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J. Phys. A: Math. Gen. **20** (1987) 1259-1268. Printed in the UK

Frustration effects in quasicrystals: an exactly soluble example in one dimension

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Received 6 March 1986

Abstract. Frustration effects due to competing interactions between magnetic atoms in quasicrystals are studied in an exactly soluble example: the Ising chain in a quasiperiodic two-valued magnetic field. At zero temperature the model exhibits an infinity of pure phases, characterised by a modulation of the order parameter which reflects the aperiodic structure of the system, up to a larger and larger length scale.

1. Introduction

Since the experimental discovery by Shechtman *et al* [1] of icosahedral symmetry associated with long-range order in Al-Mn alloys, there has been a growing interest in this new *quasicrystalline* state of matter [2]. Among the structural models that have been proposed to describe these phases, the most appealing one is certainly the *strip method* [3-5]. This algorithm generates quasiperiodic tilings of Euclidean space by projection from a regular lattice in a higher-dimensional space. Up to now, physicists have mainly focused their attention on the structural properties of quasicrystals (position of atoms, topology of defects, etc). The systematic study of their physical properties is still in its earliest stages.

In this paper, we aim to emphasise that the lack of periodicity of quasicrystals may have spectacular consequences for their magnetic properties, as soon as some *frustration* is present. A system is frustrated if some of its interactions are in competition, such that there exists no ground state which satisfies all of them [6]. Since the geometry of quasicrystals exhibits some structure at every length scale, their magnetic phase diagram may correlatively be expected to have a very rich content.

We shall illustrate these general considerations by solving a simple one-dimensional example of a frustrated quasicrystal: a ferromagnetic Ising chain in a quasiperiodic two-valued magnetic field. Section 2 describes the model, and presents some general formalism, which we have already used in the study of harmonic excitations (phonons) on the same geometrical structure, in collaboration with Petritis [7]. Section 3 is devoted to an analytic solution of the model at zero temperature. The outcome is quite remarkable: besides the two expected ordered phases, the system exhibits two infinite sequences of other pure phases. Each of these phases, labelled by an integer (L) or $(-L)$, is characterised by a non-trivial total magnetisation, due to a spatial modulation of the order parameter. This pattern reflects the quasiperiodicity of the system up to a maximal scale, which diverges as the label (L) or $(-L)$ of the phase becomes larger.

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2. The model

The geometrical model of a one-dimensional quasicrystal we have chosen to consider is generated by the well known projection method [3-5]. The line D to be tiled is drawn in the Euclidean plane, contains the origin 0 and makes an angle $\theta (0 < \theta < \pi/4)$ with the x axis. Consider the strip swept by shifting the unit square $(-1 < x \leqslant 0;\ -1 < y \leqslant 0)$ along D. If we project orthogonally onto D all points of the strip with integer coordinates, we obtain a quasiperiodic tiling of the real line with two types of segments, namely short and long ones, of length $s = \sin\theta$ and $c = \cos\theta$, respectively (see figure 1). Throughout the following, θ assumes the value θ_∞ such that $\tan\theta_\infty = \tau^{-1} = \tau - 1$, where $\tau = (\sqrt{5}+1)/2$ is the golden mean. This particular choice has two advantages: τ is the irrational number which is 'the worst approximated by rationals', and hence the value for which the effects of aperiodicity can be expected to be the most important. Moreover, the directions along which the six-dimensional hypercubic lattice has to be projected in order to get a three-dimensional tiling with icosahedral symmetry also involve the golden mean [3-5]. We expect that the essential features of our model remain qualitatively the same for any irrational value of $\tan\theta$ with typical Diophantine properties.

The magnetic model we aim to study is defined by putting two types of atoms on the *bonds* of D, according to their length, i.e. c atoms on long bonds and s atoms on short ones. Each atom has spin $\frac{1}{2}(\sigma_n = \pm 1)$ and nearest-neighbour couplings of unit strength $(J = 1)$, irrespective of its type. Moreover, each spin σ_n feels a *local field* h_n, which depends only on its type (c or s). The Hamiltonian of the model is therefore

$$\mathcal{H} = -\sum_n \sigma_n \sigma_{n+1} - \sum_n h_n \sigma_n \tag{1}$$

where $h_n = h_c$ or h_s, according to the length of the nth bond of D (see figure 2). The

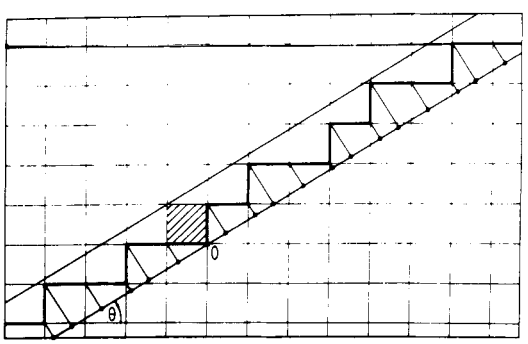

Figure 1. Construction of a quasiperiodic tiling of the line by the strip method.

