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► **To cite this version:**

Anu Jagannathan, Benjamin Motz, Elena Vedmedenko. Novel properties of frustrated low dimensional magnets with pentagonal symmetry. *Philosophical Magazine*, 2011, pp.1. 10.1080/14786435.2010.539578 . hal-00665443

HAL Id: hal-00665443

<https://hal.science/hal-00665443>

Submitted on 2 Feb 2012

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Journal:	<i>Philosophical Magazine & Philosophical Magazine Letters</i>
Manuscript ID:	TPHM-10-May-0213.R1
Journal Selection:	Philosophical Magazine
Date Submitted by the Author:	29-Sep-2010
Complete List of Authors:	Jagannathan, Anu; Université Paris-Sud, Laboratoire de Physique des Solides Motz, Benjamin; Université Paris-Sud, Physics Vedmedenko, Elena; University of Hamburg, Physics
Keywords:	aperiodic materials, low-dimensional structures, magnetic films, magnetic structure, nanosized clusters, theoretical
Keywords (user supplied):	frustrated antiferromagnet, quasiperiodic magnetic thin film, fractals

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Manuscripts

Philosophical Magazine
Vol. 00, No. 00, ?? June 2010, 1–7

RESEARCH ARTICLE

NOVEL PROPERTIES OF FRUSTRATED LOW
DIMENSIONAL MAGNETS WITH PENTAGONAL
SYMMETRY

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(v4.4 released November ????)

We consider a new type of frustrated spin networks with pentagonal loops and long range quasiperiodic structural order. Five-fold loops can be expected to occur naturally in quasicrystals, and experimental studies of icosahedral alloys show manifestations of local five-fold symmetry in a variety of different physical contexts. Our model considers classical spins placed on vertices of a tiling of the two dimensional Penrose tiling, and interacting with nearest neighbors via antiferromagnetic bonds. The ground state of this fractal system has a complex magnetic structure, and is studied analytically as well by Monte Carlo simulation on finite clusters.

Keywords: quasiperiodicity, frustration, antiferromagnetism, fractals

1. Introduction

Frustrated magnetic models have been a subject of much interest over the years, due to the new types of behaviors that can arise as a result of the frustration. Spin glasses are one well-known example of frustrated magnets. In these materials, the magnetic moments (spins) interact via exchange interactions that are random in sign and, in most cases, in magnitude as well. As a consequence, any given spin is typically unable to find an orientation that can satisfy all of the bonds that join it to its neighbors, whence the idea of frustration. Spins freeze below a certain transition temperature, with randomly oriented moments, forming a disordered magnetic glassy phase, with complex dynamical and thermodynamical properties. Periodic frustrated systems include the Ising antiferromagnet on a triangular lattice, whose interesting zero temperature properties were considered by Wannier in 1950 [1]. In the triangular antiferromagnet, the frustration has a geometric origin, due to the fact that one cannot place three vectors on the three vertices of a triangle so as to satisfy simultaneously all of the antiferromagnetic bonds. Similarly, in three dimensions, the presence of triangular loops in the face-centered cubic lattice leads to frustration. In recent years much interest has been shown in the quantum states of such frustrated antiferromagnets, and much work has been done on frustrated

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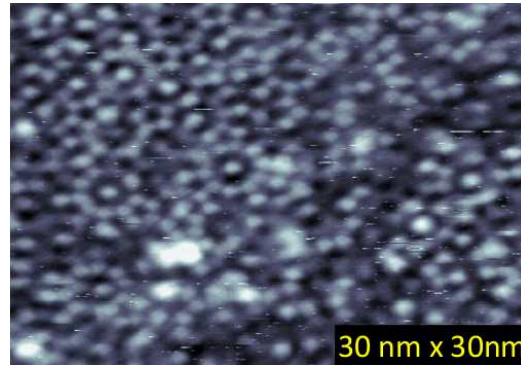


Figure 1. STM image of Pb atoms deposited on a AgInSb surface showing the presence of five and ten-fold atomic rings (figure reproduced with permission, courtesy of the Liverpool and Nancy groups)

systems such as the Kagome lattice [2], the pyrochlore lattice and many other interesting lattices in two and three dimensions (for a review see [3]).

