# Ground states of frustrated Ising quasicrystals



1993 J. Phys. A: Math. Gen. 26 2791

(http://iopscience.iop.org/0305-4470/26/12/019)

J. Phys. A: Math. Gen. 26 (1993) 2791–2802. Printed in the UK

# Ground states of frustrated Ising quasicrystals

M Duneau†, F Dunlop† and C Oguey‡§

† Centre de Physique Théorique, CNRS-UPR 14, Ecole Polytechnique, F-91128 Palaiseau, France

‡ Laboratoire de Physique des Solides, CNRS-URA 02, Bat. 510, Université de Paris-Sud, F-91405 Orsay, France

Received 27 July 1992, in final form 8 December 1992

**Abstract.** The ground states of a two-dimensional quasiperiodic Ising model are investigated. The spin variables are put on the vertices of a tiling with quasiperiodic 8-fold symmetry and the couplings are short range, ferro- or antiferro-magnetic according to the pair distances. Among our results, the ordering of the spins is neither rigid nor random, but structured in a hierarchical way. A significant degree of frustration is present in the ground states whose energy is computed exactly. The residual entropy is bounded from below and computed exactly in some cases.

## 1. Introduction

In order to investigate the magnetic behaviour of quasicrystals at low temperature, a few models were proposed and analysed by Duneau *et al* (1991). We continue this work here.

Since the atomic structure of quasicrystals is not yet entirely solved, there is no sufficiently exact model on which to make computations. Moreover the electronic problem in such materials is too involved to reach the level of reliable predictions. Nevertheless, one can raise the question of magnetic ordering on simpler models, such as Ising ones, built on quasiperiodic tilings whose structure is better known and still close to actual quasicrystals. What is the influence, on the magnetic ground state, of an underlying aperiodic symmetry such as the 8-fold point symmetry and a quasiperiodic translational order? How does the ground state depend on the detailed features (in signs and strengths) of the spin interactions? These two questions summarize the scope of the work of Duneau *et al* (1991) and the present paper.

Similar questions have been approached by exact solutions, renormalization or numerical investigations. Geerse and Hof (1991) provide a good theoretical background and also a generous list of references including experimental results on the magnetic and spin-glass properties of real quasicrystals.

The interactions are chosen to be short range and to vary only according to local geometric criteria so as to fulfil the positional symmetry. Despite these restrictions, the magnetic phase diagram at $T = 0$ shows a rich structure ranging from entirely rigid antiferro- or ferro-magnetic states to effectively uncorrelated paramagnetic-like states.

In this paper we pay attention to a model involving only first- and second-nearest neighbour interactions. The spins stand on the vertices of a quasiperiodic 8-fold symmetric tiling which is not the canonical octagonal tiling but another one, obtained as a simple and

§ Since October 1992: Université de Cergy-Pontoise, BP 8428, 47 Av. des Genottes, F-95806 Cergy-Pontoise, France.

0305-4470/93/122791+12$07.50  

locally derivable decoration of the former. The tiles of our model split into three species: two kinds of octagons and an irregular pentagon. This implies some degree of frustration provided at least one of the coupling constants is negative. Qualitatively, the frustration is neither strong enough to break the system into small and magnetically independent molecules nor weak enough to allow strict long-range order. Nevertheless, it can be solved exactly by means of the hierarchic and the spin-flip symmetries of the Hamiltonian. We will see that the ground states decompose into independent clusters whose sizes take values in a diverging subset of the natural numbers. The energy will also be evaluated exactly and the entropy will be bounded from below.

To make the connection with the work of Duneau *et al* (1991) more precise, we can say that the model examined here is analogous to a component of phase (C) there. We are convinced that the state (C) can be solved exactly by a method similar to the one followed here but an explicit and complete solution would be complicated due only to technical reasons, and so is less appealing.

Section 2 summarizes the main geometrical features of the quasiperiodic tiling under study. The Ising model is defined in section 3 which also contains the results on the ground state energy values. In sections 4 and 5, we carry out preliminary investigations on the spin-flip symmetries and on the connectivity of the graph induced by the interaction bonds. The bounds on the ground state energies are derived in section 6. Those estimates are based on a hierarchy of frustration loops which is defined and analysed in section 7.

## 2. Geometry of the 8-fold tiling

The octagonal tiling is obtained by the cut and project method (CP method) from $\mathbb{R}^4$, see the reviews by Steinhardt and Ostlund (1987), Janot and Dubois (1988), Henley (1987). In order to normalize the edges to unit length in the physical plane, the hypercubic lattice is defined as $\Lambda = \sqrt{2}\mathbb{Z}^4$. The two orthogonal planes $E^{\parallel}$ and $E^{\perp}$ are the ranges of the following orthogonal projectors:

$$p = \frac{1}{2}\begin{bmatrix} 1 & \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & 1 & \frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{1}{\sqrt{2}} & 1 & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} & 1 \end{bmatrix} \qquad p^{\perp} = 1 - p.$$

