

Polytopes (35) and (335) as frustrated spin systems with non-random interactions

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1991 J. Phys.: Condens. Matter 3 1165

(<http://iopscience.iop.org/0953-8984/3/9/011>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 171.66.16.151

The article was downloaded on 11/05/2010 at 07:07

Please note that [terms and conditions apply](#).

Polytopes {35} and {335} as frustrated spin systems with non-random interactions

J Kurzyk

Institute of Physics, Technical University of Cracow, Podchorążych 1, 30-084 Kraków, Poland

Received 29 March 1990, in final form 25 October 1990

Abstract. A new method of construction of the Hamiltonian for uniformly frustrated spin systems is proposed. In the XY case the method leads to the model which is equivalent to the well known uniformly frustrated XY model but it is more general than the latter because it makes sense for the three-dimensional spins as well. In this paper the method has been used in an atypical way because we study here two unreal spin systems. In the first system, spins are placed on the vertices of the polytope {35} which form, in the curved space S^2 , a two-dimensional triangular lattice with a fivefold symmetry axis. In the second system, spins are placed on the vertices of the polytope {335} which form, in the curved space S^3 , a three-dimensional lattice with icosahedral symmetry. In the same way as other workers, we are interested in the polytope {335} because of a topological similarity between fragments of it and fragments of amorphous materials. Using the Monte Carlo technique we have calculated the temperature dependence of the mean energy and specific heat for both ferromagnetic and antiferromagnetic interactions. The ground states of both systems have been found too. Moreover some low-lying metastable states have been found for the icosahedral spin system.

1. Introduction

The concept of frustration is very attractive for theoretically investigating spin glasses [1]. The frustration effect can be caused by competing, randomly distributed ferromagnetic and antiferromagnetic interactions (such a case occurs, for instance, in dilute alloys as a consequence of the oscillatory nature of RKKY interactions [2]). In mathematical models, however, it is often assumed that the interactions instead of being randomly distributed have some more complicated distributions because the randomness makes the problem too difficult. For example, in a model proposed by Villain [3–5] the interactions distributed in such a way that the number of ferromagnetic bonds on certain ‘elementary polygons’ is odd. One of the bonds then remains necessarily unsatisfied and consequently frustration arises. A modification of this model is the uniformly frustrated XY model [6] described by

$$H = -J_0 \sum_{\langle ij \rangle} \cos(\theta_i - \theta_j - \Psi_{ij}) \quad (1)$$

where θ_i is the angle of the planar spin at site i , $\langle ij \rangle$ denotes the nearest-neighbour pairs and Ψ_{ij} is a bond angle such that the sum around a plaquette given by

$$\Psi_{ij_1} + \Psi_{ij_2} + \dots + \Psi_{j_n i} = 2\pi f \quad (2)$$

is constant over the entire lattice. This idea is very convenient and often used. Unfortunately, it makes sense only in a case of two-dimensional (XY) spins. In this paper we

propose a more general construction. It is equivalent to the above method in the XY case but it makes sense for three-dimensional spins as well. Our idea is based on the observation by Toulouse [1] that the frustration effect is very similar to the effect of parallel transport on vectors in curved space so that it may be visualized as giving curvature to the lattice. Thus we propose the following method of the construction of the frustrated spin model. First we construct a hypothetical crystal in a curved space topologically equivalent to the real crystal which we are interested in. This is possible if the curvature of the space is small enough in comparison with the dimensions of the crystal. Next we find the Hamiltonian of the spin system related to this hypothetical crystal, and finally we use it to describe our real spin system (in flat space). The frustrations introduced into the model by this means depend on the curvature of the space and the dimensions of elementary cells of the hypothetical crystal. Thus, if the curvature is constant and small enough in order that one may neglect differences in the shapes of the elementary cells, which appear as a result of the curvature of the space, we get the uniformly (in fact nearly uniformly) frustrated spin model.

In this paper we have not exactly complied with the above scheme because the hypothetical crystals (in curved space) for which we have constructed the Hamiltonian do not have the topological counterparts in Euclidean space. First we consider the icosahedral crystal (on the three-dimensional sphere S^3) called the polytope {335}. It is very interesting because of its symmetry. It is known that, although long-range icosahedral order is prevented by the properties of Euclidean space, local icosahedral order, which is the most advantageous [7], is preferred in some conditions. Such conditions are attained in glasses and one can show that small fragments of the amorphous materials are topologically similar to fragments of the polytope {335}. Thus, we should use our Hamiltonian as a Hamiltonian of the fragments of the amorphous spin system. Because, however, a selection of the fragments and a connection between them and the fragments of the polytope is ambiguous [8], we have at the moment abandoned this idea. Instead, we studied the whole polytope. This is not new. Some workers have already tried to approximate some physical properties of amorphous materials by the corresponding properties of the polytope. Until now, structural [8–10], some electronic [10], acoustic and vibrational [11–13], and melting [13, 14] properties of the polytope have been studied. In this paper we investigate some magnetic properties of the polytope {335}. We think that it may shed new light on the nature of amorphous spin systems because many effects in magnetic glasses often result from the frustrations caused by the topology of the amorphous systems. For instance, the spin-glass behaviour of some amorphous structures with antiferromagnetically interacting ions (e.g. insulating transition-metal aluminosilicates [15]) arises from the topology of the structure. In the two-dimensional case this type of frustration exhibits the antiferromagnetic triangular XY model. Here, just as in the amorphous materials, the topology of the lattice makes it impossible to satisfy simultaneously all antiferromagnetic bonds. In the three-dimensional case, none of the usual regular lattices has this property but the {335} lattice does.

Because it is very difficult to imagine effects connected with the curvature of three-dimensional space we have decided to study also a lattice in two-dimensional curved space. The lattice which we have chosen is the polytope {35}. We are interested in it because many simple properties of the unimaginable polytope {335} may be inferred by pure analogy to the properties of the polytope {35}. On the vertices of the polytope we have placed the two-dimensional spins so that it is a specific XY system.