In this report, we will introduce a new type of frustrated model which is based on five-fold symmetry, present in many quasicrystals. Motivation for considering such a quasiperiodic magnet comes from the experimental progress in recent years in producing quasiperiodic atomic layers on the surfaces of quasicrystals. Many different atomic species have been shown to form pseudomorphic films with a connectivity that reflects the underlying quasiperiodic organisation as can be seen in Fig. 1 which shows an STM image of adsorbed Pb atoms on the surface of AlPdMn (for more details see the review in [4]). It is thus likely that magnetic structures could eventually be obtained as such techniques are refined and extended. We note in passing that three-dimensional antiferromagnetic quasicrystals with antiferromagnetic interactions have been investigated in many preceding works [5].

As a simple theoreticians model of a frustrated two dimensional quasiperiodic magnetic layer, we consider antiferromagnetically coupled vector classical spins on vertices of a subtiling of the Penrose tiling. We find that the resulting structure is frustrated on an infinity of length scales, with, as the starting point the elementary pentagonal five-fold rings. The frustration leads naturally to a macroscopic entropy of the ground states of this system, as has been shown for the six-fold symmetric Kagome lattice antiferromagnet, which is based on the triangular elementary unit. This quasiperiodic antiferromagnet provides a new playground for exploration of the physics of frustrated systems, and is of course expected to have different properties compared to unfrustrated quasiperiodic antiferromagnets (such as the quantum spin models on the Penrose and Ammann Beenker tilings considered in [6]).

We present the model in the following section 2. The first subsection outlines some details regarding the geometrical properties of the model. The following subsection outlines the methods of analysis that we have used. Section 3 presents results, along with a discussion and conclusions.

2. A model of a frustrated quasiperiodic antiferromagnet

We consider two-component vector spins (XY spins) \vec{S}_i placed on vertices, labeled by the index i , of a subtiling of the Penrose rhombus tiling (PT), as shown in Fig.2. The Hamiltonian is

$$H = J \sum_{i,j} \vec{S}_i \cdot \vec{S}_j \quad (1)$$

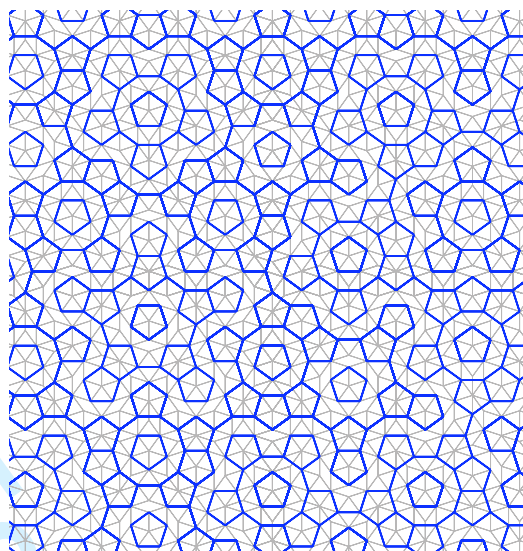


Figure 2. The vertices of the subtiling, along with the couplings are shown in blue, with the original Penrose tiling shown in light gray for comparison.

where J is the strength of the spin-spin interactions. All the couplings are anti-ferromagnetic ($J > 0$), they are of equal strength and act along the short diagonals of the fat rhombuses, indicated by blue bonds in Fig. 2.

Spins are clearly frustrated due to the presence of the pentagonal rings. The ground state degeneracy is easily calculated. In the case of Ising variables, it is five, since there are five ways to have one frustrated bond in a given pentagon. For the vector spin case, the degeneracy is reduced to just two, as we explain below. However, the frustration is also present at larger length scales, and this is a consequence of the geometrical properties of the structure, some of which we outline in the next subsection. This in turn is reflected in the ground state entropy of this frustrated antiferromagnet.