The projections $L = p(\Lambda)$ and $L^{\perp} = p^{\perp}(\Lambda)$ are dense $\mathbb{Z}$-modules respectively generated by $\{e_1, \ldots, e_4\}$ and $\{e_1^{\perp}, \ldots, e_4^{\perp}\}$, projections of the standard basis of the hypercubic lattice. In orthonormal coordinates in each plane:

$$e_1 = (1, 0) \qquad e_1^{\perp} = (1, 0)$$

$$e_2 = \frac{1}{\sqrt{2}}(1, 1) \qquad e_2^{\perp} = \frac{1}{\sqrt{2}}(-1, -1)$$

$$e_3 = (0, 1) \qquad e_3^{\perp} = (0, 1)$$

$$e_4 = \frac{1}{\sqrt{2}}(-1, 1) \qquad e_4^{\perp} = \frac{1}{\sqrt{2}}(1, -1).$$

The standard octagonal tilings correspond to a cut region $E = E^{\parallel} \times W$ where the acceptance domain $W$ is, up to a translation, the projection of the unit cube of $\mathbb{R}^4$ into the perpendicular space. $W$ is a regular octagon generated by the four vectors $\{e_1^\perp, \ldots, e_4^\perp\}$ (see figure 1). The tilings in the physical space involve two types of tiles: a square, in two possible orientations, and a rhombus, in four possible orientations, which are the projections of the six different two-dimensional facets of the 4-cube.

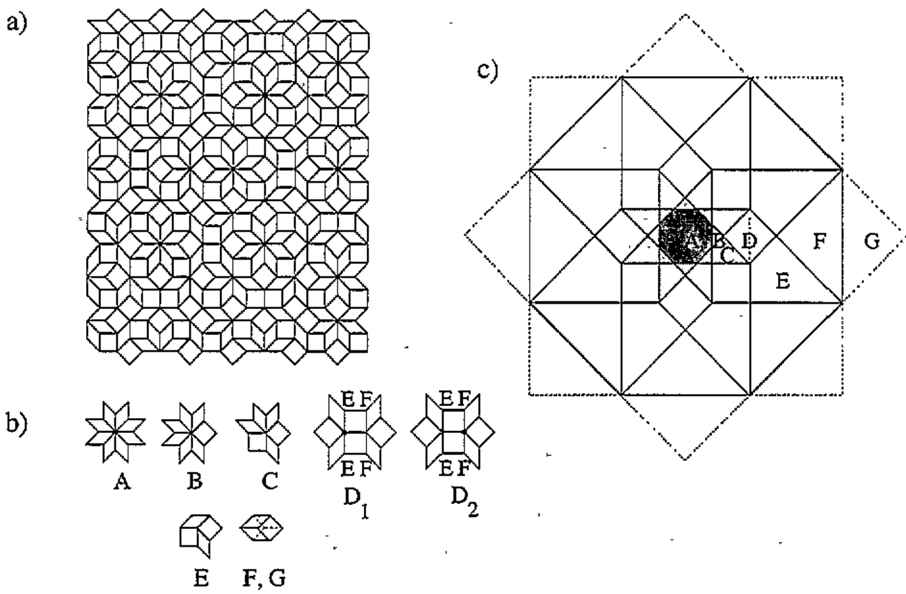


**Figure 1.** (*a*) Canonical octagonal tiling. (*b*) Local environments of the octagonal tiling with the position of the G-sites to be added to the tiling. (*c*) The acceptance domain $W$ of the octagonal tiling is the octagon spanned by the four vectors $e_1^\perp$, $e_2^\perp$, $e_3^\perp$ and $e_4^\perp$. $W$ splits into 7 domains, A, B, C, $D_1$, $D_2$, E and F, corresponding to the neighbourhoods of the selected nodes. The F-sites are surrounded by a square and two rhombi forming a hexagon. The symmetric position of the F-site in the hexagon is called a G-site and corresponds to an acceptance domain made of 8 triangles, outside $W$, similar to those of the F-sites.

The octagonal tiling shows a perfect inflation symmetry, due to the existence of an invertible integral linear transformation $J$ in $\mathbf{R}^4$ which commutes with the action of the 8-fold rotation group $C_8$. $J$ has the following equivalent expressions:

$$J = \begin{bmatrix} 1 & 1 & 0 & -1 \\ 1 & 1 & 1 & 0 \\ 0 & 1 & 1 & 1 \\ -1 & 0 & 1 & 1 \end{bmatrix} = \lambda p - \lambda^{-1} p^\perp$$

where $\lambda = (1 + \sqrt{2})$ is the inflation ratio. As a consequence the $\mathbb{Z}$-modules $L$, $L^\perp$ are invariant under scaling by an integral power of $\lambda$.

