be rewritten as

$$c(p)=\frac{pl_1-2\pi\ \mathrm{Int}(pl_1/2\pi)}{2\pi q-p\delta} \tag{2.25a}$$

and *only* depends on the integer p. The wavevector of the modulation is given by (2.18*b*) as

$$\omega=2\pi\frac{l_1+2\pi r-s\delta}{2\pi q-p\delta}. \tag{2.25b}$$

ω needs to be determined only modulo 2π. We note that if r and s are integer solutions of (2.24), $r'=r+q$ and $s'=s+p$ are also integer solutions but then ω is changed by

2π, which is an equivalent solution. It is then sufficient to seek the solutions of (2.24) where, for example, we have

$$0 \leqslant s < |p|. \tag{2.26}$$

Note that when p and q are relatively prime, there is always a unique solution to equation (2.24a) under the condition (2.26). If equation (2.24b) is also fulfilled then the wavevector ω is uniquely defined by equation (2.25b) and depends only on p. On the other hand, there is a finite probability that equations (2.24a, b) are fulfilled with p and q *not* relatively prime. In such cases the wavevector could be reduced from ω given in (2.25b). To see this consider the largest common divisor, K, of p and q and define the relatively prime numbers $p_0 (= p/K)$ and $q_0 (= q/K)$. Then the set of solutions (r, s) to equation (2.24a) can be obtained from *one* solution (r_0, s_0):

$$\begin{aligned} s_i &= s_0 + ip_0 \\ r_i &= r_0 + iq_0 \qquad \text{(integer } i\text{)}. \end{aligned} \tag{2.27}$$

There are K solutions (2.27) fulfilling (2.26). Consequently, there are K possible wavevectors ω_i defined by (2.25b):

$$\omega_i = \omega_0 + 2\pi i/K \qquad i = 1, \ldots, K. \tag{2.28}$$

Very interestingly, in this situation we have found *numerically* (see § 3) that the function $\sigma(x)$ (and any related periodic function) is periodic with the reduced period $2\pi/K$. If this is always the case, we may quite generally define the *fundamental* wavevector Q by

$$Q = 2\pi \frac{l_1 + 2\pi r_0 - s_0\delta}{2\pi q_0 - p_0\delta} \tag{2.29}$$

where p_0 and q_0 are defined above and satisfy

$$\begin{aligned} &q_0 s_0 - p_0 r_0 = \mathrm{Int}(pl_1)/K \\ &0 \leqslant s_0 < |p_0|. \end{aligned} \tag{2.30}$$

We prove in appendix 2 that there exists an infinite sequence of p_i for which conditions (2.23) are fulfilled. The density of these integers is exactly $(3/\pi^2)\zeta(3) \simeq 0.365\,38$, which is approximately found by numerical tests ($\simeq 0.37 \pm 0.01$). In addition the corresponding values of C_i given by (2.25a) are found to be dense on the interval $[0, 1]$ (but not with a uniform density) because the sequence of points $(p_i l_1/2\pi, p_i\delta/2\pi)$ is dense on the triangle $((0, 0), (0, 1), (1, 1))$.

In the next section, we numerically investigate the plateaux of $l(\mu)$ and the corresponding configurations. In many cases we identify a corresponding set of numbers (p, q, r, s) and thus a one-circle band structure. Then we can exhibit simple hull functions $\sigma(x)$ and $f(x)$ which describe the shape of the configuration. (The precise shape of these functions are not determined by this approach, which is purely topological, but depends on the particular choice of potential $V(x)$.)

3. Numerical results

We have obtained the numerical results presented here by using the procedure described in appendix 3 for calculating the minimum energy states of the model (1.1) (including

the non-convex interaction (1.4)). We illustrate the properties of this model for irrational values l_1 and l_2 with the specific choice $l_1 = (\sqrt{3.5}+\sqrt{5}-2-\sqrt{2})\pi = 2.1761$ and $l_2 = (\sqrt{3.5})\pi = 5.8774$ (and hence $\delta = (2+\sqrt{2}-\sqrt{5})\pi = 3.7013$).

Figure 2 shows the (free) energy per particle F_M^N/N as a function of the 'configuration magnetisation' M $(0 \leq M \leq N)$, i.e. the sequences of 0 and 1 (cf appendix 3). The chemical potential μ has been set to zero; adding a term $\mu(u_n - u_0) = \mu M$ simply tilts the whole function F_M. We observe that the function $F(M)$ is apparently continuous (as $N \to \infty$), convex, and has several (sharp) corners which become minima of $F(M)$ as μ is varied. The locations $c = M/N$ (or $\tilde{c} = 1 - c$) of these minima as a function of μ are displayed in figure 3 (here $N = 5000$). $c(\tilde{c})$ denotes the concentration of l_2 (l_1) distances in a pure l_1 (l_2) chain; the mean distance l is then given by $l = (1-c)l_1 + cl_2 = \tilde{c}l_1 + (1-\tilde{c})l_2$. We can clearly see a typical devil's staircase behaviour; the magnification also shown in figure 3 suggests that the staircase may be complete. Also, within the accuracy of our numerical computation, F_M seems to be convex, since $\tilde{c}(\mu)$ appears to increase monotonically. The numbers assigned to each step of the staircase will be explained below.