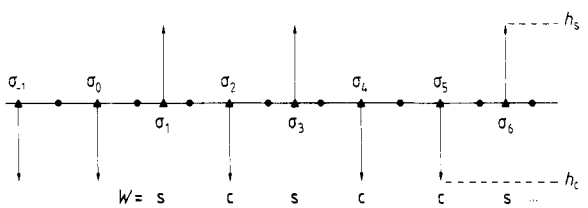

Figure 2. Definition of the almost periodic magnetic fields h_n in connection with the word W coding the geometry of the model.

two values h_s and h_c of the quasiperiodic magnetic field are the basic parameters of the model. Its thermodynamical properties are clearly invariant under a global change of sign of the field: $(h_c; h_s) \to (-h_c; -h_s)$. The model is frustrated if h_c and h_s have different signs, i.e. $h_s < 0 < h_c$ or vice versa.

The implementation of a transfer matrix formalism for the present model is very easy. Our presentation will closely follow the lines of our previous work [7] on the phonon spectrum of the very same structure. We shall recall some useful results on the geometry of the model, referring the reader to our previous publication for a detailed derivation. Consider the infinite word $W = \text{scscc}\ldots$ built by the succession of long and short segments of the tiling, starting from the origin (see figure 2). W is the limit of a sequence of *finite* words W_L, which obey a three-term recursion relation

$$W_L = W_{L-1} W_{L-2} \qquad L \text{ even}$$
$$W_L = W_{L-2} W_{L-1} \qquad L \text{ odd} \tag{2a}$$

together with the initial conditions

$$W_{-1} = \text{s} \qquad W_0 = \text{c}. \tag{2b}$$

The finite word W_L is the basic cell of the *periodic* tiling of D generated by the projection algorithm, if the angle θ_L between D and the x axis is such that

$$\tan \theta_L = t_L = F_L / F_{L+1} \tag{3}$$

where the rational t_L is the Lth principal convergent of the reciprocal golden mean τ^{-1}. The integers F_L are the well known Fibonacci numbers, defined by the recursion ($L \geqslant 1$)

$$F_L = F_{L-1} + F_{L-2} \tag{4a}$$

and the initial values

$$F_{-1} = 1 \qquad F_0 = 0. \tag{4b}$$

This sequence of numbers plays an important role in the following; we have in particular made use of numerous identities among them, which can all be easily derived from their simple expression in terms of τ:

$$F_L = [\tau^L - (-\tau)^{-L}]/\sqrt{5}. \tag{5}$$

Note that the length of W_L is F_{L+2}.

We are interested in the free energy $f(\beta)$ of the model defined by the Hamiltonian (1) at temperature β^{-1}. This quantity is simply given by

$$f = -\beta^{-1} \lim_{N \to \infty} (N^{-1} \ln \operatorname{Tr} T(N)) \tag{6}$$

where $T(N)$ is the product of N elementary transfer matrices $M(h_n)$

$$T(N) = \prod_{1 \leqslant n \leqslant N} M(h_n). \tag{7}$$

The numbers h_n are equal to h_c or h_s, according to the value of the nth letter of the infinite word W. The 2×2 matrix $M(h)$ is

$$M(h) = \begin{bmatrix} \exp[\beta(1+h)] & \exp[\beta(-1-h)] \\ \exp[\beta(-1+h)] & \exp[\beta(1-h)] \end{bmatrix}. \tag{8}$$