Up to rotations, there are seven possible environments of tiles sharing a common vertex, labelled A through F as shown on figure 1. This classification of sites corresponds to a partition of the octagonal window into seven different orbits (under $C_8$) of acceptance domains. For instance all the A-sites come from nodes which project into the small octagon of edge length $\lambda^{-2}$. For convenience, the D-sites are decomposed into $D_1$-sites and $D_2$-sites according to the following rule: $D_1$ sites have four E-sites and one D-site as neighbours, while $D_2$ sites have two E-sites, two F-sites and one D-site as neighbours (see figure 1(*b*)). The F-sites correspond to eight triangular domains at the boundary of the octagon. These sites are surrounded by a square and two rhombi which build up a characteristic hexagon. Upon translation of the window in the perpendicular space $E^\perp$, the octagonal tiling undergoes a series of flips which mainly affect these hexagons: the F-sites jump to the symmetric positions at a distance $\lambda^{-1} = \sqrt{2}-1$. These sites, unoccupied in the standard octagonal tiling, are labelled G-sites; they are associated to acceptance domains in $E^\perp$ which fall, of course, outside the octagon $W$ and build up eight peripheral triangles as shown in figure 1.

The patterns obtained by adding all the G-sites to the set of vertices of the octagonal tilings are of particular interest for our purposes. By the cut and project method, they can be obtained directly from an extended window, the 8-fold star shown in figure 1. All the hexagons of the underlying canonical tiling contain an F-site and a G-site, now equivalent up to second neighbours. These sites are separated by the shortest pair distance $d_1 = \lambda^{-1}$ which is, up to symmetry and the scaling by $\sqrt{2}$, the projection of a lattice vector of type$(1, -1, 0, 1)$. The next nearest-neighbour distance is the small diagonal $d_2 = \sqrt{2-\sqrt{2}}$ of the rhombus, corresponding to a lattice vector of type $(1, -1, 0, 0)$; the third one is the edge length $d_3 = 1$.

By inflation symmetry, the extended tiling, with sites A, B, C, D, E, F and G, selected by the 8-fold star in $E^\perp$ is equivalent to:

- the set of A, B, C and D sites of a standard octagonal tiling at scale $\lambda^{-1}$;
- the set of A and B sites of a standard octagonal tiling at scale $\lambda^{-2}$.

A last feature which will be useful in the following is parity. Since each site $x$ is the projection of a unique lattice node $\xi = \sqrt{2}(n_1, n_2, n_3, n_4)$ of $\Lambda$ we can define the parity of $x$ as that of $n_1+n_2+n_3+n_4$; consequently any structure $S$ built by the CP algorithm splits into an even subset $S_+$ and an odd subset $S_-$.

## 3. The Ising model and its ground state energy

We consider a system of Ising spins $\sigma_x = \pm 1$ placed on the vertices of the extended octagonal tiling, and coupled through the Hamiltonian

$$H(\sigma) = -J_1 \sum_{|x-y|=d_1} \frac{\sigma_x\sigma_y - 1}{2} - J_2 \sum_{|x-y|=d_2} \frac{\sigma_x\sigma_y + 1}{2}$$

where $d_1$ and $d_2$ are the nearest and next-nearest neighbour distances.

The spins on A, B, C and $D_1$ sites do not interact with anyone and will therefore be forgotten. The rest of the sites, namely those on $D_2$, E, F and G sites, are coupled by either $J_1$ or $J_2$. This system of nodes and bonds is tightly connected (figure 2). It even induces a tiling of the plane by three types of tiles: a pentagon P, an octagonal moon crescent M and a regular octagon O. Since the prescriptions to derive this tiling from the former extended octagonal one amount to remove the A, B, C and $D_1$ sites—and redefine the edges—the corresponding selection window is now the 8-fold star without the central octagon. This tiling obeys inflation rules which follow, in a straightforward way, from the inflation of the original octagonal tiling (this also appears on figure 2).

As easily checked, $J_1$ couples the odd subset with the even subset whereas $J_2$ couples only spins belonging to the same parity class. In absence of applied magnetic field, the sign

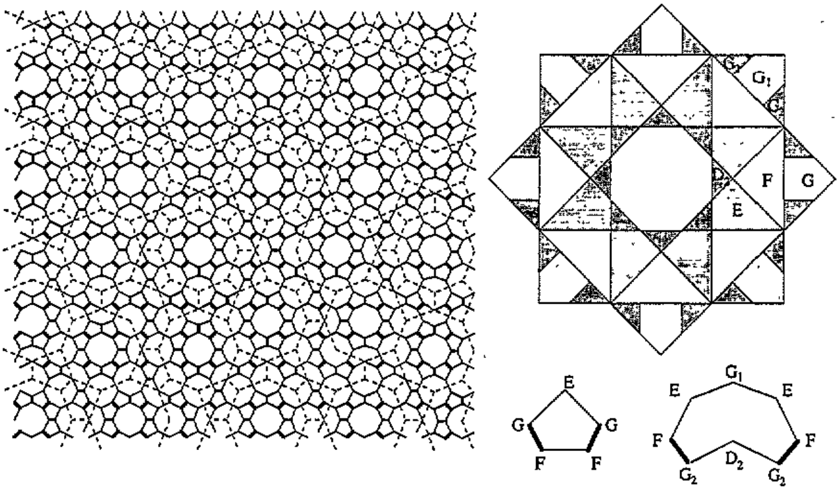


**Figure 2.** The extended octagonal tiling is made of A, B, C, D, E, F and G sites. The two nearest neighbour interactions $J_1$ and $J_2$ only couple $D_2$, E, F and G sites which correspond, in $E^{\perp}$, to a stellated octagonal window with a hole in the middle. The uncoupled A, B, C and $D_1$ nodes sit at the centres of octagons. The dashed tiling corresponds to an inflated tiling.