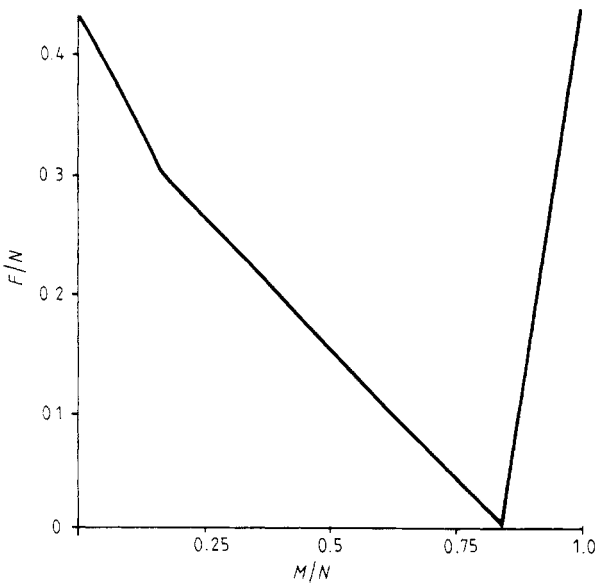

Figure 2. (Free) energy per particle F/N as a function of the mean 'magnetisation' $\tilde{M} = M/N$ or concentration $\tilde{c}$, for $\mu \equiv 0$.

For each state we now examine the distribution of particles within a periodicity interval of the potential $V(x)$: $\{u_i \bmod 2\pi\}$. Towards this end we calculate the integrated probability $D(\nu)$ to find a particle between 0 and $\nu < 2\pi$:

$$D(\nu) = \frac{1}{N}\sum_{i=1}^{N} \theta(\nu - u_i \bmod 2\pi). \tag{3.1}$$

This function is shown in figures 4(*a*) and 4(*b*) for the configurations $\{u_i\}$ corresponding to the corners of F_M^N (or plateaux of $\tilde{c}(\mu)$) at $M = 49$ and $M = 253$ or $\tilde{c} = 0.157$ and $\tilde{c} = 0.832$, respectively. We observe that the u_i are distributed in a finite number of

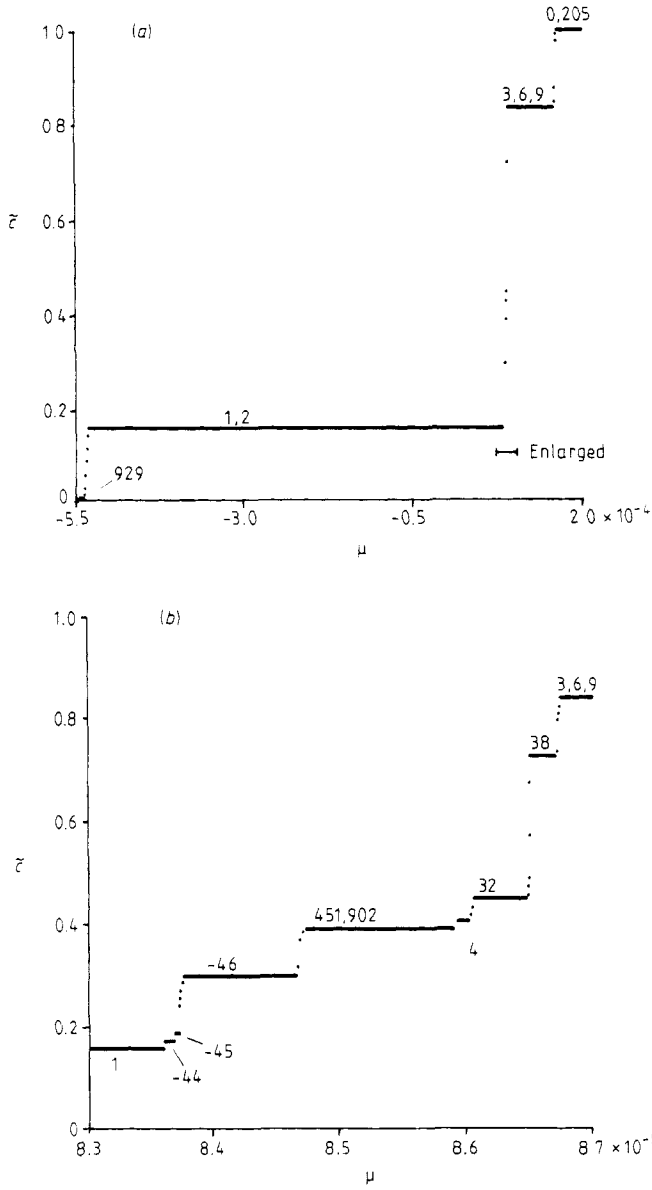

Figure 3. (*a*) Minimal concentration $\tilde{c}$ of $F(M)$ as a function of the chemical potential μ. (*b*) Enlargement of region marked in (*a*). Each step is labelled with allowed values of p in the range $(-2{,}000, +2{,}000)$. Associated values of q, r, s can be computed from the equations in appendix 2.

bands within the interval $[0, 2\pi]$; these bands correspond to the non-horizontal parts in the figures. In addition to these simple one- and three-band structures we show a more complicated 21-band structure in figure 4(*c*) for $\tilde{c} = 0.309$. It is these observations about the band structures which lead us to the analysis of the model as described in § 2.