Owing to the properties of the approximants t_L, the free energy $f(\beta)$ can also be evaluated through

$$f = \lim_{L\to\infty} f_L \tag{9a}$$

$$f_L = -(\beta F_{L+2})^{-1} \ln \mathrm{Tr}\, \mathscr{C}_L \tag{9b}$$

where $\mathscr{C}_L$ is the product of the F_{L+2} matrices $M(h)$ associated with the F_{L+2} letters of the word W_L. Moreover f_L has a simple interpretation: it is the free energy of the *periodic* model defined by the angle θ_L (see equation (3)). The matrices $\mathscr{C}_L$ obey by definition the recursion relation (2*a*), with the factors in the opposite order, since matrix products are conventionally read from right to left ($L \geqslant 1$)

$$\begin{aligned} &\mathscr{C}_L = \mathscr{C}_{L-1}\mathscr{C}_{L-2} \qquad && L \text{ odd} \\ &\mathscr{C}_L = \mathscr{C}_{L-2}\mathscr{C}_{L-1} \qquad && L \text{ even} \end{aligned} \tag{10a}$$

together with the initial conditions

$$\mathscr{C}_{-1} = M(h_s) \qquad \mathscr{C}_0 = M(h_c). \tag{10b}$$

This last property can easily be shown to imply that the *traces* x_L and *determinants* y_L of $\mathscr{C}_L$ obey the following recursion:

$$\begin{aligned} &x_L = x_{L-1}x_{L-2} - x_{L-3}y_{L-2} \qquad && L \geqslant 2 \\ &y_L = y_{L-1}y_{L-2} \qquad && L \geqslant 1 \end{aligned} \tag{11a}$$

while the initial conditions (10*b*) are now

$$\begin{aligned} &x_{-1} = 2\,\mathrm{e}^{\beta}\cosh(\beta h_s) \\ &x_0 = 2\,\mathrm{e}^{\beta}\cosh(\beta h_c) \\ &x_1 = 2\mathrm{e}^{2\beta}\cosh[\beta(h_s+h_c)] + 2\mathrm{e}^{-2\beta}\cosh[\beta(h_s-h_c)] \\ &y_{-1} = y_0 = 2\sinh(2\beta). \end{aligned} \tag{11b}$$

The recursion (11*a*) generalises to arbitrary 2×2 matrices the mapping introduced by several authors [8–12] in the case of matrices with determinant unity, which was the starting point of a renormalisation group analysis of Schrödinger equations with quasiperiodic potentials. We have also made use of this mapping in [7] in order to study the low-frequency behaviour of the phonon model.

The recursion relations (11*a*) and the initial conditions (11*b*) allow one to determine the free energy of the model through the simple formula (see equation (9*b*))

$$f = -\beta^{-1} \lim_{L\to\infty} \left(F_{L+2}^{-1} \ln x_L \right) \tag{12}$$

which can indeed be used to compute $f(\beta)$ numerically at finite temperature. The zero-temperature limit is a more subtle point, to be discussed in the next section.

3. Exact solution at zero temperature

In this section, we derive an exact expression of the *ground-state energy* E_0 of the model, which is by definition

$$E_0 = \lim_{\beta\to\infty} f(\beta). \tag{13}$$

The mapping (11*a*) acting on the traces and determinants of $\mathscr{C}_L$ contains a minus sign, and hence involves huge compensations at low temperature ($\beta \to \infty$), where x_L and y_L become large. It is therefore preferable to go back to the matrix equations (10). Let us first remark that the free energy $f(\beta)$ depends on the matrices $\mathscr{C}_L$ only through their *invariants* x_L and y_L, and hence remains unchanged if we forget about the ordering prescription (10*a*) and always put $\mathscr{C}_{L-1}$ at the left of $\mathscr{C}_{L-2}$, say. From a geometrical point of view, this modification amounts to performing a cyclic permutation of letters on each finite word W_L, which leaves the quantity f_L invariant.

In order to obtain the ground-state energy E_0 of the model, it is sufficient to follow the leading behaviour as $\beta \to \infty$ of each entry of the matrix $\mathscr{C}_L$ (see, for instance, [13]). The exponents $a_L, \ldots, d_L$ such that

$$\mathscr{C}_L \underset{\beta\to\infty}{\sim} \begin{bmatrix} \exp(\beta a_L) & \exp(\beta b_L) \\ \exp(\beta c_L) & \exp(\beta d_L) \end{bmatrix} \tag{14}$$

obey the following recursion:

$$\begin{aligned} a_L &= \mathrm{Sup}(a_{L-1} + a_{L-2};\ b_{L-1} + c_{L-2}) \\ b_L &= \mathrm{Sup}(a_{L-1} + b_{L-2};\ b_{L-1} + d_{L-2}) \\ c_L &= \mathrm{Sup}(c_{L-1} + a_{L-2};\ d_{L-1} + c_{L-2}) \\ d_L &= \mathrm{Sup}(c_{L-1} + b_{L-2};\ d_{L-1} + d_{L-2}) \end{aligned} \tag{15a}$$

and the initial conditions (10*b*) imply

$$\begin{aligned} a_{-1} &= -b_{-1} = 1 + h_s & d_{-1} &= -c_{-1} = 1 - h_s \\ a_0 &= -b_0 = 1 + h_c & d_0 &= -c_0 = 1 - h_c. \end{aligned} \tag{15b}$$

The ground-state energy is then given by

$$E_0 = -\lim_{L\to\infty} [F_{L+2}^{-1}\, \mathrm{Sup}(a_L;\ d_L)] \tag{16}$$

where Sup denotes the larger of its two arguments.