of $J_1$ is therefore irrelevant since the energy is invariant—up to an overall constant—by changing the sign of $J_1$ and flipping all the spins of one definite parity. For definiteness, we will assume $J_1 > 0$.

Frustration follows from the coupling $J_2$ which is assumed to be antiferromagnetic ($J_2 < 0$). The smallest frustration loop is the elementary pentagon {E, G, G, F, F} giving rise to a minimal energy equal to $\min(|J_1|, |J_2|)$. For $|J_1| \geqslant 2|J_2|$, the frustration is local, being completely restricted to those elementary pentagons. The situation is quite different when $|J_1| < 2|J_2|$, where frustration loops of all sizes—roughly, pentagons inflated to all scales—give 'non-local' contributions to the ground state energy. The energy will be given as a function of the number of sites of different types, e.g. $N_G$ will denote the extensive contribution to the number of G-sites in a large but finite tiling, proportional to the area of the associated acceptance domain. Boundary contributions to the energy will be neglected. The result is the following:

$$\min_{\sigma} H(\sigma) = \begin{cases} |J_1|N_G/2 & \text{if } |J_1| \leqslant -J_2 \\ |J_1|N_{G_1}/2 + |J_2|N_{G_2}/2 & \text{if } -J_2 \leqslant |J_1| \leqslant -2J_2 \\ |J_2|N_{G_1} + |J_2|N_{G_2}/2 & \text{if } -2J_2 \leqslant |J_1|. \end{cases}$$

The $G_1$ sites are meeting points of two Ps and either an M or an O. The $G_2$ sites are those G that are meeting points of a P, an M and an O. See figure 2 where the corresponding acceptance domains are shown. We now proceed to derive these estimations.

## 4. Spin flip symmetries

The connectivity associated to the $J_2$ coupling alone is like that of a Sierpinski gasket (Mandelbrot 1977) where each vacancy is occupied by an independent cluster (gasket) of the suitable size. The $J_2$ bonds are lattice vectors of type $(1, -1, 0, 0)$ (and cyclic permutations; the cyclic permutations of the four coordinates correspond to 45° rotations in $E^{\parallel}$) which couple separately $S_+$ to $S_+$ and $S_-$ to $S_-$. The even subset $S_+$ splits into $S_{++}$, $S_{+-}$, according to the parity of $n_1 + n_3$ and, similarly, the odd subset $S_-$ splits into $S_{-+}$ and $S_{--}$. Since the $J_2$ bonds only couple $S_{++}$ with $S_{+-}$ and $S_{-+}$ with $S_{--}$ we conclude that the antiferromagnetic ground states are not frustrated. In other words, any closed loop made of only $J_2$ bonds is even so that the minimum energy associated to the $J_2$ term in the Hamiltonian is zero. Such a ground state is specified for instance by letting spins up on $S_{++}$ and down on $S_{+-}$, and similar mutually opposite signs on $S_{-+}$ and $S_{--}$. The degeneracy of the ground state energy follows from the occurrence of infinitely many connected components in either $S_+$ or $S_-$. Any connected component, for instance in $S_+$, has all its $S_{++}$ spins equal whereas the $S_{+-}$ spins have the opposite sign.

Each block contributes to a factor 2 in the number of ground states. The total number $\mathcal{N}$ of blocks is equal to the total number of isolated octagons at all scales of inflation. Therefore:

$$\log(\mathcal{N}) = \lambda^{-2} N_{\mathrm{O}}(1 + \lambda^{-2} + \lambda^{-4} + \ldots) \log 2 = \lambda^{-2} N_{\mathrm{O}}(1 - \lambda^{-2})^{-1} \log 2 = N_{\mathrm{O}} \log 2/(2\lambda)$$

where $N_{\mathrm{O}}$ is the average number of octagons in the pentagon–octagon–moon tiling. It follows that the residual entropy, when $J_1 = 0$, is simply $S(J_1 = 0) = kN_{\mathrm{O}} \log 2/(2\lambda)$, where $k$ is the Boltzmann constant.

