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A NEW TWO-DIMENSIONAL LATTICE OF COORDINATION NUMBER FIVE*

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An introduction is given to the symmetrical square and triangular two-dimensional Bravais lattices. Next the two most symmetric two-dimensional, non-Bravais regular lattices are introduced - the honeycomb and the kagome - each derived from the triangular lattice. These four lattices have coordination numbers of four, six, three and four respectively. A third high symmetry two dimensional non-Bravais regular lattice, also derived from the triangular lattice is introduced. The remarkable fact about this previously unknown lattice is that its coordination number is five.

On introduit des treillages Bravais symétriques qui sont carrés et triangulaires et qui ont deux dimensions. On présente ensuite des treillages non-Bravais réguliers les plus symétriques qui ont deux dimensions, le rayon de miel et le kagone, chacun desquels découle du treillage triangulaire. Ces quatre treillages ont des numéros de coordination de valeur quatre, six, trois et quatre respectivement. On présente enfin un treillage régulier, de haute symétrie, bidimensionné et non-Bravais, une dérivation du treillage triangulaire. L'aspect remarquable de ce treillage, préalablement inconnu, est le fait que cinq est son numéro de coordination.

Introduction

Bulk solid materials are most commonly found in a crystalline state. Their constituents - atoms, molecules or ions - typically occupy the sites or vertices of a three dimensional lattice. Familiar examples are the simple cubic, body centered cubic, face centered cubic, hexagonal close packed and diamond lattices. Descriptions and drawings of these lattices can be found in most textbooks on solid state physics.

Less familiar but not uncommon are two-dimensional lattices. Kittel (1956) provides an exceptionally good introduction to them. They may occur as monatomic layers well separated from one another within the structure of a complex three-dimensional crystal and these have become of greater interest since the discovery of high temperature superconductors (Bednorz and Müller, 1986). In typical high T_c cuprate superconductors such as $YBa_2Cu_3O_{6+x}$ or $La_{2-x}Sr_xCuO_2$ two-dimensional layers of CuO_2 within the parent compound appear to serve as the medium in which the current flows without resistance (Manousakis, 1991).

For many years it has been accepted that there are four regular two-dimensional lattices of high symmetry - the square, triangular, honeycomb and kagome; in each, all vertices are equivalent. In the four lattices each vertex has four, six, three or four nearest neighbour vertices or sites respectively. In this paper a previously unknown two-dimensional lattice of high symmetry in which all the vertices are equivalent and each vertex has five neighbours is presented.

Two Bravais lattices - square and triangular

A Bravais lattice is a simple lattice in which any two vertices are equivalent under translation alone (in more complex lattices two vertices are in general equivalent only under a combination of translation and rotation). The two most symmetric and common two dimensional Bravais lattices are the square (Fig 1a) and triangular (Fig 1b).

* Dedicated to the memory of Walter J. Chute

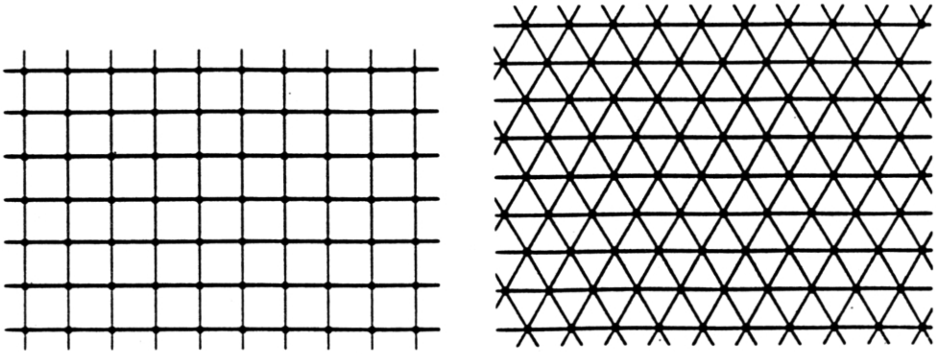

Fig 1 The two most symmetric two-dimensional Bravais lattices (a) the square lattice; (b) the triangular lattice.

Suppose you were a small but highly intelligent insect. You could walk along the nearest neighbour bonds from one vertex of a Bravais lattice to any other vertex and your view, facing the same direction, would be identical to that from the first vertex. This is a demonstration of the translational invariance of a Bravais lattice.