In our model we have in mind nearest-neighbour interactions of Heisenberg type between classical spins. However, because the scalar product of two vectors in curved

space is not defined for vectors fixed at different points, we must give the interpretation of the Hamiltonian. This is done in section 3.

In this paper we confined ourselves to finding a ground state and temperature dependence of the mean energy (and then the specific heat) of both spin systems. The calculations were performed by the Monte Carlo technique for both positive and negative coupling constants.

2. Polytopes {35} and {335}

The polytope is a general term for such geometric forms as segment (in one-dimensional space), polygon (in two-dimensional space), polyhedron (in three-dimensional space), etc (in higher-dimensional spaces). The polytope {35} (the notation following that of Schläfli, see [16]) is a polyhedron in which each vertex is surrounded by five triangles (denoted {3}). This polytope is known by the name icosahedron. It is one of the five Platonic solids. However, we look at the polytope in another way. Its faces, instead of being flat, are spherical triangles and they lie on the same sphere as vertices of the polytope (see figure 2). Because we are interested in a space which is the surface of a sphere, the polytope is a two-dimensional triangular lattice in the non-Euclidean curved space S^2 . Unlike the usual triangular lattice in the flat space, in our lattice each vertex has five (instead of six) neighbours. The crystal consists of 12 vertices, 20 faces and 30 edges, but it has no borders. Because of this, our model needs no boundary conditions.

The set of five Platonic solids can be extended to analogical constructions in higher-dimensional spaces. In the four-dimensional space, one can construct six Platonic solids (regular polytopes). One of them is the polytope {335}. It is composed of tetrahedral cells (denoted {33}), with five tetrahedra per near-neighbour bond. As in the previous case, we are considering the construction on the sphere on which the vertices of the polytope lie; so our polytope is composed of spherical tetrahedra. Because the polytope fills the surface of a four-dimensional hyper-sphere S^3 , which is a three-dimensional curved space, it is a three-dimensional crystal without borders. It consists of 120 vertices, 720 edges, 1200 faces and 600 cells. The crystal has icosahedral symmetry at every vertex (the orthogonal projection of one of the atoms with its 12 near-neighbours from S^3 onto Euclidean space can be seen later in figure 3).

Usually one of the vertices of the polytope is placed at the point $(0, 0, 0, R)$ [16] which we shall call the pole of sphere S^3 (R is its radius). Such a choice of a coordinate system is, however, inconvenient for us because of the divergences in equation (10). In order to avoid them, we put the pole in the centre of one of the cells. In that case the vertices of the polytope can be displayed on 15 two-dimensional spheres ($x^2 + y^2 + z^2 = R^2 - w^2$) to get polyhedra. The spheres are the sections of our three-dimensional sphere S^3 by three-dimensional spaces parallel to X - Y - Z space [8, 16]. Icosahedra are inscribed into the spheres $w = 0$, $w = \pm 0.2185R$, $w = \pm 0.3536R$, $w = \pm 0.5721R$. Tetrahedra are inscribed into the spheres $w = \pm 0.1350R$, $w = \pm 0.7906R$, $w = \pm 0.9256R$. Dipyramids are inscribed into the spheres $w = \pm 0.7071R$. By analogy, in our polytope {35} the centre of one of the faces is the pole of the sphere. Cutting the two-dimensional sphere ($x^2 + y^2 + z^2 = R^2$) by two-dimensional spaces parallel to the X - Y space (i.e. planes parallel to the X - Y plane) we get one-dimensional spheres (i.e.

circles $-x^2 + y^2 = R^2 - z^2$). The vertices of the polytope lie on four circles. Triangles are inscribed into all these circles.

3. Description of the model

Let us consider a four-dimensional (three-dimensional) flat space with a Cartesian coordinate system x, y, z, w (x, y, z) and a spherical coordinate system $\rho, \psi, \vartheta, \phi$ (ρ, ϑ, ϕ). The relationships between the coordinates are as follows:

$$\begin{aligned} x &= \rho \sin \psi \sin \vartheta \cos \phi \\ y &= \rho \sin \psi \sin \vartheta \sin \phi \\ z &= \rho \sin \psi \cos \vartheta \\ w &= \rho \cos \psi \end{aligned} \quad (3a)$$

for four-dimensional space, and

$$\begin{aligned} x &= \rho \sin \vartheta \cos \phi \\ y &= \rho \sin \vartheta \sin \phi \\ z &= \rho \cos \vartheta \end{aligned} \quad (3b)$$

for three-dimensional space. In the above expressions, $0 \leq \psi \leq \pi$, $0 \leq \vartheta \leq \pi$ and $0 \leq \phi < 2\pi$.

We define a four-dimensional sphere (three-dimensional sphere) with the radius R by the equation $x^2 + y^2 + z^2 + w^2 = R^2$ ($x^2 + y^2 + z^2 = R^2$). The surface of the sphere is the non-Euclidean three-dimensional space S^3 (two-dimensional space S^2). We can connect a coordinate system r, ϑ, ϕ (r, ϕ) with this space. Here $r = R\psi$ ($r = R\vartheta$) is the geodesic distance from a given point to the reference point called the pole of the sphere, and ϑ, ϕ (ϕ) are the angle coordinates receiving the same values as the coordinates in equation (3a) (equation (3b)). Then the metric tensor of S^3 is

$$g_{ij} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & R^2 \sin^2(r/R) & 0 \\ 0 & 0 & R^2 \sin^2(r/R) \sin^2 \vartheta \end{pmatrix} \quad (4a)$$

and the metric tensor of S^2 is

$$g_{ij} = \begin{pmatrix} 1 & 0 \\ 0 & R^2 \sin^2(r/R) \end{pmatrix}. \quad (4b)$$

In the curved space S^3 or S^2 , respectively, we build the crystal topologically corresponding to our real crystal in Euclidean space. In the present work, we have built the tetrahedral close-packed structure on the sphere S^3 (i.e. the polytope {335}) and the triangle close-packed structure on the sphere S^2 (i.e. the polytope {35}). We recall that only fragments of these structures have their topologically counterparts in flat space. In both cases the counterparts are fragments of the three- and two-dimensional amorphous structures, respectively.