The $J_1$ bonds are found in the 'corridors' between the gaskets, one such bond being attached to every G-site. The perturbation of the system with $J_1 = 0$ by small $J_1$ couplings can be handled in the following way. First notice that the $J_1$ bonds, of type $(1, -1, 0, 1)$ (+ cyclic permutations), split into two classes according to the two possible orientations modulo $\pi/2$ (i.e. 0 or $\pi/4$). One class couples $S_{++}$ with $S_{--}$ and $S_{+-}$ with $S_{-+}$; the other couples $S_{++}$ with $S_{-+}$ and $S_{+-}$ with $S_{--}$. If $J_1$ is positive (ferromagnetic) and smaller than $|J_2|$, then the antiferromagnetic ground states described above for $J_1 = 0$ yield $J_1$ bonds which are satisfied when they belong to the first class and frustrated when they belong to the second class. By symmetry, the four orientations of $J_1$ bonds have the same density, therefore the corresponding energy is $J_1 N_G/2$ since the number of $J_1$ bonds is equal to $N_{\mathrm{G}}$. It will turn out that this upper bound to the ground state energy is actually also a lower bound when $|J_1| \leqslant -J_2$. This implies that the value of the residual entropy computed above for $J_1 = 0$ is a lower bound to the entropy when $|J_1| \leqslant -J_2$.

## 5. Structure of the $J_2$ bonds

The gasket-like features of the $J_2$ bonds pattern, shown in figure 3, result from a nice self-similarity property. This can be seen as follows. The $J_2$ bonds build up (regular) octagons which are either isolated or connected to other octagons by either a common $J_2$ edge or a double $J_2$ coupling via a G-site. All these octagons can be labelled by their centre which is of type A, B, C or $\mathrm{D}_1$. Since the union of the corresponding domains is a deflated octagonal window ($\lambda^{-1} W$), these centres are the sites of an inflated octagonal tiling (by a factor $\lambda$) and the associated octagons decorate this tiling. Adjacent octagons transform into small diagonals of rhombi and it can be checked that all such diagonals are obtained. Octagons coupled by a double $J_2$ transform into diagonals of squares and all squares are involved with their unique diagonal which does not contain an F-site (in the new underlying tiling).

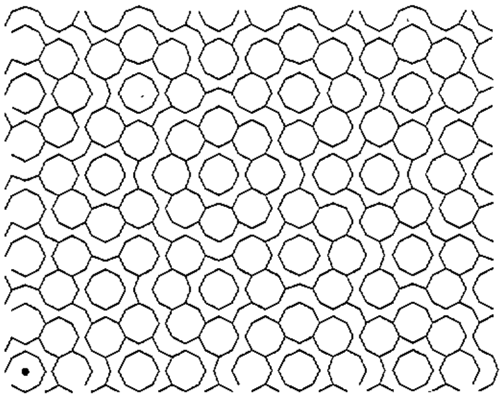

**Figure 3.** The pattern made by the $J_2$ bonds showing a hierarchy of 8-fold symmetric clusters of all sizes. The point marked with a dot is the centre of a globally 8-fold symmetric pattern.

Isolated octagons transform into isolated sites. Finally, the structure of the $J_2$ couplings is isomorphic to a standard tiling with a different connectivity which we call the skeleton.

The skeleton is made of octagons O, pentagons P, hexagons $H_6$ and heptagons $H_7$. The hierarchical structure follows from a substitution rule which is the following (Duneau *et al* 1991):

$$\mathrm{O} \longrightarrow \mathrm{O} + 8\mathrm{P}$$
$$\mathrm{P} \longrightarrow \mathrm{O} + \mathrm{H}_7 + 4/2\mathrm{H}_6$$
$$\mathrm{H}_6 \longrightarrow \mathrm{O} + 2\mathrm{P} + 2\mathrm{H}_6 + 2/2\mathrm{H}_6$$
$$\mathrm{H}_7 \longrightarrow \mathrm{O} + 5\mathrm{P} + 2\mathrm{H}_6.$$

In the above formula the halves refer to hexagons shared by two adjacent iterated objects. The octagons and all their iterations of any order build up isolated clusters of all sizes, hence the similarity with a Sierpinski gasket.

Due to inflation symmetry the POM (pentagon–octagon–moon) tilings show a hierarchy of self similar units. More precisely, the inflation of a frustrated pentagon is a pentagon of type $\{C, D_2, D_2, D_1, D_1\}$. A simple substitution rule transforms this pentagon into a new frustrated loop of larger scale and so on. These will be described in detail in section 7.

## 6. Energy and entropy bounds

### 6.1. Case $|J_1| \geqslant -2J_2$

*6.1.1. Upper bound for the ground state energy.* We use the $D_2$ E F G description, and make the ansatz that only EG couplings can be frustrated. This implies that the spins on the two G sites of a pentagon have opposite signs, so that the E site is effectively decoupled from the other sites of the pentagon, with an energy contribution equal to $|J_2|$ for any configuration satisfying the ansatz. If we remove all EG bonds, we observe that the network of remaining bonds is decoupled into isolated pairs of E-sites coupled by $J_2$, and quasi-one-dimensional structures with exactly one loop, of unbounded size but not frustrated. These loops are in one-to-one correspondence with the corridors previously described. Choosing arbitrarily one of the two ground states of each decoupled structure yields a global configuration satisfying the ansatz.