2.1. Geometrical properties of the pentagonal cluster model (PCM)

The system illustrated in Fig. 2 can be obtained from the Penrose rhombus tiling by retaining only those pairs of sites which are linked by the diagonals of the fat rhombuses. It can also be obtained very simply by the cut and project method (which will not be described here). A two-component – or XY – spin is attached to each of these sites. Figure 2 shows the resulting sites and bonds of length $\tau = (\sqrt{5} + 1)/2$ (in units in which the edge length of a rhombus is equal to 1). All bonds have the same strength and are antiferromagnetic.

The PCM is an assembly of interpenetrating clusters of increasing size, which are five-fold symmetric and fractal. They are labeled C_n , where n is the “generation” of the cluster. The smallest clusters are isolated pentagons (C_0 and C_1 , which have opposite orientations and occur with different frequencies). Next, there are clusters of five pentagons arranged around a decagonal ring (C_2). C_3 has five pairs of pentagons arranged around a decagon, as will be illustrated further below. Each cluster can be constituted recursively from three preceding ones.

The properties of the infinite cluster, which percolates through the system can thus be calculated to great accuracy by a recursive method. We thus find the fractal dimension of the infinite cluster to be 1.799. The probability of occurrence of each type of cluster, p_n , falls off with the cluster linear size $l_n = \tau^n$ (the length of the side of the pentagonal cluster) as a power law. Fig. 3 shows the distribution obtained

numerically for the PCM for large finite samples obtained using the method of cut-and-projection. The slope gives the exponent of the power law dependence $p \propto l^{-\gamma}$ with $\gamma = 2.089$.

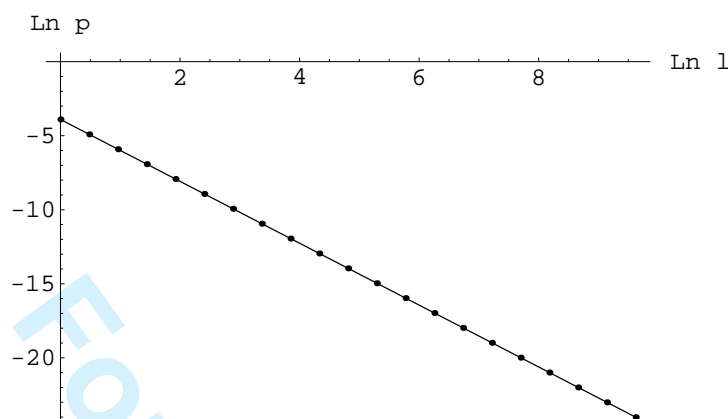


Figure 3. A log-log plot of the probability p of each cluster plotted against its linear size l , showing the power law dependence. The slope is equal to -2.089 .

2.2. Magnetic ground states

For XY spins on the vertices of a pentagon, the minimal energy states correspond to configurations in which the spins angles are rotated by $\pm 4\pi/5$ as one passes from one vertex to the next. The bond energies are all equal, and have the value $b = J \cos(4\pi/5)$. For a given pentagon, we can define $\chi = \sum_{bonds} (\phi_i - \phi_{i+1})/4\pi$ where χ is the sum of changes of angle around the five bonds of the pentagon. The overall change of angle is thus $\pm 4\pi$ and there is a two-fold chiral degeneracy of the ground state, $\chi = \pm 1$.