The geodesic distance between near neighbours in the polytopes is equal to $0.6283R$ in the {335} and to $1.1072R$ in the {35} polytope. In both cases we place classical spins

tangent to the sphere on the vertices of the polytope; so the spin dimensionality is 3 for the sphere S^3 and 2 for S^2 . We assume that the spins interact through nearest-neighbour Heisenberg interactions:

$$H = -J_0 \sum_{\langle AB \rangle} S_A \cdot S_B \quad (5)$$

where $\langle AB \rangle$ denotes near-neighbour pairs. Unfortunately, as is well known, in a curved space the scalar product of two vectors located at different points is undefined; thus we must specify what we understand by it.

Let us consider two vectors A and B at the points A and B in a curved space. Because the vectors are connected with different local coordinate systems, in order to calculate their scalar product, we must somehow find the components of one of these vectors in the local coordinate system of the other. The same situation appears also in the usual Euclidean space if we use some curvilinear (e.g. spherical) coordinate system (incidentally it should be noted that our coordinate systems in S^3 and S^2 resemble spherical (r, ϑ, ϕ) and polar (r, ϕ) coordinate systems, respectively). In that case we can work out the problem by moving one of the vectors via parallel transport from one point to the other. In a curved space this operation is not unequivocal because it depends on the path followed. However, from the physical point of view it seems that the best path is the geodesic line connecting both points because interactions are usually transmitted the shortest way. In this sense the scalar product of the vectors A and B is determined by the following expression:

$$A \cdot B = g_{ij}^A a^i \beta_k^j(A, B) b^k \quad (6)$$

where a^i and b^k are the contravariant components of the vectors A and B , g_{ij}^A are the components of the metric tensor at the point A , and $\beta_k^j(A, B)$ are the contravariant components of the basic vectors of the coordinate system at the point B after parallel transport to the point A along the geodesic line connecting these points. Because our metric tensor is diagonal, we may, instead of using the tensor components a^i of the vector A , use the physical components $A^i = a^i \sqrt{g_{ii}}$ (sum over i is not taken). Equation (6) is then given by

$$A \cdot B = G_{ij}^{AB} A^i B^j \quad (7)$$

where

$$G_{ij}^{AB} = \sqrt{g_{ii}^A g_{jj}^B} \beta_j^i(A, B) \quad (8)$$

(do not sum over i and j in the above expression). Consequently our Hamiltonian (5) takes the following form:

$$H = -J_0 \sum_{\langle AB \rangle} G_{ij}^{AB} S_A^i S_B^j. \quad (9)$$

For the lattice on the sphere S^2 (e.g. the polytope {35}) the matrix \mathbf{G} can easily be found using spherical trigonometry (see figure 1) but for the lattice on S^3 (e.g. the polytope {335}) we must find it numerically. First we find the β matrix for a given pair of vertices A and B . In order to do this, we start from the basic vectors in B : $\hat{e}_1(B)$, $\hat{e}_2(B)$, $\hat{e}_3(B)$. Then, we successively compute contravariant components of the vectors parallel to the

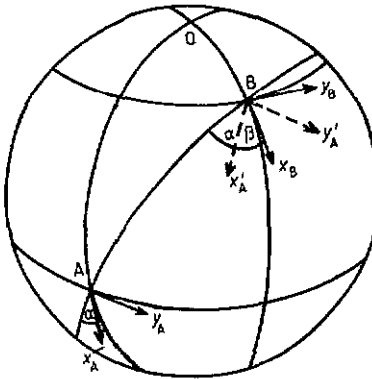


Figure 1. Local coordinate systems at points A and B of the sphere. The axes x'_A, y'_A are obtained after parallel transport of the axes x_A, y_A along the geodesic line AB. The point O is the pole of the sphere. The angle β is the angle of rotation matrix G^{AB} (see text).

first, point by point, in N points on the geodesic line BA in accordance with the following expressions:

$$\begin{aligned}
 e_i^r(k) &= e_i^r(k-1) + R \sin(r/R) \cos(r/R) [e_i^r(k-1) \Delta x^\theta(k) \\
 &\quad + \sin^2 \vartheta e_i^r(k-1) \Delta x^\phi(k)] \\
 e_i^\theta(k) &= e_i^\theta(k-1) - (1/R) \cot(r/R) [e_i^\theta(k-1) \Delta x^r(k) + e_i^r(k-1) \Delta x^\theta(k)] \\
 &\quad + \sin \vartheta \cos \vartheta e_i^\theta(k-1) \Delta x^\phi(k) \\
 e_i^\phi(k) &= e_i^\phi(k-1) - (1/R) \cot(r/R) [e_i^\phi(k-1) \Delta x^r(k) + e_i^r(k-1) \Delta x^\phi(k)] \\
 &\quad - \cot \phi [e_i^\phi(k-1) \Delta x^\theta(k) + e_i^\theta(k-1) \Delta x^\phi(k)]
 \end{aligned}
 \tag{10}$$

where $i = 1, 2, 3; k = 1, 2, \dots, N$ (in our calculations $N = 500$); $e_1^r(0) = 1, e_1^\theta(0) = 0, e_1^\phi(0) = 0; e_2^r(0) = 0, e_2^\theta(0) = 1, e_2^\phi(0) = 0; e_3^r(0) = 0, e_3^\theta(0) = 0, e_3^\phi(0) = 1; \Delta x(k) = x_k - x_{k-1}; x_k$ is the vector pointing to the k th point on the geodesic line connecting the points A and B; $x_0 = x_B, x_N = x_A$.

Finally we multiply the elements of the β matrix by the factor appearing in equation (8).