Therefore, for any $J_2 \leqslant 0$,

$$\min_\sigma H(\sigma) \leqslant |J_2| N_P = |J_2| N_{G_1} + |J_2| N_{G_2}/2.$$

The residual entropy of this state is the sum of the entropy associated to the loops, equal to $S(J_1 = 0)$ computed in section 4, plus the contribution of the isolated E–E pairs the number of which is equal to $(N_E - N_D)/2$.

There exist in fact other configurations with the same energy and not satisfying the ansatz, in particular with some FF bonds frustrated, so that the above estimate of the residual entropy is only a lower bound.

*6.1.2. Lower bound for the ground state energy.* The frustration on a pentagon may be located on a $J_2$ bond, in which case it is not shared with any other pentagon, or on a $J_1$ bond, in which case it can be shared with a neighbouring pentagon. The energy attached to an individual pentagon is thus larger than or equal to $\min(|J_1|, |J_1|/2)$. Therefore, for any $J_2 \leqslant 0$,

$$\min_\sigma H(\sigma) \geqslant \min(|J_2|, |J_1|/2) N_P$$

which concludes the proof in the case $|J_1| \geqslant -2J_2$.

### 6.2. Case $|J_1| \leqslant -J_2$

*6.2.1. Upper bound of the ground state energy.* The parity argument presented in section 4 provides an upper bound in any case. Taking into account the identity $N(J_1) = N_G$, it yields

$$\min_\sigma H(\sigma) \leqslant |J_1| N_G/2.$$

*6.2.2. Lower bound of the ground state energy.* Pentagons come isolated or in groups of four or eight. In addition to pentagons $L_0 = P$, we shall count frustration loops $L_n$, $n = 1, 2, \ldots$, built by iteration of a substitution process, as explained in the next section. The main properties of this family of loops, including the pentagons $L_0$ at the original scale, is that any given bond $J_2$ or $J_1$ belongs to at most two loops. Therefore, for any $J_2 \leqslant 0$,

$$\begin{aligned}\min_\sigma H(\sigma) &\geqslant \min(|J_1|, |J_2|)(1/2) \sum_{n\geqslant 0} N(L_n) \\ &= \min(|J_1|, |J_2|) N_G/2\end{aligned}$$

according to the counting performed at the end of section 7. This concludes the case $|J_1| \leqslant -J_2$.

When $|J_1| < -J_2$, the residual entropy is equal to $S(J_1 = 0)$ as computed in section 4.

### 6.3. Case $-J_2 \leqslant |J_I| \leqslant -2J_2$

*6.3.1. Upper bound of the ground state energy.* We start from a configuration which would be a ground state if $|J_1| < -J_2$, where half of the $J_1$ couplings are frustrated; more precisely, half of the $FG_1$ couplings and half of the $FG_2$ couplings are frustrated. The $FG_2$ couplings belong to moon crescents, made of two $FG_1$ bonds (coupling $J_1$) and six $J_2$ couplings. We now change the configuration by flipping the spins on the three sites $G_2$, $D_2$, $G_2$, in every frustrated crescent. This has the effect of removing frustration from the crescent, and taking it onto the regular octagons in the concavity of the corresponding crescents.

The resulting configuration has an energy $\frac{1}{2}|J_1|N_{G_1} + \frac{1}{2}|J_2|N_{G_2}$, as desired.

These configurations, which are shown below to be ground state configurations, provide a lower bound to the residual entropy equal to $S(J_1 = 0)$.

*6.3.2. Lower bound of the ground state energy.* Let us consider again the frustration loops already introduced. At first sight, we only have

$$\min_\sigma H(\sigma) \geqslant |J_2|(1/2) \sum_{n \geqslant 0} N(\mathrm{L}_n)$$

but this bound can be improved. The count of energy resulting from frustration can in fact be optimized as follows:

(i) Isolated pentaton $\{\mathrm{F\,G_2\,E\,G_2\,F}\} : |J_2|$
(ii) 'Inner' pentagon $\{\mathrm{F\,G_1\,E\,G_1\,F}\} : |J_1|/2$
(iii) 'Border' pentagon $\{\mathrm{F\,G_2 E\,G_1\,F}\} : (|J_1| + |J_2|)/4$
(iv) Inflated isolated pentagon: $|J_2|/2$.

This count is easily verified when the frustrated segments of all the inflated loops are of the type $EG_2$, and are thus shared with 'border' pentagons. Half of the 'border' pentagons then have $EG_2$ frustrated, the other half must then have $FG_1$ frustrated, hence (iii).

Whenever an inflated loop has frustration on a segment other than $EG_2$, two associated 'border' pentagons get a $|J_1|$ frustration, hence an additional energy $(|J_1| - |J_2|)/2$ which cancels the gain in energy which may have come from the displacement of the frustration of the inflated loop.

The count (i)–(iv) gives the desired lower bound.

## 7. The hierarchical sequence of frustration loops

In this section, we draw loops $\mathrm{L}_n$, $n = 0, 1, 2, \ldots$, along the edges of the POM tiling (figure 2), in such a way that any given edge belongs to at most two loops. These loops will be made of two $J_1$ couplings and an odd number of $J_2$ couplings, and will therefore be frustrated for $J_2 < 0$.