Most of the observed minimum energy configurations are characterised by a set of numbers p, q, r, s (cf § 2, figure 3). These numbers determine the total width of the

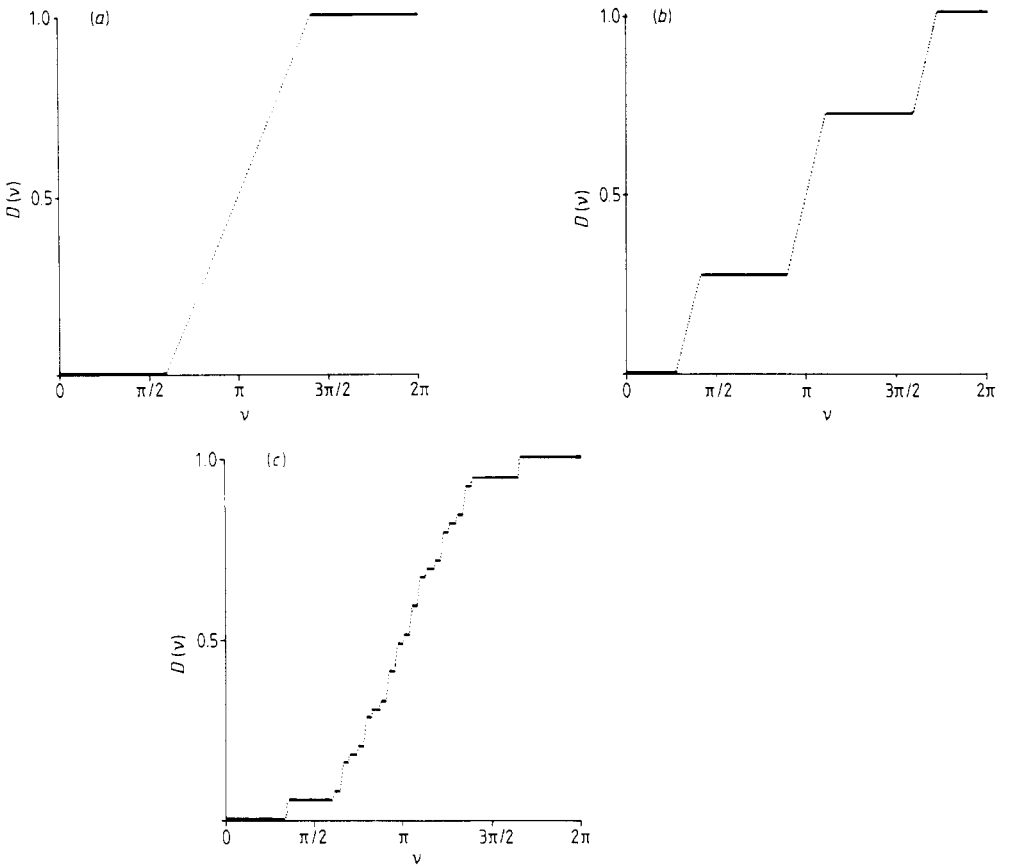

Figure 4. Integrated probabilities $D(\nu)$ (see § 3) for (*a*) a one-band configuration, (*b*) a three-band configuration, and (*c*) a 21-band configuration.

bands as well as the mean distance of the concentrations c, $\tilde{c}$. The numbers in figure 5 are the various values of p which can be associated with these plateaux. Some of the values for p which are allowed according to the prediction of our topological theory do not appear in our actual example. This could be due to the fact that the total width of these bands is too large and costs too much energy. But, of course, the finite size ($N < 5000$) of our calculation also limits a more detailed assignment of p values to the plateaux. The widths of the plateaux apparently depend on the detailed properties of the specifically chosen potential $V(x)$ and cannot be predicted by the analysis in § 2.

The numbers p, q, r, s determine the rotation number ω (cf equation (2.25*b*)) which is necessary in order to test the predictions about the functions $\sigma(x)$ and $h(x)$. Note that there can be several choices of rotation numbers for a single configuration labelled by p since the mean distance (or concentration) does not depend on r and s whereas the winding number depends on r and s as well as p and q. Table 1 lists all possible combinations of these numbers together with the corresponding values for winding number, concentrations and total bandwidth for $|p| < 10$.

First we plot the pseudo-spin variables $\sigma_i \equiv \sigma(i\omega + \beta)$ $\{0, 1\}$ of a given configuration as a function of $y_i = \omega i \bmod 2\pi$. According to the predictions of § 2, this corresponds

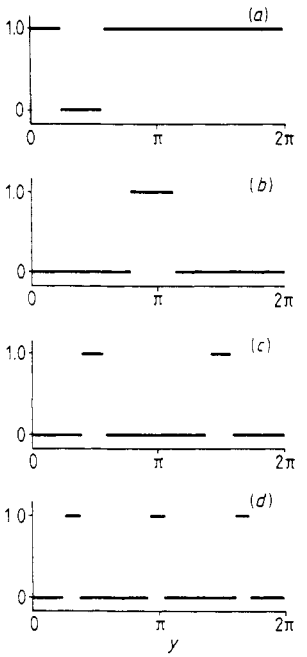

Figure 5. Hull function $\sigma(y)$ for different states labelled by p. Note the independence of $\sigma(y)$ on s when there are several choices, and the periodicity $2\pi/K$ with $K=1$ (a, b), 2 (c), 3 (d), corresponding to 1, 2 or 3 solutions, respectively (see discussion in §§ 2 and 3). (a) $p=1$, $s=0$; (b) $p=3$, $s=2$; (c) $p=6$, $s=2, 3$; (d) $p=9$, $s=2, 5, 8$.