When the curvature of the space approaches zero (the space becomes flat) the matrix G approaches the rotation matrix

$$G_{ij}^{AB} = \begin{pmatrix} s\vartheta_B C\phi_{BA} s\vartheta_A + C\vartheta_B C\vartheta_A & s\vartheta_B C\phi_{BA} C\vartheta_A - C\vartheta_B s\vartheta_A & s\vartheta_B s\phi_{BA} \\ C\vartheta_B C\phi_{BA} s\vartheta_A - s\vartheta_B C\vartheta_A & C\vartheta_B C\phi_{BA} C\vartheta_A + s\vartheta_B s\vartheta_A & C\vartheta_B s\phi_{BA} \\ -s\phi_{BA} s\vartheta_A & -s\phi_{BA} C\vartheta_A & C\phi_{BA} \end{pmatrix} \tag{11a}$$

(where $s = \sin$ and $C = \cos$) in the three-dimensional case, and

$$G_{ij}^{AB} = \begin{pmatrix} \cos \phi_{BA} & \sin \phi_{BA} \\ -\sin \phi_{BA} & \cos \phi_{BA} \end{pmatrix} \tag{11b}$$

in the two-dimensional case. Here $\phi_{BA} = \phi_B - \phi_A$ and ϑ_A, ϕ_A and ϑ_B, ϕ_B are the spherical coordinates of the points A and B. The Hamiltonian (9) with the matrix (11a) is equivalent to the usual Heisenberg Hamiltonian, and with the matrix (11b) it is equivalent to the usual XY Hamiltonian.

Below, for comparison, we give two G matrices for a pair of points $A(r_A = 0.388, \vartheta_A = 0.116\pi, \phi_A = \pi)$ and $B(r_B = 0.388, \vartheta_B = 0.500\pi, \phi_B = 0.116\pi)$ and for a pair of points $C(r_C = 2.356, \vartheta_C = 0.200\pi, \phi_C = 0.176\pi)$ and $D(r_D = 2.754, \vartheta_D = 0.304\pi, \phi_D = 1.750\pi)$ on the sphere S^3 with $R = 1$ (the left-hand matrices) and in the flat space (the right-hand matrices):

$$G_{ij}^{AB} = \begin{pmatrix} -0.264 & -0.895 & -0.366 \\ -0.956 & 0.292 & -0.026 \\ 0.131 & 0.343 & -0.932 \end{pmatrix} \quad G_{ij}^{AB} = \begin{pmatrix} -0.333 & -0.873 & -0.357 \\ -0.934 & 0.357 & 0 \\ 0.127 & 0.333 & -0.934 \end{pmatrix}$$

$$G_{ij}^{CD} = \begin{pmatrix} 0.676 & 0.169 & 0.717 \\ 0.526 & 0.571 & -0.631 \\ -0.516 & 0.803 & 0.297 \end{pmatrix} \quad G_{ij}^{CD} = \begin{pmatrix} 0.577 & -0.188 & -0.795 \\ -0.583 & 0.587 & -0.562 \\ 0.572 & 0.787 & 0.230 \end{pmatrix}.$$

Note that our matrix G is very similar to the matrix (11) for the pair of points lying near the pole of the sphere, where $\sin(r/R) \approx r/R$.

For a crystal on the sphere S^2 , the matrix G can be expressed as a rotation matrix

$$G_{ij}^{AB} = \begin{pmatrix} \cos \psi_{AB} & \sin \psi_{AB} \\ -\sin \psi_{AB} & \cos \psi_{AB} \end{pmatrix}. \quad (12)$$

For the polytope {35} the angle ψ_{AB} takes the values $0, \pm\pi/5$ and $\pm 3\pi/5$ depending on which pair of near-neighbour vertices of the polytope is considered (in the case of the flat two-dimensional space defined by the polar coordinates r, ϕ the angles $\psi_{AB} = \phi_B - \phi_A$ and for the pairs of points with the same coordinates r, ϕ as our vertices we get the values $0, \pm\pi/3, \pm 2\pi/3$).

Using the form (12), the Hamiltonian (9) for the crystal on S^2 can be rewritten as follows:

$$H = -J_0 \sum_{(AB)} \cos(\theta_B - \theta_A + \psi_{AB}) \quad (13)$$

where θ_A is the angle which the planar spin at the point A makes with an axis parallel to the local meridian (see figure 1). If deformations of cells of our hypothetical crystal, caused by the curve of the space, are very small (i.e. the curvature is very small), the frustrations of each elementary cell are approximately equal because they depend on the curvature of the space (which is constant here) and on the surface of the cells (which are about constant). In the case of polytope {35}, all cells are identical so that the frustration

$$\psi_{AB} + \psi_{BC} + \psi_{CA} = 2\pi f \quad (14)$$

is exactly the same for every elementary triangle and it is equal to $f = \frac{1}{16}$.

The next step of the proposed method is the use of the Hamiltonian (9) to the real crystal which is topologically similar to the hypothetical crystal in curved space. Now (in Euclidean space) we may relate the spins to the global coordinate system instead of relating them to the local coordinates. A transformation of the Hamiltonian (9) to the