Next suppose that you, the intelligent insect, remain at the same vertex of the square lattice but you rotate counter-clockwise by 90°, 180° or 270°, your view does not change at any of the four positions. This demonstrates the rotational invariance of the square lattice. Similarly rotation by 60°, 120°, 180°, 240° or 300° at a vertex of a triangular lattice provides an identical view. Thus the square lattice has fourfold rotational invariance and the triangular lattice has sixfold rotational invariance. This rotational invariance is intimately related to the fact that a vertex on the square lattice has four nearest neighbours (coordination number four) while a vertex on the triangular lattice has coordination number six.

These two lattices each have a third type of invariance. If several fellow insects erected a large mirror perpendicular to the lattice plane and orientated along one of the nearest neighbour bonds the reflection in the mirror would be identical to the view before it was obscured by the mirror. This is reflection invariance.

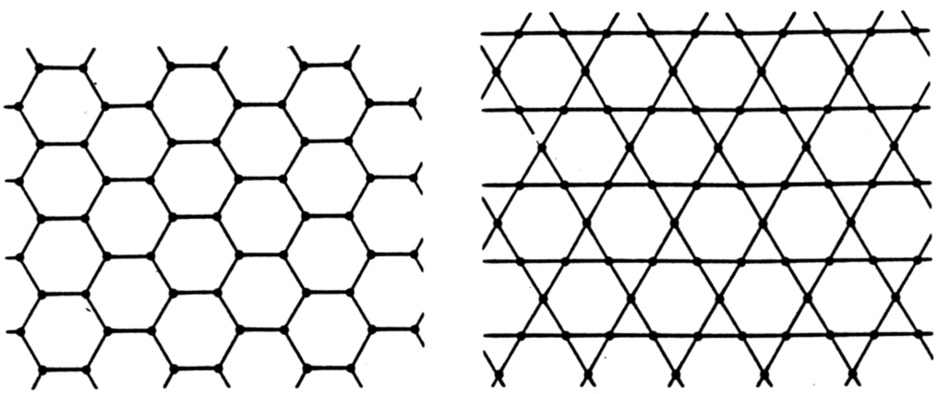

Fig 2 The two most symmetric two-dimensional non-Bravais lattices (a) the honeycomb lattice; (b) the kagome lattice.

Two non-Bravais lattices - the honeycomb and the kagome

The two most symmetric two-dimensional non-Bravais lattices are the honeycomb and the kagome lattices illustrated in Fig 2a and Fig 2b respectively. Note that the honeycomb lattice has coordination number 3 and that the kagome lattice has coordination number four. Now if you, bright insect, standing on the honeycomb lattice, walk from your initial vertex to one of its three nearest neighbour vertices without turning, the appearance of the lattice in front of you appears different. However, if you also turn through 60°, 180° or 300° at the second vertex the lattice looks the same as you saw it initially. This is a manifestation of the invariance of the honeycomb lattice under a combination of translation and rotation.

If you are standing on a vertex of the kagome lattice and walk to the next vertex you must also turn through an angle of 60° or 240°, clockwise or counter-clockwise depending on which vertex you walked to, for the lattice scenery to remain the same. This is a second example of a non-Brevais lattice being invariant under a combination of translation and rotation. If you now stand at the center of one of the hexagon "holes", the lattice from this vantage point is more symmetric for it is invariant under rotation about 60°, 120°, 180°, 240° or 300°. That is, it has sixfold rotational invariance. The honeycomb lattice also has reflection invariance in any mirror erected to run through the center of a hexagon and any one of the 6 vertices nearest to the center. The kagome lattice has the same reflection and sixfold rotation invariances when observed from the center of one of its hexagons.

The reader may observe in Fig 2a that the honeycomb lattice is invariant under translation if the translation is to a *second-nearest* neighbour of the initial vertex. Similarly, an examination of Fig 2b reveals that the kagome lattice is invariant under translation if the translation is to a third-nearest neighbour.

Construction of other lattices from the triangular lattice

Fig 3a demonstrates that the triangular lattice may be considered as consisting of 3 identical triangular sublattices whose vertices are labelled A, B, and C. Deleting any one of three sublattices produces a honeycomb lattice consisting of two triangular sublattices as illustrated in Fig 3b. The triangular lattice may be considered also as consisting of four identical triangular sublattices. Eliminating any one of the four sublattices yields the kagome lattice. Thus the kagome lattice consists of 3 triangular sublattices.