Table 1. Set of solutions to equations (A2.1a)-(A2.1c) for $l_1=\pi(\sqrt{3.5}+\sqrt{5}-\sqrt{2}-2)$ and $l_2=\pi\sqrt{3.5}$ together with the corresponding concentrations and winding numbers (mod 2π) up to $|p|<10$.

p	q	r	s	ω	c	$\tilde{c}$	Φ
0	1	0	0	0.3463	0.000	1.000	1.000
1	1	0	0	0.8428	0.843	0.157	0.41
2	2	0	0	0.4214	0.843	0.157	0.82
2	2	1	1	0.9214	0.843	0.157	0.82
3	2	1	2	0.7225	0.168	0.832	0.23
4	3	2	3	0.8997	0.599	0.401	0.64
−5	−2	0	1	−0.2568	0.284	0.716	0.95
6	4	1	2	0.3613	0.168	0.832	0.47
6	4	3	5	0.8613	0.168	0.832	0.47
7	5	4	6	0.9263	0.484	0.516	0.88
9	6	1	2	0.2408	0.168	0.832	0.70
9	6	3	5	0.5742	0.168	0.832	0.70
9	6	5	8	0.9075	0.168	0.832	0.70

to the function $\sigma(y)$ defined in equation (2.18a) (see equation (2.20)). Figure 5 shows several cases with different configurations and winding numbers, all of them in agreement with the theory of § 2. Note that a single configuration can be described with different values for r and s (and hence different winding numbers) but the function

$\sigma(y)$ depends on p only. Remarkably, the complicated band structures can often be described by such a simple function $\sigma(y)$. We have checked several examples with p and q *not* relatively prime. In all such examples we find that $\sigma(y)$ is periodic with period $2\pi/K$ and is independent of the K solutions (r, s) to equations (2.24*a*, *b*) (cf figures 5(*c*) and (*d*) where $K = 2, 3$, respectively). Therefore, as discussed in § 2, the fundamental wavevector Q is given by equation (2.29).

In addition the function $h(y)$ is obtained by plotting

$$h_i = \sum_{j=1}^{i} \sigma_j - p \operatorname{Int}(\omega i/2\pi) + is \tag{3.2}$$

as a function of $y_i = \omega i \bmod 2\pi$. According to equation (2.21*c*) we should thus obtain the function f. Figure 6 shows the function $h(x)$ (from which $f(x)$ and $g(x)$ can be derived) for the same cases as in figure 5. Again we notice that the shape of the function h does indeed only depend on p. The predictions of the topological analysis (§ 2) are fulfilled for the most important plateaux. For the corresponding configurations, the mere existence of these functions clearly demonstrates the *finiteness* of the fluctuations of the positions u_i.

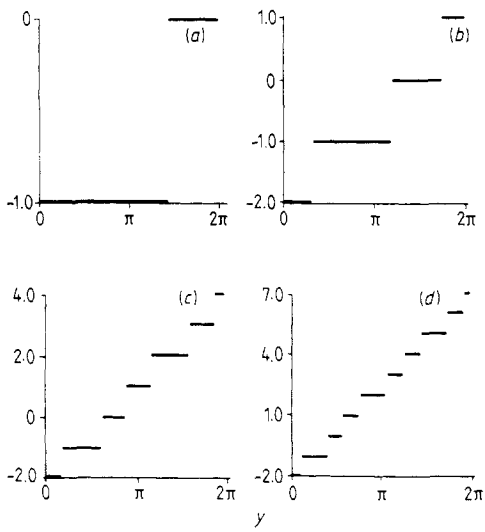

Figure 6. Hull function $h(y)$ for the same states as in figure 5.

If there is only one rational relationship between the three lengths, e.g. equation (2.4) has an integer solution, then the energy curve $F(M)$ looks qualitatively the same as in the irrational case, whereas the minimum energy configurations are now periodic (commensurate). A small perturbation therefore has little effect on the $F(M)$ curve but changes the configurations quite drastically: a periodic state becomes a band structure.

Finally, we show an example of *rational* l_1 and l_2: $l_1 = 4\pi/7 = 1.7952$ and $l_2 = 12\pi/7 = 5.3856$ (and $\delta = 8\pi/7 = 3.5904$). In this case the curve $F^N(M)$ has only a few corners with straight lines between; in the irrational case we had (infinitely) many corners which show up as curved lines between the more pronounced ones due to the finite size of the calculation. As a consequence the devil's staircase becomes harmless

with only a few steps corresponding to those few corners. Figure 7 shows this staircase with no additional plateaux appearing under magnification. If we add a small number (6×10^{-4}) to l_2 and thus destroy the property of rationality we again obtain a more complicated behaviour as shown in figure 8.