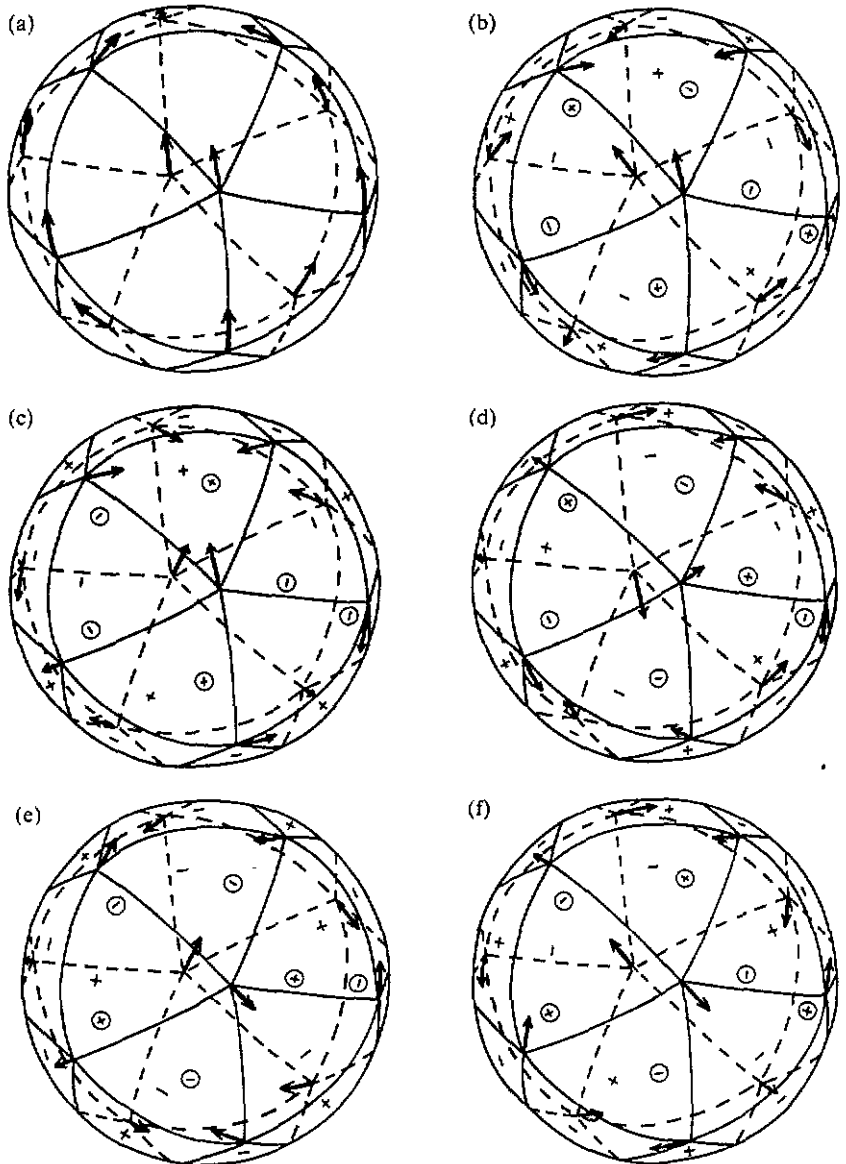


Figure 2. The lowest-energy configuration of the spin system on the polytope {35} for (a) positive and (b)–(f) negative coupling constants. The plus and minus signs in (b)–(f) indicate the helicity of each triangle. The signs in the circles concern the unseen triangles.

Cartesian coordinate system modifies the matrix G . For example, in the two-dimensional case, the matrix (12) takes the form

$$G_{ij}^{AB} = \begin{pmatrix} \cos(\psi_{AB} + \phi_{AB}) & \sin(\psi_{AB} + \phi_{AB}) \\ -\sin(\psi_{AB} + \phi_{AB}) & \cos(\psi_{AB} + \phi_{AB}) \end{pmatrix} \quad (15)$$

where $\phi_{AB} = \phi_A - \phi_B$ and ϕ_A, ϕ_B are the angular coordinates of the points A and B.

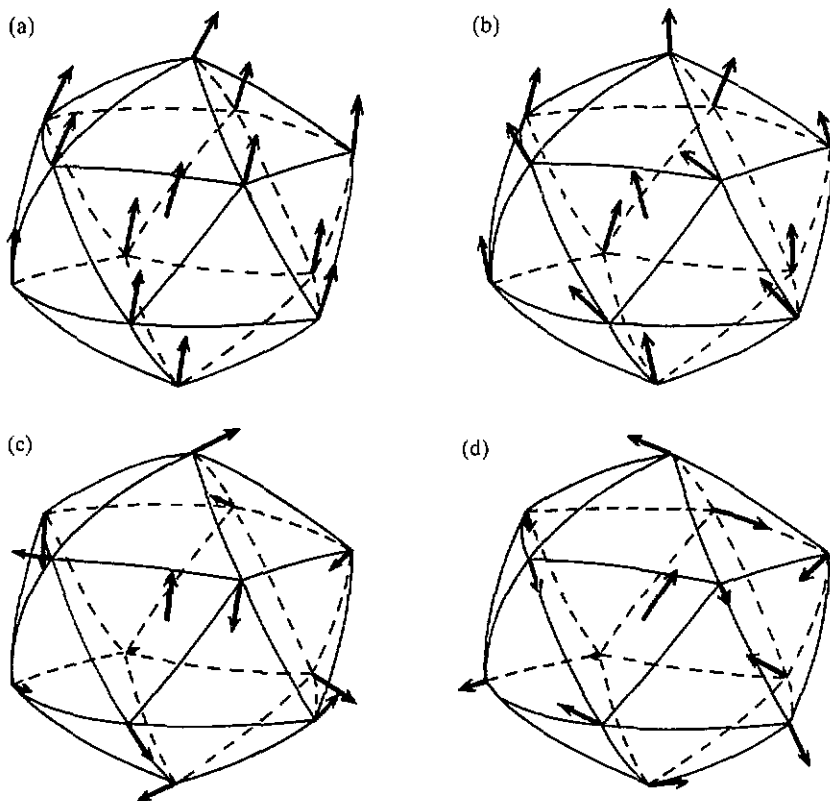


Figure 3. The orthogonal projection of a 'spherical icosahedron' from S^3 onto Euclidean space: (a), (b) $J_0 > 0$; (c), (d) $J_0 < 0$. The spin configurations relate to the ground state and the low-lying metastable state of the polytope {335}. The energies of the central spin are equal to (a) $-11.97J_0$, (b) $-10.47J_0$, (c) $-3.22|J_0|$ and (d) $-2.32|J_0|$.

Note that the transformation does not change the frustration since the sum of the angles ϕ_{AB} around a plaquette is equal to zero.

As one can see, in the case of two-dimensional spins, the model constructed according to that scheme is equivalent to the uniformly frustrated XY model described by the Hamiltonian (1). The Hamiltonian (9), however, is superior to the Hamiltonian (1). The superiority consists of the fact that the former makes sense for both two- and three-dimensional spins while the latter may be used only in the XY case.