The first loops $\mathrm{L}_0 = \mathrm{P}$ are the basic pentagons. Edges $FG_1$ separating adjacent pentagons already belong to two loops, and cannot be used any further. We thus remove these edges and obtain a new tiling made of the original octagons O and moons M, the original isolated pentagons $\mathrm{P}_1$, plus strings $\mathrm{P}^4$ and $\mathrm{P}^8$ of adjacent pentagons now considered as single tiles. This $\mathrm{P_1OMP^4P^8}$ tiling will be the starting point of a substitution rule yielding a whole hierarchy of tilings of the plane defined as follows.

The original $P_1OMP^4P^8$ tiles are given the inflation index $n = 1$, and are accordingly denoted by $P_1$, $O_1$, $M_1$, $P_1^4$, $P_1^8$. The substitution rule is the following (see figure 4):

$$P_n + 3O_n + 2M_n = P_{n+1}$$

$$O_n + P_n^8 = O_{n+1}$$

$$O_n + P_n^4 = M_{n+1}$$

$$4P_n + 9O_n + 5M_n = P_{n+1}^4$$

$$8P_n + 16O_n + 8M_n = P_{n+1}^8.$$

The tiling at scale $n + 1$ can also be obtained from the tiling at scale $n$ in the following way.

(i) First of all, define the centre of P as the centre of its circumscribed circle (the five vertices stand on a common circle, avoiding ambiguities); the centre of $P_n$ will be defined similarly, by induction.

(ii) Scale (homothetically) each $P_n$, from its centre, by the factor $-\lambda$. The scaled $P_n$ is denoted $-\lambda P_n$.

(iii) If $n$ is even, define $\widetilde{P}_{n+1}$ as the maximal union of original POM tiles contained in $-\lambda P_n$; else (if $n$ is odd) define $\widetilde{P}_{n+1}$ as the minimal union of original POM tiles containing $-\lambda P_n$. The set of $\widetilde{P}_{n+1}$ is made of three types of connected components, which are isolated $\widetilde{P}_{n+1}$ or strings of 4 or 8 (overlapping) $\widetilde{P}_{n+1}$. These components define the tiles $P_{n+1}$, $P_{n+1}^4$, $P_{n+1}^8$ respectively.

(iv) Dilate, from their centre and by the factor $-\lambda$, only those $O_n$ which are surrounded by a $P_n^8$ pattern.

(v) If $n$ is odd, define $O_{n+1}$ as the maximal union of original POM tiles contained in $-\lambda O_n$, else ($n$ even) define $O_{n+1}$ as the minimal union of original POM tiles containing $-\lambda O_n$.

(vi) Define the $M_{n+1}$ patterns by scaling the $O_n$ which are half-surrounded by a $P_n^4$ pattern and applying the same rule as for the $O_{n+1}$ pattern, but amputating it of all the overlaps with the already defined patterns $P_{n+1}$, $P_{n+1}^4$, $P_{n+1}^8$ and $O_{n+1}$.

To summarize the main features of these tilings, remark that, at all stage $n$, the number of prototiles is 5 and the prototiles $P_n$, $O_n$, $M_n$, $P_n^4$, $P_n^8$ are unions of the original tiles. The ordering of the tiles coincides with the ordering of the $n$th inflated tiling, which is at scale $\lambda^n$. In particular, the linear size of the tiles is of the order of $\lambda^n$ but the boundaries become more and more sinuous as $n$ grows, due to the fact that each step is an exact partition of the original POM tiling.

We shall use the following properties of boundaries of patterns:

$$\partial\widetilde{P}_{n+1} \cap \partial(-\lambda P_n) = \emptyset$$

$$\partial O_{n+1} \cap \partial(-\lambda O_n) = \emptyset$$

$$\partial O_{n+1} \subset \partial P_n^8$$

$$\partial(OM)_{2n+1} \subset \partial P_{2n}^8 \cup \partial P_{2n}^4$$

where $(OM)_n$ denotes a union of nearest neighbours $O_n \cup M_n$. The last relation holds because $(OM)_{2n+1} = O_{2n} + P_{2n}^8 + O_{2n} + P_{2n}^4$ and $O_{2n}$, being strictly inside the associated $-\lambda O_{2n-1}$, cannot meet any $P_{2n+1}$ which are also strictly inside their associated $-\lambda P_{2n}$.

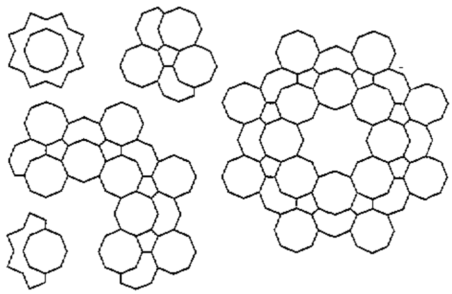

**Figure 4.** Substitution rule for the patterns $P_n$, $O_n$, $M_n$, $P_n^4$ and $P_n^8$.

The loops $L_n$, $n \geqslant 0$, are defined as the boundaries of the transformed pentagons: $L_n = \partial P_n$. In order to obtain a lower bound to the energy in terms of half the number of loops, we must check that any given bond belongs to at most two loops. The argument goes as follows.