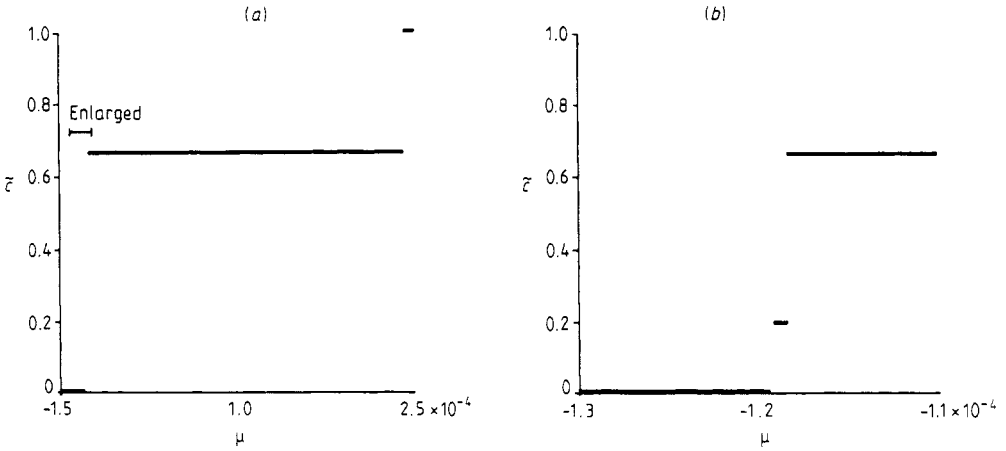

Figure 7. (*a*) Minimal concentration $\tilde{c}$ of $F(M)$ as a function of the chemical potential μ for rational l_1, l_2. (*b*) Enlargement of the region marked in (*a*).

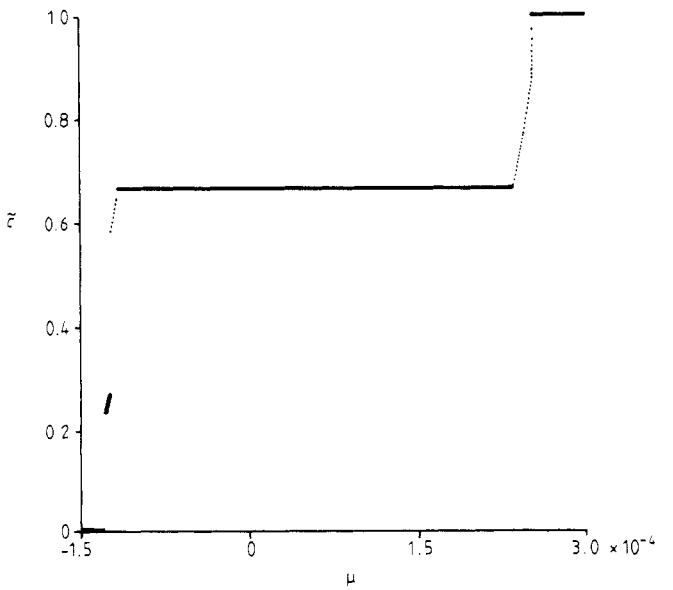

Figure 8. Same as figure 7(*a*), but with a small perturbation on the ratio l_1/l_2 (see § 3).

4. Conclusions

Our major conclusion, within the modified FK model introduced in § 1, has been that the presence of *non-convex* interactions does *not* in general give rise to a single first-order

transition (as anticipated on approximate grounds (e.g. Villain and Gordon 1980)), but rather results in many intermediate phases, quite probably an infinite number. It is important to note that our model involves competition of *three* lengths. According to some suggestions of Ruelle (1983), we might therefore have expected a structurally 'chaotic' ground state, but we have not observed this. There is, however, a possibility of 'marginal chaos' in the form of 'weak periodicity' (Aubry 1983a), occurring either in the limit of large p (i.e. many bands) or in special band structures. It is also important to note that the locking phases correspond, surprisingly, to incommensurate values of c and ω. In the special cases of $l_1/2\pi$ and $l_2/2\pi$ both rational, the ground states are commensurate and we find only a finite number of first-order transitions (cf figure 7 and the discussion in § 3). For l_1, l_2, 2π not rationally related there cannot exist *any* commensurate ground state. This assertion can be proved by contradiction. Assume we found a commensurate ground state, then there is an integer n so that $u_{i+n} - u_i = L$ which is independent of i and a combination of l_1 and l_2: $nl_1 + n_2 l_2 = L$. $L/2\pi$ is necessarily irrational from which we conclude that the sequence of points u_{i+kn} (mod 2π) is uniformly dense on the interval $[0, 2\pi]$ for any i. Consequently the energy of this configuration is just the average of the external potential $V(u)$ over one period which is always larger than any of the configurations we have obtained. Therefore it cannot be a ground state.

It is not necessarily easy to generalise our model. Nevertheless, it should be instructive to analyse complementary models with *three competing* lengths, e.g. the FK model extended to exclude two inequivalent periodic potentials. Also, non-Ising effects may modify our conclusions. For instance the devil's staircase we observed (§ 3) may become incomplete or we might find a mixture of this devel's staircase and that found for the usual purely convex FK model (i.e. locking at commensurate values of the local potential (V) period and the mean atomic distance). In our model the interatomic interaction is assumed to be dominant. We note that, in the usual convex FK model, if the interatomic potential dominates then the domain walls are wide (on the scale of a lattice spacing) and thus lattice pinning is weak. In our model the locking of phases is *not* due to the periodic potential, but mostly due to the barrier potential which must be overcome to change the atom's location from l_1 to l_2. Relaxing the Ising limit will mix these influences.