The next biggest cluster is composed of 25 spins arranged in five linked pentagons. The minimal energy configurations for two of the clusters are shown in Fig. 4. The resulting structure is frustrated, both at the level of the pentagonal rings and, as a result, at the level of the decagonal loop as well. One can distinguish three types of bonds: b_1 , bonds belonging to the pentagons, b_2 , the bonds that belong both to a pentagon and the decagon and b_3 , the bonds of the decagon that connect two different neighboring pentagons. By a direct minimization of the cluster Hamiltonian, we can easily determine the optimal values of each of the bond energies. b_1 and b_2 correspond to a difference of angles close to $4\pi/5$, while b_3 is close to the optimal value of $-J$, or equivalently to a difference of angles close to π . These last are the least frustrated bonds in the cluster. Bigger clusters have a greater number of inequivalent bonds, but one finds that the values of bonds belong in one of three main groups. This is shown in fig. 5 which shows a color coded representation of the main classes of bond energies expected in the ground state of a large cluster.

Coming now to the question of degeneracy, we have shown that the C_2 clusters have many degenerate states, one of which is illustrated in 6, and that the degeneracy grows with cluster size. The calculation of the configurational entropy of the entire system is in progress will be reported elsewhere. We note here simply that this feature is an consequence of the chiral degeneracy already mentioned for the C_0 and C_1 elementary pentagons.

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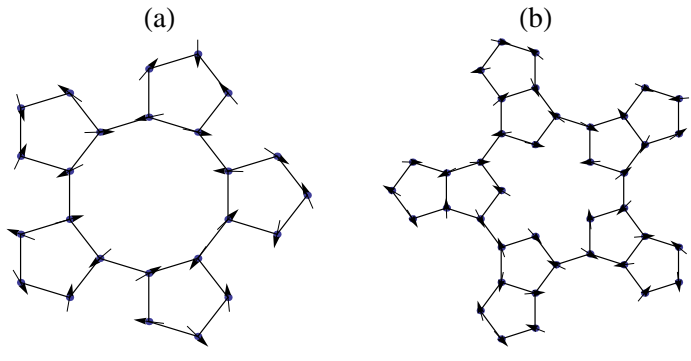


Figure 4. One of the ground state spin configurations for the clusters C_2 and C_3 containing 25 and 40 spins respectively

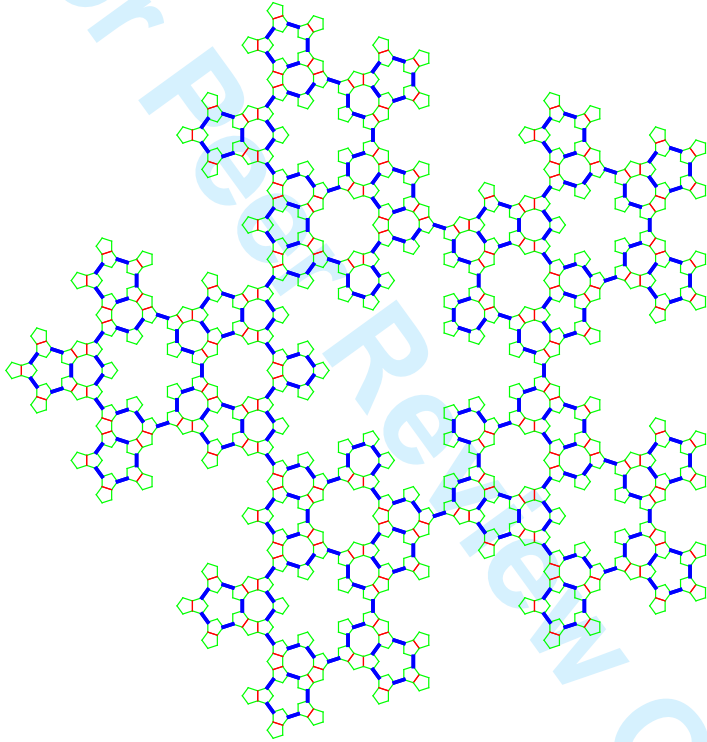


Figure 5. A cluster of 1515 spins, with the bonds colored according to the expected corresponding energies in the ground state. Theoretical predictions show that bonds fall into three categories : the most frustrated bonds (red), intermediate frustrated green bonds (thin bonds) and the least frustrated blue bonds (thick bonds).