Let us first illustrate how this formalism works in the simple case where both magnetic fields h_s and h_c are positive. Under these conditions, it is easy to realise that a_L is larger than d_L, and that a_L obey the very same three-term recursion relation (4*a*) as the Fibonacci numbers. Since F_{L+1} and F_{L+2} form a basis of the solutions of equation (4*a*), there exist two constants α, β such that

$$a_L = \alpha F_{L+2} + \beta F_{L+1}. \tag{17a}$$

The ground-state energy then becomes

$$E_0 = -(\alpha + \beta\tau^{-1}). \tag{17b}$$

In the present case (h_s and h_c positive), the initial conditions (15*b*) fix $\alpha = 1 + h_s$ and $\beta = h_c - h_s$ and yield

$$E_0^{(1)} = -(1 + \tau^{-1}h_c + \tau^{-2}h_s) \qquad (h_c > 0;\ h_s > 0). \tag{18}$$

This is indeed the expected expression for the ground state of a fully ordered phase ($\sigma_n = +1$), since atoms of types c and s have densities τ^{-1} and τ^{-2}, respectively. In other words, the zero-temperature magnetisation

$$M_0 = -\left(\frac{\partial}{\partial h_c} + \frac{\partial}{\partial h_s}\right) E_0 \tag{19}$$

is identically equal to +1 in this phase.

Let us now turn to the interesting case where h_c and h_s have different signs, and lead to a frustrated model. We shall present the results for $h_c < 0 < h_s$. The main idea is that the quantities $\mathrm{Sup}(a_L; d_L)$ still obey the recursion relation (4*a*) for large enough L, and hence the ground-state energy is still given by (17*b*), where α and β are two functions of h_c and h_s to be determined.

The study of the recursion (15) involves many inequalities and it would be tedious to translate it into words. We prefer to summarise it in a flow chart (figure 3), where the comparisons implied by (15*a*) are represented by tests. At each new value of the iteration label L, four new regions of the parameter plane $(h_c; h_s)$ arise: two of them join the totally ordered (+) or (−) phases, denoted (1) and (−1), respectively, while a third region builds a new pure phase, labelled $(L+1)$, and the fourth and last region remains undecidable and needs at least one more iteration.

The phase diagram of our model is hence as follows: besides two totally ordered phases, denoted (1) and (−1), there exist *an infinity of other pure phases*, denoted (L), and their transforms under $(h_s; h_c) \to (-h_s; -h_c)$, denoted $(-L)$. The end of this section is devoted to a quantitative study of these phases.

For the pure phase (L), the quantities

$$S_N^{(L)} = \mathrm{Sup}(a_N; d_N) \tag{20}$$

obey the recursion (4*a*) for $N \geqslant L$. $S_{L-2}^{(L)}$ assumes the same value as in one of the totally ordered phases, namely (1) for even L and (−1) for odd L (see figure 3, left)

$$S_{L-2}^{(L)} = F_L + (-1)^{L-1}(F_{L-1}h_c + F_{L-2}h_s). \tag{21a}$$

$S_{L-1}^{(L)}$ is a slightly more delicate quantity; it is shown by inspection to obey a linear recursion between two consecutive pure phases

$$S_{L-1}^{(L)} = S_{L-2}^{(L-1)} + S_{L-3}^{(L-1)}. \tag{21b}$$

After solving this last equation, we determine the ground-state energy by means of (17*b*). Our final result is $(L \geqslant 2)$

$$E_0^{(L)} = -1 + (-1)^L(\tau^{-1}h_c + \tau^{-2}h_s) + 2(\tau^{-1}F_L - F_{L-1}) \times [F_{L-1}h_c + F_{L-2}h_s + (-1)^L(h_s - h_c - 2)]. \tag{22}$$