The potential barrier for changing between lengths l_1 and l_2 clearly leads us to anticipate the existence of many *metastable* states, corresponding to random distributions of l_1 and l_2. In particular, note that when $c(p)$ changes, p changes through arbitrarily large values (cf the hull functions in figure 6), implying large amplitude global rearrangements of atoms for large p. It would also be interesting to study the distribution in energy of the metastable states. In any experimental situation close to our model, we expect relaxation times for decay to the true ground state to be very long and perhaps even infinite (as, is probably the case in spin glasses). We have, of course, not included any explicit dynamics, but we should expect that very slow experiments are necessary. Extrinsic impurities and defects are likely to play an important role in this regard. On the other hand, our results may actually be relevant to modelling incommensurate systems with *mobile* defects, at least for ground-state properties, since such systems present three competing length scales—the lattice spacing, the mean defect separation and the period of the incommensurate potential. Interestingly, in the ferroelectric $Ba_2Na\,Nb_5O_5$, where there are intrinsic mobile vacancy defects (probably Na ions), locking to incommensurate structures has been observed (Schneck *et al* 1982).

To the extent that our basic model is experimentally relevant without more realistic modifications, we should expect a 'smeared first-order' transition to be observed, accompanied by broadened satellites of the incommensurate pattern or additional substructure (cf neutron scattering studies of Rb_2ZnBr_4 (Iizumi and Gesi 1983)). High resolution, slow experiments might show remnant effects of the theoretically implied devil's staircase, i.e. structure within the satellites. (The width should arise from the distribution of metastable states since the system cannot make instantaneous transitions between these.) The dominant modulation wavevector may still show remnants of the devil's staircase if the metastable states are not too disjoint. (Theoretically, the wavevector is probably very discontinuous everywhere.)

Acknowledgments

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Appendix 1

Here we describe in detail two examples of one-circle band structures which we have observed numerically as ground states.

Example 1. One-band structure

Figure 4(a) shows a ground state for which the $u_i \bmod 2\pi$ are uniformly distributed on a unique interval $[A_1B_1]$. The transformation T exchanges the intervals as shown in figure A1. The interval $[A_1B_1']$ is translated by l_1 on $[A_1'B_1]$. The interval $[B_1'B_1]$ is translated by l_2 on $[A_2A_2']$. The assumptions of § 2 are all fulfilled. Glueing B_1 and A_2, this transformation becomes a rotation by the length l_1 on the circle of length

$$\Phi = \overline{A_1B_1} = \overline{A_1A_2} + \overline{A_2B_1'} + \overline{B_1'B_1} = 2\pi - l_2 + l_1.$$

This example corresponds to

$$p = q = 1 \qquad \text{and} \qquad r = s = 0$$

for the conditions given in § 2.

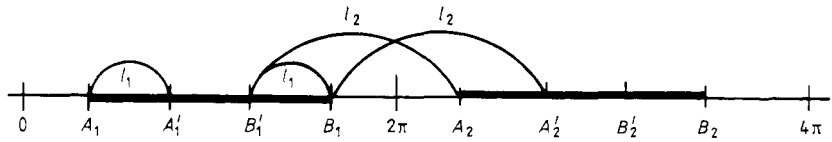

Figure A1. Schematic graph of a one-band structure.

Example 2. Three-band structure

There exist several possible three-band structures. The ground state which has the distribution of $u_i \bmod 2\pi$ shown in figure 3 is associated with the graph shown in figure A2. (Note that for didactic convenience we use a slightly modified notation

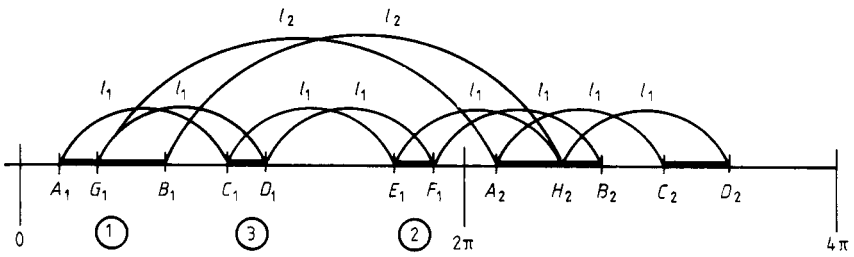

Figure A2. Schematic graph of a three-band structure.