As was mentioned in section 1, we do not pass to the Euclidean space in the present work. Here, we have used the Hamiltonian (9) directly for hypothetical crystals in curved space.

4. Monte Carlo simulation

We have studied the behaviour of the Hamiltonian (9) for both systems (i.e. the polytopes {35} and {335}) by the Monte Carlo simulation. In order to find the ground state, we started from a random spin configuration and then, stepping sequentially through the

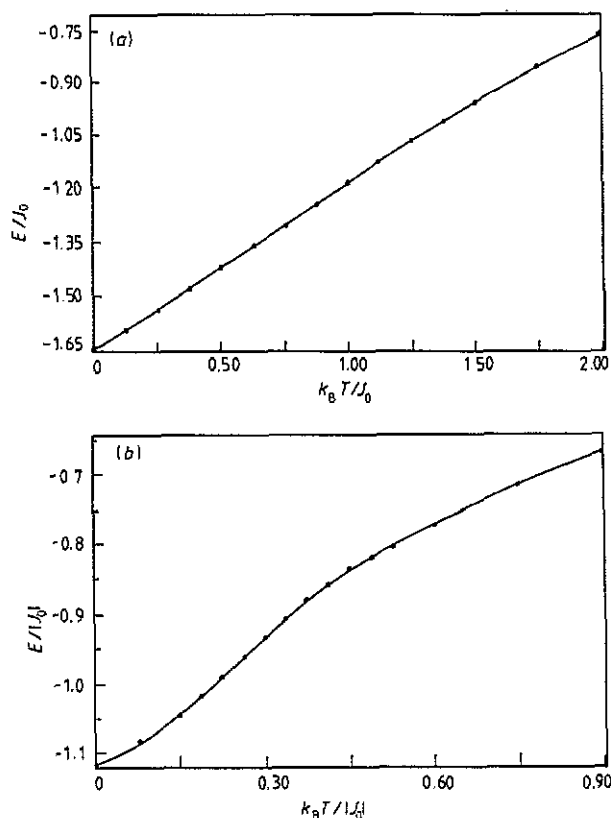


Figure 4. Mean energy per spin versus temperature for the {35} spin system with (a) positive and (b) negative couplings. The full curves are composed of straight lines between neighbouring data points.

lattice, we turned each encountered spin to minimize its energy. In this procedure each spin was turned over 1000 times and finally all spins had, almost, the most profitable directions with respect to their environments. For the polytope {335}, the quantity

$$\chi = \sqrt{\sum_{i=1}^n (E_{i\min} - E_i)^2 / n} \quad (16)$$

where E_i is the energy of the i th spin and $E_{i\min}$ is its actual minimal energy was about $10^{-9}|J_0|$.

The minimal energy of the polytope {35} is equal to $-1.655J_0$ per spin for ferromagnetic interactions and $-1.118|J_0|$ per spin for antiferromagnetic interactions. Thus the system is frustrated for both positive and negative bonds. In the lowest-energy configuration no spin is parallel (for $J_0 > 0$) or antiparallel (for $J_0 < 0$) with respect to each of its nearest neighbours. In the case of a positive coupling constant the ground-state configuration is, energetically, heterogeneous; the spins located near the poles have the energy $-2.000J_0$ and each of the remaining six spins have the energy $-4.618J_0$ (in the ferromagnetic state it should be $-5J_0$). For a negative coupling constant the spin energy is not differentiated; each of the spins has the energy $-2.236|J_0|$.

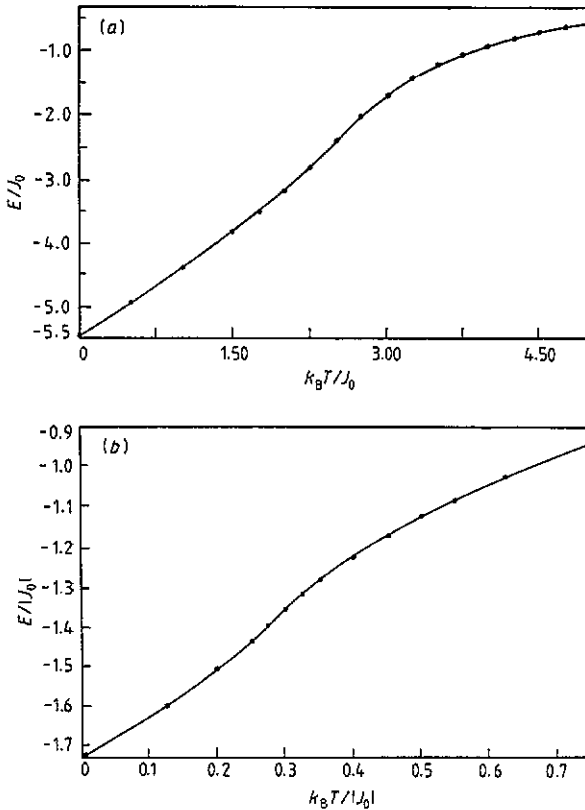


Figure 5. Mean energy per spin versus temperature for the {335} spin system with (a) positive and (b) negative couplings. The full curves are composed of straight lines between neighbouring data points.

Like the usual antiferromagnetic planar model on a triangular lattice [17] or other regularly frustrated systems [18] the ground state of our antiferromagnetic {35} system has an extra discrete degeneracy, in addition to the invariance under an overall rotation of the spins. The full set of ground states consists of five disconnected manifolds (the usual antiferromagnetic triangular lattice has a higher symmetry than ours and therefore its ground state has only two topologically distinct classes of patterns) characterized by different 'helicities'. The helicity of a triangle is defined as $\Sigma(\Delta\theta/2\pi)$, where $\Delta\theta$ is the smallest clockwise change in an angle when the triangle is traversed in a clockwise direction (if two spins happen to be parallel or antiparallel, the helicity is defined to be zero). The ground-state configurations of {35} for positive and negative coupling constants are shown in figure 2(a) and figures 2(b)–2(f), respectively. In these figures the plus and the minus signs indicate the helicities $+0.9$ and -0.6 . In the configuration with the lowest energy for $J_0 > 0$ (figure 2(a)) the helicity of all the triangles are -0.1 except for two polar triangles the helicity of which is equal to 0.9 . Naturally the sum of the helicities of all the triangles is zero for all the above-mentioned cases.