This rather lengthy expression contains all information of physical interest. The boundary between phases (L) and $(L-1)$ is a part of the line defined by the equation $(L \geqslant 3)$

$$F_{L-3}h_c + F_{L-4}h_s + (-1)^L(h_s - h_c - 2) = 0. \tag{23}$$

Figure 4 shows the complete phase diagram of the model. As the label L is increased, the phases (L) become smaller and smaller, and accumulate onto a limit point

$$\Omega: (h_s = 2\tau^{-1};\ h_c = -2\tau^{-2}). \tag{24}$$

The whole diagram is completed by symmetry WRT the origin. Figure 5 shows an enlargement of the vicinity of Ω. For $L \geqslant 4$, the domain of existence of the pure phase (L) is a triangle defined by its vertices $P^{(L)}$, $P^{(L+1)}$, $P^{(L+2)}$. Conversely, $P^{(L)}$ is the coexistence point of three consecutive phases (L), $(L-1)$, $(L-2)$. Its coordinates are $(L \geqslant 4)$

$$P^{(L)}: \left(h_s = \frac{2F_{L-2}}{F_{L-1} - 1};\ h_c = \frac{-2F_{L-3}}{F_{L-1} - 1} \right). \tag{25}$$

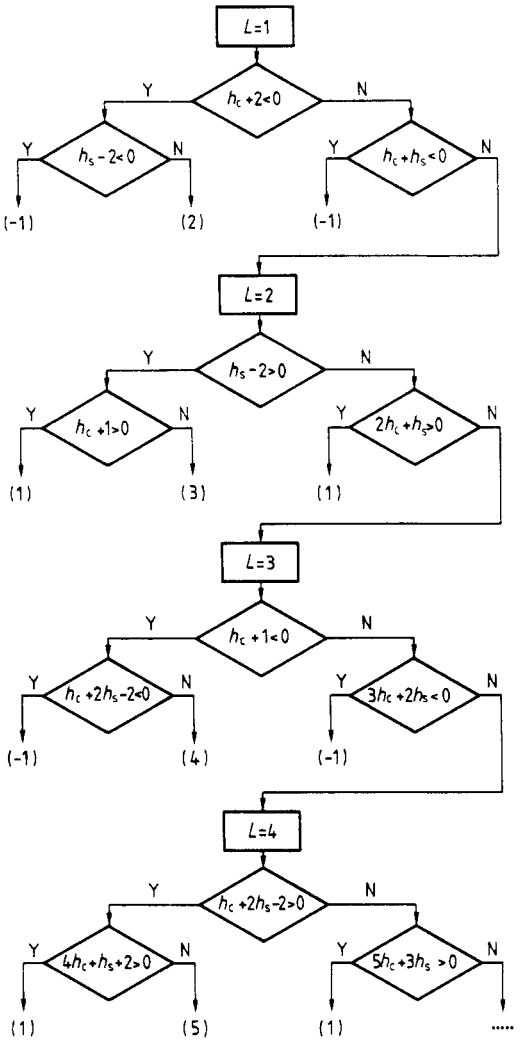

Figure 3. Flow chart of the iterative solution of (15). A new pure phase arises at each step of the recursion.

Among the six unbounded phases, (2), (−2), (3), (−3) have very simple shapes, while the boundaries of the totally ordered phases (1) and (−1) are made of an infinity of segments, including $\Omega\Omega'$. The equation of this last line is $\bar{h}=0$, where

$$\bar{h}=\tau^{-1}h_c+\tau^{-2}h_s \tag{26}$$

is the averaged applied field.

Let us now characterise the physical properties of this infinity of pure phases. Their zero-temperature magnetisation, given by (19), becomes

$$M_0^{(L)}=2F_L(F_{L-1}-\tau^{-1}F_L)-(-1)^L. \tag{27}$$

It is constant in each of the phases, which is characterised by a specific ordering of the spins at zero temperature. For the first five values of L, we have been able to determine this ordering by inspection, since it coincides with the one of the model

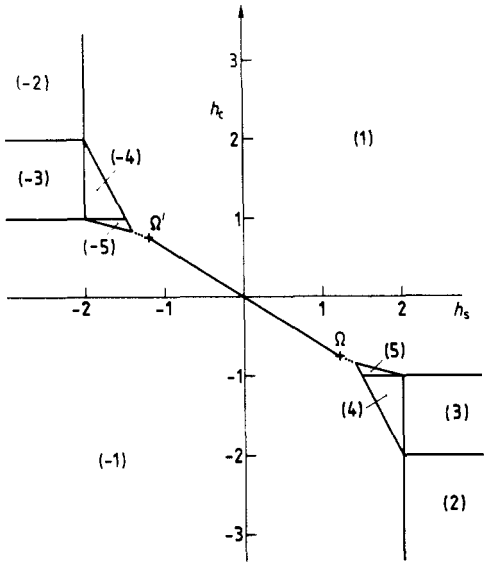

Figure 4. Zero-temperature phase diagram in the $(h_s; h_c)$ plane, showing the domains of existence of the phases (L) and $(-L)(L \leqslant 5)$ and their accumulation points Ω, Ω'.