First, notice the following properties ($n \geqslant 1$):

(i) odd patterns $P_{2n-1}$ lie strictly inside patterns $P_{2n}$ or $P_{2n}^4$ or $P_{2n}^8$ (by construction);

(ii) the boundary of any given pattern $P_{2n}$, $P_{2n}^4$, $P_{2n}^8$, $O_{2n-1}$ or $(OM)_{2n-1}$ does not meet any $P_{n'}$ contained in the given pattern.

This last property is proven by induction. If it is true for $P_{2n-2}^8$ and $P_{2n-2}^4$, then it is true for $O_{2n-1}$ and $(OM)_{2n-1}$ because of the inclusion relations above. If it is true for $O_{2n-1}$ and $(OM)_{2n-1}$, then it is true for $P_{2n}$, $P_{2n}^4$, $P_{2n}^8$ because $P_{2n} = P_{2n-1} + O_{2n-1} + 2(OM)_{2n-1}$ and $P_{2n-1}$ satisfies (i) by induction, and $O_{2n-1}$, $(OM)_{2n-1}$ satisfy (ii) by induction. Similarly for $P_{2n}^4$, $P_{2n}^8$.

Next, being boundaries of isolated transformed pentagons, two loops $L_n$, $n \geqslant 1$, at the same scale cannot get into contact. So, all we need to verify is that any given loop $L_n = \partial P_n$ shares any of its particular bonds with at most one $L_{n'} = \partial P_{n'}$, $n' < n$. We first observe that, according to (i) and (ii),

$$\partial P_{n'} \cap \partial P_n \neq \emptyset \qquad \text{and} \qquad P_{n'} \subset P_n \Rightarrow n' \text{ even and } n \text{ odd.}$$

If $n$ is odd, $P_n$ is surrounded by $O_n$ and $(OM)_n$, because of (i). Then (ii) implies that $\partial P_n$ cannot meet outside loops of smaller index. As for inside loops, the parity rule just above does not allow three nested loops to meet on a bond. If $n$ is even, (ii) implies that $\partial P_n$ can meet only outside loops of smaller index. Such an outside loop $\partial P_{n'}$ must be of even index because of (i), and then cannot meet loops inside $P_{n'}$ because of (ii). This concludes the proof.

To be complete, we still have to count the loops. Since the ordering of the $n$th tiling is the same as the ordering of the $n$ times inflated tiling, the total number $N_L$ of loops in $\cup_{n\geqslant 0} L_n$ is

$$\sum_{n\geqslant 0} N(L_n) = N_P(1 + \lambda^{-2} + \lambda^{-4} + \ldots) = N_P(1 - \lambda^{-2})^{-1} = N_P\lambda/2.$$

Now the number of Ps (at scale 1) is $N_P = N_E$. So that $N_L = N_E\lambda/2 = N_F = N_G$.

The direct consequence for spins is that, if all the loops $L_n$ are frustrated, the ground state energy is bounded by:

$$E(\sigma) = \frac{1}{2} \sum_{\text{bonds}} (-J_b \sigma_{b_1} \sigma_{b_2} + |J_b|) \geqslant \frac{1}{2} \sum_{\text{loops}} E_g(\mathrm{L})$$

where $b_1$ and $b_2$ stand for the ends of bond $b$ and $E_g(\mathrm{L})$ is the minimal energy of the loop. $E_g(\mathrm{L})$ is strictly larger than zero if L is frustrated.

## 8. Conclusion

Compared to the high translational homogeneity of the model, as ensured by quasiperiodicity, the magnetic ground states display some loss of regularity. Because of frustration, only hierarchical symmetry is preserved by the states to some degree. This provides a theoretical support to a magnetic behaviour analogous to the one of amorphous materials rather than to the one of fully ordered crystals.

## References

Duneau M, Dunlop F, Jagannathan A and Oguey C 1991 Frustrated Ising models on quasiperiodic lattices in two dimensions *Mod. Phys. Lett.* B **28** 1895–1903

Geerse C P M and Hof A 1991 Lattice gas models on self-similar aperiodic tilings *Rev. Mod. Phys.* **3** 163

Henley C L 1987 Quasicrystal order, its origin and its consequences: a survey of current models *Comm. Cond. Mat. Phys.* **13** 59

Janot Ch and Dubois J M (ed) 1988 *Quasicrystalline Materials* (Singapore: World Scientific)

Mandelbrot B B 1977 *Fractals: Form Chance and Dimension* (San Francisco: Freeman)

Steinhardt P J and Ostlund S (ed) 1987 *The Physics of Quasicrystals* (Singapore: World Scientific)