The ground-state energy of the polytope {335} is $-5.455J_0$ per spin for ferromagnetic and $-1.726|J_0|$ per spin for antiferromagnetic interactions. In accordance with what has

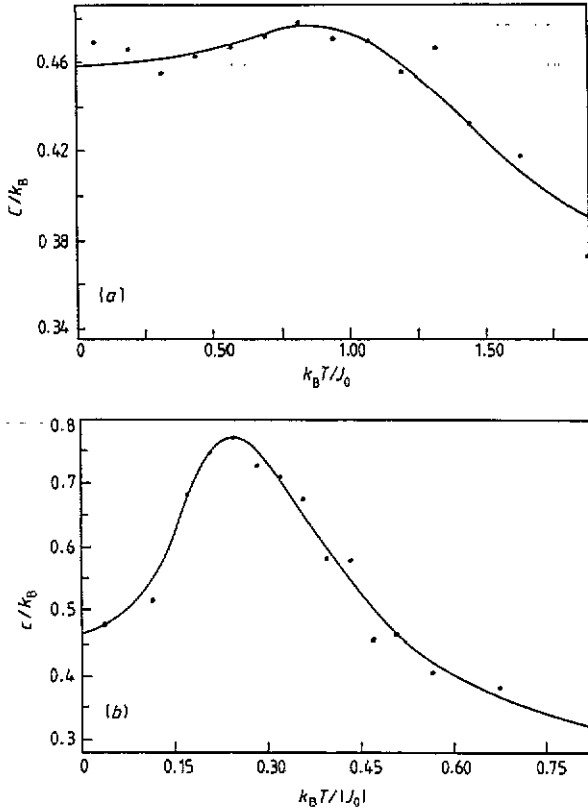


Figure 6. Specific heat per spin versus temperature for the {35} spin system with (a) positive and (b) negative couplings. The smooth curves through the data are drawn as guides to the eye and are not the result of any theoretical computation.

already been shown by Wannier [19], the ground-state energy for the antiferromagnetic case is only about a third of that for the ferromagnetic case.

In the case of positive J_0 the energy of the spins increases moderately as we remove away from the 'equator'. The 12 spins on the equator have the energy $-11.97J_0$ (neighbouring spins are almost parallel to the central spin) and the energies of spins on the other 'layers' (see section 2) are $-11.93J_0$ (eight spins), $-11.88J_0$ (24 spins), $-11.71J_0$ (24 spins), $-11.13J_0$ (24 spins), $-10.14J_0$ (12 spins), $-8.99J_0$ (8 spins) and $-5.37J_0$ (8 spins). For the negative coupling constant in the lowest-energy configuration the spins have the following energies: $-3.78|J_0|$ (20 spins), $-3.55|J_0|$ (40 spins), $-3.40|J_0|$ (20 spins) and $-3.22|J_0|$ (40 spins).

We have not investigated the discrete degeneracy and the helicity of the ground state yet. The problem of the helicity (and especially the question of whether the system sustains the helicity) is very interesting. In two-dimensional and most probably in three-dimensional XY spin glasses the helical ordering occurs only at $T = 0$ [18], but a numerical study by Henley [20] suggested that a Heisenberg spin glass could sustain helicity.

Looking for the ground state we have found, in both coupling cases, a low-lying metastable state. For the positive J_0 , the energy of this state is $-5.236J_0$ per spin and for

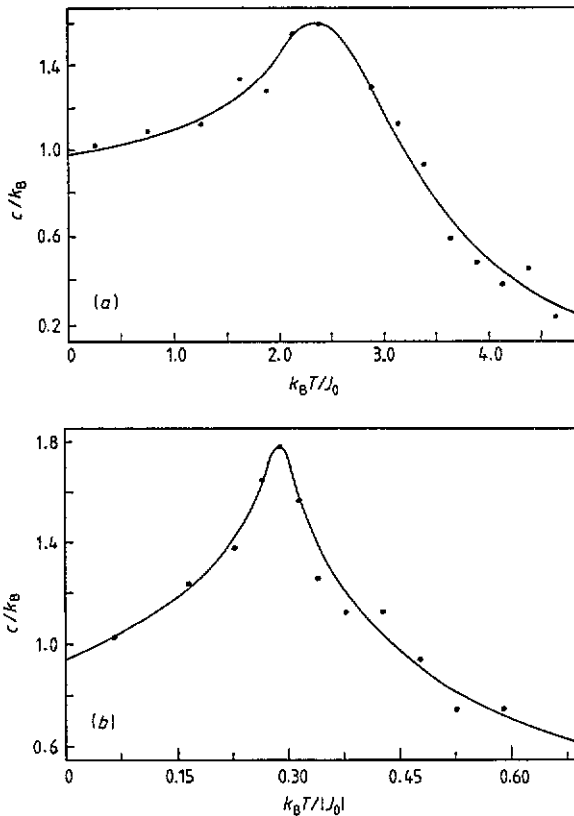


Figure 7. Specific heat per spin versus temperature for the {335} spin system with (a) positive and (b) negative couplings. The smooth curves through the data are drawn as guides to the eye and are not the result of any theoretical computation.

the negative J_0 it is $-1.674|J_0|$ per spin. The first state is energetically very homogeneous, even more homogeneous than the ground state. In this state each spin has the energy $-10.47J_0$. The second state is very heterogeneous. The spin energy varies almost uniformly from about $-2.2|J_0|$ to about $-4.6|J_0|$. Of these two states the former is considerably easier to achieve by Monte Carlo simulation. It follows from this that the former state is more stable than the latter (its potential barrier is higher).