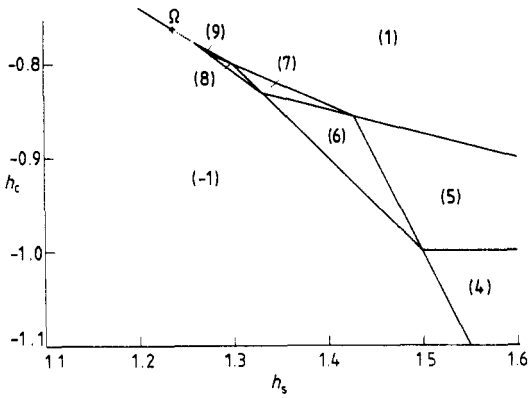

Figure 5. Enlargment of figure 4 around the accumulation point Ω, showing the domains of existence of the first nine pure phases.

Table 1. Spin orientations and total magnetisation of the first five pure phases (L), showing the larger and larger size of ordered clusters.

Phase	Spin orientations at zero temperature														
W	s	c	s	c	c	s	c	s	c	c	s	c	c	···	Magnetisation M_0
1	+	+	+	+	+	+	+	+	+	+	+	+	+	···	1
2	+	−	+	−	−	+	−	+	−	−	+	−	−	···	$1-2\tau^{-1}=-0.236\,07$
3	+	+	+	−	−	+	+	+	−	−	+	−	−	···	$5-8\tau^{-1}=0.055\,73$
4	+	+	+	−	−	+	+	+	−	−	−	−	−	···	$11-18\tau^{-1}=-0.124\,61$
5	+	+	+	+	+	+	+	+	−	−	−	−	−	···	$31-50\tau^{-1}=0.098\,30$

defined by the approximant θ_L (see (3)) for the same values of the magnetic fields. We present these results in table 1, together with the associated values of the zero-temperature magnetisation $M_0^{(L)}$. It is remarkable that the sequence of values $M_0^{(L)}$ does not go to zero, but approaches a simple oscillating law

$$M_0^{(L)} \underset{L\to\infty}{\sim} (-1)^{L-1}(1-2/\sqrt{5}) \tag{28}$$

with $1-2/\sqrt{5}=0.105\,57$, while the averaged applied field $\bar{h}$ (see (26)) goes uniformly to zero on the domain of existence of phase (L) as L gets large.

It can be shown recursively that the zero-temperature spin orientations in phase (L) are deduced from those in phase $(L-1)$ by flipping the *smallest* clusters of up (or down) spins. These smallest clusters are indeed the most fragile ones. The order parameter (succession of spin orientations) hence develops some structure at larger and larger length scales: the largest ordered cluster appearing in phase (L) has indeed length F_{L+1}.

The boundaries between any two phases are first-order transition lines (the magnetisation is indeed discontinuous). The zero-point entropy vanishes inside each pure phase, since the spin configurations listed in the table are the *unique* ground states of the phases. Along the transition lines, the entropy is non-trivial, since *at least* the two ground states of the adjacent phases become degenerate.

The existence of modulation in the order parameter at an arbitrarily large length scale is certainly one of the most spectacular physical properties induced by the geometry of quasicrystals. It would be very interesting to find evidences that analogous modulated phases survive at finite temperature in two- or three-dimensional magnetic quasicrystals.

Acknowledgment

It is a pleasure to thank Claude Godrèche for useful discussions.

Note added. After completion of the present work, the author became aware of a recent article by Achiam *et al* [14], which also concerns the Ising model on a one-dimensional quasiperiodic structure. The emphasis is put on quite different and complementary aspects in [14] and in the present paper. Achiam *et al* examine in detail the *scaling* properties and the corrections to scaling around the zero-temperature fixed point by means of an exact real space renormalisation procedure, both with and without an external magnetic field. We focus our attention on the effects of *frustration* on the complexity of the zero-temperature phase diagram and on the structure of the ground states.

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