from § 2.) The interval $[AG_1]$ is translated by l_1 in $[C_1D_1]$. The interval $[G_1B_1]$ is translated by l_2 in $[A_2H_2]$. The interval $[C_1D_1]$ is translated by l_1 in $[E_1F_1]$. The interval $[E_1F_1]$ is translated by l_1 in $[H_2B_2]$. The assumptions of § 2 are all fulfilled if these intervals are glued in the order $[A_1B_1]$, $[E_1F_1]$, $[C_1D_1]$. The width and the relative positions of these intervals are easily found by solving linear equations. We define the parameters

$$\Delta_1 = \overline{A_1B_1}$$

$$\Delta_2 = \overline{A_1G_1} = \overline{C_1D_1} = \overline{E_1F_1} = \overline{H_2B_2}$$

$$\delta_1 = \overline{B_1C_1} \qquad \delta_2 = \overline{D_1E_1}.$$

By inspection of figure A2, we write

$$\overline{A_1C_1} = \Delta_1 + \delta_1 = l_1 \qquad \overline{G_1A_1} = 2\pi - \Delta_2 = l_2$$

$$\overline{C_1E_1} = \Delta_2 + \delta_2 = l_1 \qquad \overline{F_1B_2} = 2\pi - B_1F_1 = 2\pi - (\delta_1 + \delta_2 + 2\Delta_2) = l_1$$

which yields

$$\Delta_1 = 3l_1 - l_2 \qquad \Delta_2 = 2\pi - l_2$$

$$\delta_1 = l_2 - 2l_1 \qquad \delta_2 = l_1 + l_2 - 2\pi.$$

To have non-overlapping intervals we must have $\Delta_1 > 0$, $\Delta_2 > 0$, $\delta_1 > 0$, $\delta_2 > 0$, which yields

$$\tfrac{1}{3}l_2 < l_1 < \tfrac{1}{2}l_2$$

and

$$0 < l_1 + l_2 < 2\pi.$$

The total bandwidth is

$$\Phi = \Delta_1 + 2\Delta_2 = 4\pi - 3(l_2 - l_1)$$

and the rotation length θ is

$$\theta = \Delta_1 + \Delta_2 = l_1 + 2\pi - 2(l_2 - l_1)$$

which corresponds to the set of integers

$$p = 3 \qquad q = 2$$

$$r = 1 \qquad s = 2$$

according to formulae (2.13*a*) and (2.16).

Appendix 2

The purpose of this appendix is to prove that, for an integer p, the probability P, that there exist two integers r and s such that with

$$q(p) = 1 + \mathrm{Int}(p\delta/2\pi) \tag{A2.1a}$$

we have

$$qs - pr = \mathrm{Int}(pl_1/2\pi) \tag{A2.1b}$$

and

$$\mathrm{Int}(pl_2/2\pi) = \mathrm{Int}(pl_1/2\pi) + \mathrm{Int}(p\delta/2\pi), \tag{A2.1c}$$

is equal to

$$P = \frac{3}{\pi^2} \sum_{n=1}^{\infty} \frac{1}{n^3} \simeq 0.365\,38. \tag{A2.2}$$

(Independent of δ, l_1 providing these are not rationally related to 2π.) Consequently the sequence of p_i such that it is possible to find q, r, s fulfilling (A2.1) is *infinite*. In addition we prove that the sequence of points $(p_i\,\delta/2\pi \bmod 1,\ p_i\,l_1/2\pi \bmod 1)$ is *uniformly dense* in the triangle $((0,0), (0,1), (1,0))$.

Before proving these results, we make some preliminary remarks.

Remark 1. Let be m, n, k be three given integers (possibly equal) and p a random integer. The events

(i) p divisible by m,

(ii) $q(p)$ divisible by n,

(iii) Int $pl_1/2\pi$ divisible by k,

are independent.

Proof. The probability for an integer p to be divisible by m is $1/m$. We first show that the probability for $q(p)$ to be divisible by n is $1/n$. Indeed $q(p)$ is divisible by n when there exists an integer j such that

$$q = jn = 1 + \mathrm{Int}(p\delta/2\pi). \tag{A2.3a}$$

This condition is equivalent to

$$jn - 1 < p\delta/2\pi < jn \tag{A2.3b}$$

or

$$1 - \frac{1}{n} < \frac{p\delta}{2\pi n} \bmod 1 < 1. \tag{A2.3c}$$

Since $\delta/2\pi n$ is an irrational number the sequence $p\delta/2\pi n \bmod 1$ is uniformly dense on $[0, 1]$. Then the probability that (A2.3) be fulfilled is $1/n$. The same result is obtained for the conditional probability of the event $q(p)$ being divisible by n assuming that p is divisible by m. We first have to reproduce the same argument with $p = mp'$ and to use the fact that $m\delta/2\pi n$ is also an irrational number. Consequently the events (i) and (ii) are independent. In the same way, we prove that the events (i) and (iii)

are independent. We now prove that the event (iii) is independent of the unique event (ii) (and also of the simultaneous event (i) and (ii)). Int$(pl_1/2\pi)$ is divisible by k when we have

$$0 < \frac{pl_1}{2\pi k} \bmod 1 < \frac{1}{k}. \tag{A2.4}$$

q is divisible by n when (A2.3c) is fulfilled. Since δ/n and l_1/k are not rationally related to 2π the sequence of points $(p\delta/2\pi n \bmod 1,\ pl_1/2\pi k \bmod 1)$ is uniformly dense in the square $[0, 1]\times[0, 1]$. Consequently, the probability to fulfil both events (ii) and (iii) is $1/nk$, the product of the separate probabilities of these events. The same result holds for the conditional probability of (ii) and (iii) if (i) holds. This proves that the events (i), (ii) and (iii) are independent.

Remark 2. The probability that p and q be relatively prime is $6/\pi^2$.