3. Results and Conclusions

Figs. 6 and 7 show some results of a Monte Carlo simulation of a cluster of 1515 spins. The spin orientations for this sample follow the theoretically predicted schema. Deviations occur because of the low dimensionality of the system despite the low temperature ($T=0.05$ in units of J) used for the simulation. There is a good accord between the analytically and numerically determined states.

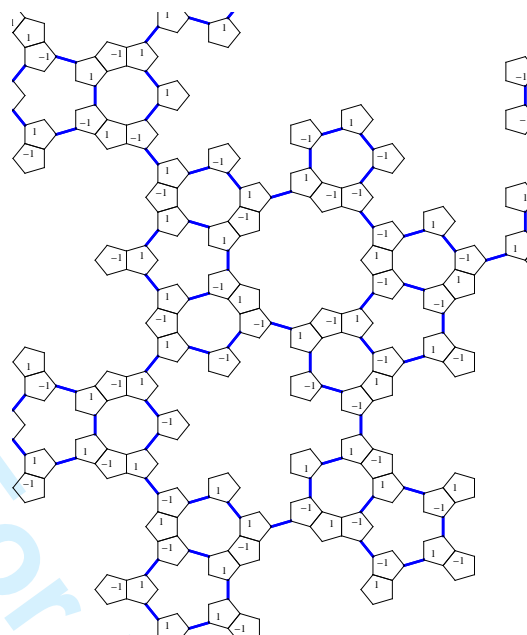


Figure 6. A small region of a large cluster, representing one of the possible low energy spin configurations, with the chirality indices shown for each of the pentagons (Nb. one defect is present in this figure.)

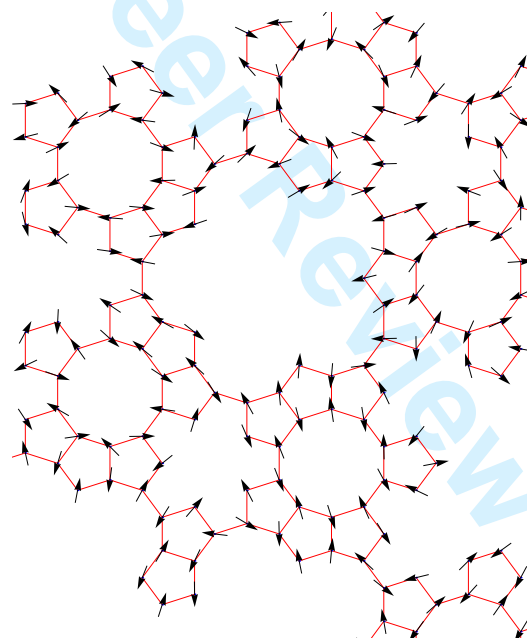


Figure 7. A portion of a large cluster showing the local spin orientations as obtained by Monte Carlo simulation ($T=0.05J$). The agreement between theory (fig. 5) and calculations is found to be good.

3.1. Conclusions

We have presented a new class of frustrated antiferromagnet based on five-fold frustrated units. The structure is fractal, and has characteristic scaling properties in real space as well as perpendicular that follow from the algebraic properties of the underlying Penrose tiling. On the theoretical side, the subtiling is an interesting geometrical object in its own right, as it forms a percolating subsystem. It is conceivable that this type of structure could be realized by atomic deposition on quasiperiodic substrates, in which the adsorbate atoms sit on preferential sites. This would provide an exciting opportunity for exploring the physics of frustrated

1 magnets. Problems we would like to address in the near future concern the spin
2 dynamics and magnetic response of this type of magnetic material. The quantum
3 version of this model, similar to what was discussed for the unfrustrated Penrose
4 tiling case in [6] will be an interesting theoretical challenge. Studies of the low
5 energy magnetic states for the long range dipolar spin-spin interactions considered
6 in [7] are also in progress, and results will be reported elsewhere.

10 3.2. Acknowledgements

11 We would like to thank Pavel Kalugin for useful discussions. Benjamin Motz was
12 supported by a CNRS contract for the duration of this work.

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