Certainly the system has more than these two local minima. For example once during all runs the system with antiferromagnetic interactions attained a metastable configuration with energy equal to $-1.644|J_0|$ per spin. Perhaps the {35} system has metastable configurations too, but we have not studied it.

Figure 3 shows the orthogonal projection of one of the spins with its 12 near neighbours from S^3 onto the Euclidean space. It is a fragment of the polytope {335} in the ground state and in the metastable state for the ferromagnetic (figures 3(a) and 3(b)) and antiferromagnetic (figures 3(c) and 3(d)) couplings. The energies of the central spin are $-11.97J_0$, $-10.47J_0$, $-3.22|J_0|$ and $-2.32|J_0|$ in figures 3(a), 3(b), 3(c) and 3(d) respectively.

Both the lowest-energy configuration and the metastable configurations are non-collinear. Considering the curvature of our lattice it is impossible to compare the total

spin configurations of our crystal with configurations of any real structures but it is visible that locally they resemble the speromagnetic and the asperomagnetic structures for ferromagnetic and antiferromagnetic interactions, respectively. The spin correlation functions $\langle S_0 \cdot S_1 \rangle / S^2$ for the first shell of neighbours are equal to 0.909 (the ground state) and 0.873 (the metastable state) for ferromagnetic interactions and to -0.288 (the ground state) and -0.279 (the metastable state) for antiferromagnetic interactions.

The temperature dependence of the average energy of both systems has been studied using the standard Metropolis method. As was mentioned in section 2 the systems need no boundary conditions since they have no borders. Data for the polytope {35} are the result of runs averaged over 5×10^4 – 10^5 Monte Carlo steps per spin with 3×10^3 initial passes discarded for equilibrium. For the polytope {335} each averaging was performed over 5×10^3 passes with the initial 10^3 discarded.

Figures 4 and 5 exhibit our results for the temperature dependences of mean energy for both systems for the positive and negative interactions. Figure 4 relates to the {35} system and figure 5 relates to the {335} system. As shown in these figures the energy curve is very smooth so that we have approximated the value of the specific heat at a temperature T between two neighbouring temperatures T_1 and T_2 by $(E_1 - E_2) / (T_1 - T_2)$. To check the method we also used a cubic-spline fit to the values of the mean energy and differentiated it to find the specific heat. The two methods give the same results within the uncertainty of the data.

The specific-heat results are shown in figures 6 and 7. Since our system is classical, the specific heat does not vanish for $T \rightarrow 0$. We have found a specific-heat peak for all cases. The specific heat of the {35} system has a peak at a temperature equal to about $0.9J_0/k_B$ for a positive coupling constant and $0.25|J_0|/k_B$ for a negative coupling constant. The curve of specific heat for $J_0 > 0$ is very rounded so that the temperature of the peak is less certain than for the other cases. For the polytope {335} the specific-heat peak is at a temperature $2.4J_0/k_B$ for $J_0 > 0$ and at $0.28|J_0|/k_B$ for $J_0 < 0$. For both systems in the antiferromagnetic case the specific-heat peak is sharper, its height is greater and the temperature of the peak is considerably lower than for the ferromagnetic case.

5. Summary

The main result of this paper is the Hamiltonian (9) which describes the uniformly frustrated spin systems. It may be used not only in the XY case, as the Hamiltonian (1), but in the Heisenberg case as well. The elements of the matrix G , which occurs in this Hamiltonian, should be calculated according to the scheme proposed in section 3. In order to do this, we must first build, in curved space, the topological counterpart of our crystal. In this paper, however, instead of studying real crystals, we have studied directly hypothetical crystals in curved space—the polytopes {35} and {335}. We think that some properties of the polytope {335} relate to the properties of some amorphous materials because of the topological compatibility between the local structures of the glasses and the polytope. For example, the magnetic order of the ground state (and the metastable states), which we have found for the polytope, resemble locally the speromagnetic structure (for ferromagnetic interactions) and asperomagnetic structure (in the antiferromagnetic case). Both non-collinear forms of magnetic order are typical of the amorphous magnetic systems.

References

- [1] Toulouse G 1977 *Commun. Phys.* **2** 115
- [2] Poon S J and Durand J 1977 *Solid State Commun.* **21** 793
- [3] Villain J 1977 *J. Phys. C: Solid State Phys.* **10** 1717
- [4] Villain J 1977 *J. Phys. C: Solid State Phys.* **10** 4793
- [5] Villain J 1978 *J. Phys. C: Solid State Phys.* **11** 745
- [6] Teitel S and Jayaprakash C 1983 *Phys. Rev. B* **27** 598
- [7] Frank F C 1952 *Proc. Roy. Soc. A* **215** 43
- [8] Sadoc J F 1981 *J. Non-Cryst. Solids* **44** 1
- [9] Nelson D R 1983 *Phys. Rev. B* **28** 5515
- [10] Nelson D R and Widom M 1984 *Nucl. Phys. B* **113**
- [11] Widom M 1986 *Phys. Rev. B* **34** 756
- [12] Fradkin M A 1987 *Zh. Eksp. Teor. Fiz.* **93** 1442
- [13] Dong-Ping Deng and Widom W 1987 *J. Phys. C: Solid State Phys.* **20** L449
- [14] Straley J S 1986 *Phys. Rev. B* **34** 405
- [15] Nägle W 1981 *Z. Phys. B* **42** 135
- [16] Coxeter H S M 1973 *Regular Polytopes* (New York: Dover) pp 118–64
- [17] Lee D H, Joannopoulos J D and Negele J W 1986 *Phys. Rev. B* **33** 450
- [18] Kawamura H and Tanemura M 1987 *Phys. Rev. B* **36** 7177
- [19] Wannier G H 1950 *Phys. Rev.* **79** 357 (erratum 1973 *Phys. Rev. B* **7** 5017)
- [20] Henley C L 1984 *Ann. Phys., NY* **156** 324, 368