Proof. The event p (or q) divisible by a prime number ρ_1 is independent of the event p (or q) divisible by another prime number ρ_2 because both conditions are equivalent to the unique condition: p (or q) divisible by the product $\rho_1\rho_2$. To be relatively prime, a necessary and sufficient condition for p and q is that they are not both divisible by any prime number ρ_i. This probability is $(1-1/\rho_i^2)$. Then the probability that p and q be relatively prime is the product

$$Q = \prod_{\rho_i} \left(1 - \frac{1}{\rho_i^2}\right) \tag{A2.5}$$

over all prime numbers. A well known method due to Riemann allows us to calculate this infinite product. We calculate $1/Q$ which can be written

$$\begin{aligned} \frac{1}{Q} &= \prod_i \frac{1}{1-1/\rho_i^2} = \prod_i \left(\sum_{n=0}^{\infty} \frac{1}{\rho_i^{2n}}\right) \\ &= \sum_{\{n_i\}} \frac{1}{(\Pi_i \rho_i^{2n_i})}. \end{aligned} \tag{A2.6}$$

The last term in (A2.6) contains all the possible products $\rho_1^{n_1}\rho_2^{n_2}\ldots\rho_i^{n_i}\ldots$ with $n_i = 0, 1, 2, \ldots$. These products are the unique decompositions into prime numbers of the series of integers. Then, we find

$$\frac{1}{Q} = \sum_{m=1}^{\infty} \frac{1}{m^2} = \frac{\pi^2}{6}. \tag{A2.7}$$

Using these two remarks, we can now calculate the probability that (A2.1b) be fulfilled. This condition is equivalent to requiring that Int$(pl_1/2\pi)$ be a multiple of the largest common divisor of p and q. The probability that this number takes a given value m is equal to the product of the probability, $1/m^2$, that p and q be both divisible by m multiplied by the independent probability, $6/\pi^2$, that the quotients of p and q by m be relatively prime. The probability of the independent events that m also divides Int(pl_2) is $(1/m^2)(6/\pi^2)(1/m)$. Then the probability that (A2.3b) be fulfilled is equal to the sum of the probabilities of all the (excluded) events for which (A2.1b) is fulfilled

with the largest common divisor m, i.e.

$$P = \frac{6}{\pi^2} \sum_{m=1}^{\infty} \frac{1}{m^3}. \tag{A2.8}$$

The second event (A2.1c) is equivalent to

$$\frac{pl_1}{2\pi} \bmod 1 + \frac{p\delta}{2\pi} \bmod 1 < 1. \tag{A2.9}$$

It is fulfilled with probability $\frac{1}{2}$ since the sequence $(pl_1/2\pi \bmod 1,\ p\delta/2\pi \bmod 1)$ is uniformly dense in the square $[0, 1]\times[0, 1]$. Using the same arguments as in remark 1, it is easy to prove that the event (A2.1c) is independent of the divisibility events of p, q and $\mathrm{Int}(pl_1/2\pi)$ by any integers used for finding the probability for the event (A2.1b). Consequently, the probability of fulfilling both (A2.1b) and (A2.1c) is the product of the two independent probabilities for (A2.1b) and (A2.1c) which yields (A2.2). The final assertion of uniform density is an obvious consequence of this independence.

Appendix 3

Here we derive the simple recursion relation for calculating the ground state of the free energy (1.1) (with non-convex interaction (1.4)). Since the distance between u_{n+1} and u_n can only be l_1 or $l_2 = l_1 + \delta$ we can write, for a chain with N particles,

$$F = \sum_{n=1}^{N} V(u_n) = \sum_{n=1}^{N} V\left(u_0 + nl_1 + \left(\sum_{i=1}^{n} \sigma_i\right)\delta\right) \tag{A3.1}$$

with $\sigma_i \in \{0, 1\}$. The Ising-like variables σ_i denote whether the distance $u_{n+1} - u_n$ is l_1 or l_2. If we introduce a magnetisation

$$M = \sum_{n=1}^{N} \sigma_n \qquad 0 \leqslant M \leqslant N \tag{A3.2}$$

for the sequence $u_0, u_1, \ldots, u_N$, then the energy of a chain with $N+1$ particles becomes

$$F_M^{N+1} = F_M^N + V(u_0 + M\delta + (N+1)l_1) \qquad \text{if } \sigma_{N+1} = 0 \tag{A3.3a}$$

or

$$F_M^{N+1} = F_{M-1}^N + V(u_0 + M\delta + (N+1)l_1) \qquad \text{if } \sigma_{N+1} = 1. \tag{A3.3b}$$

Note that the additional term is the same in both cases (A3.3a, b), which now determine a simple recursion relation for calculating the states of lowest energy, namely

$$\{F_{M-1}^N, F_M^N\} \to \{F_M^{N+1}(\sigma_{N+1} = 1), F_M^{N+1}(\sigma_{N+1} = 0)\}$$

where either $\sigma_{N+1} = 0$ or 1 is taken according to which energy (F_M^N or F_{M-1}^N) is the lowest. The sequences for F_0^{N+1} and F_{N+1}^{N+1} are trivial. u_0 is an arbitrary initial phase and is chosen as $u_0 = 0$. (Other choices of u_0 affect only initial iteration transients.)

The chemical potential μ is set to zero for these calculations. If we want to obtain the ground state for a different value of μ we simply add $-\mu M$ to F_M^N for all M and search for the new minimum.

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