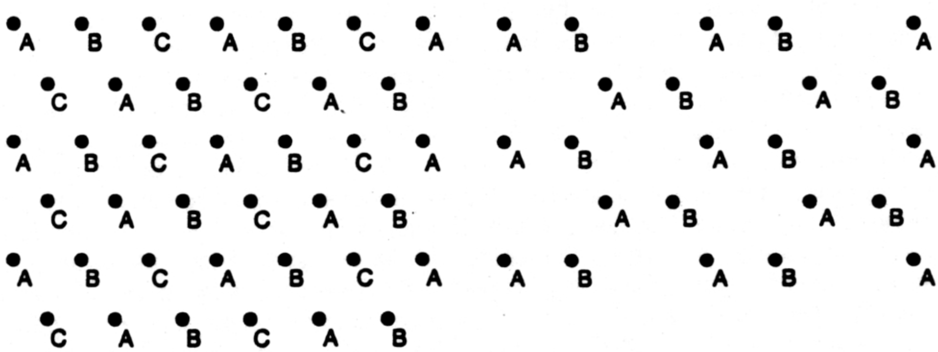

Fig 3 Deriving the honeycomb lattice from the triangular lattice (a) the triangular lattice as composed of three triangular sublattices A, B, and C; (b) the honeycomb lattice as composed of triangular sublattices A and B.

The triangular lattice can not be considered as consisting of two, five, six or eight triangular sublattices, but it can be considered as consisting of *seven* equivalent triangular sublattices as shown in Fig 4a. To make this comparison more obvious the vertices of sublattice G have been joined by solid lines. If any one of the seven sublattices is eliminated (e.g. G) a lattice of coordination number five, illustrated in Fig 4b, is obtained. It is like the honeycomb and kagome lattices in containing an array of hexagonal "holes" created by the deletion of one of the triangular sublattices.

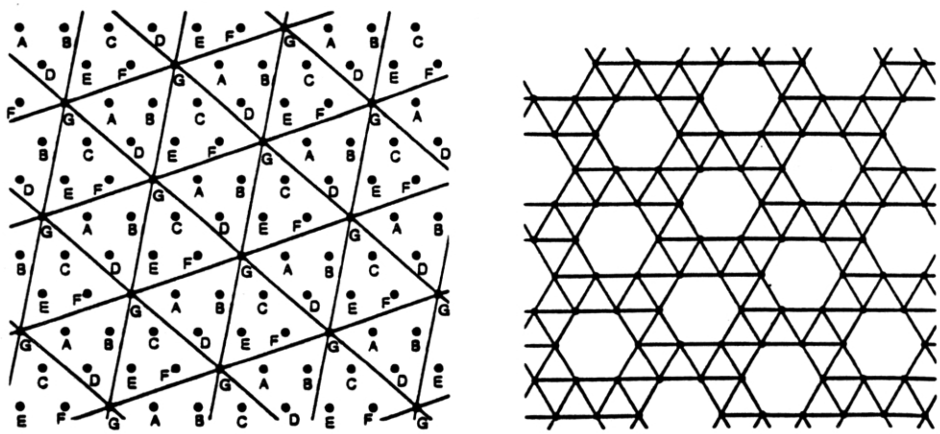

Fig 4 Deriving the new lattice from the triangular lattice (a) the triangular lattice as composed of seven triangular sublattices A, B, C, D, E, F, and G; (b) the coordination five lattice as composed of all but one of the seven sublattices in Fig 4a.

Consider the symmetry of this new lattice; seen from the center of one of the hexagons it is, like the honeycomb and kagome lattices, invariant under rotation through a multiple of 60°. However, unlike the other two non-Bravais lattices, the new lattice does not have invariance under reflection in any line through the center of a hexagon. Indeed it does not have reflection invariance in any straight line drawn anywhere on the lattice. What is important for any lattice is its symmetry with respect to the vertices of the lattice.

To facilitate understanding of the translation-rotation invariance of the new coordination five lattice, it has been decorated in Fig 5 with stylized maple leaves.

Each vertex is now directly underneath the point on the leaf where its veins meet, the leaf's vertex. Pick any leaf as central, and notice that each of its five nearest neighbours is orientated at 60°, 120°, 180°, 240° and 300° with respect to it. Suppose once more that you are an intelligent insect. What the leaves are telling you, for example, is that if you are initially standing on the vertex of a leaf facing the end point of the leaf and walk in that direction to the vertex of the next leaf, you must then turn counter-clockwise by 120° for the lattice with all its leaves to look identical to its appearance when you left your starting point. If you walk to any one of the other four nearest leaves then the angle you must rotate through for the lattice to appear unchanged is one of 60°, 180°, 240° or 300° depending on which neighbouring leaf you reach.

The translation-rotation invariance relation between any pair of nearest neighbour vertices means that this coordination five lattice is regular and has point group symmetry 6 and space group symmetry p6 (Kittel, 1956).

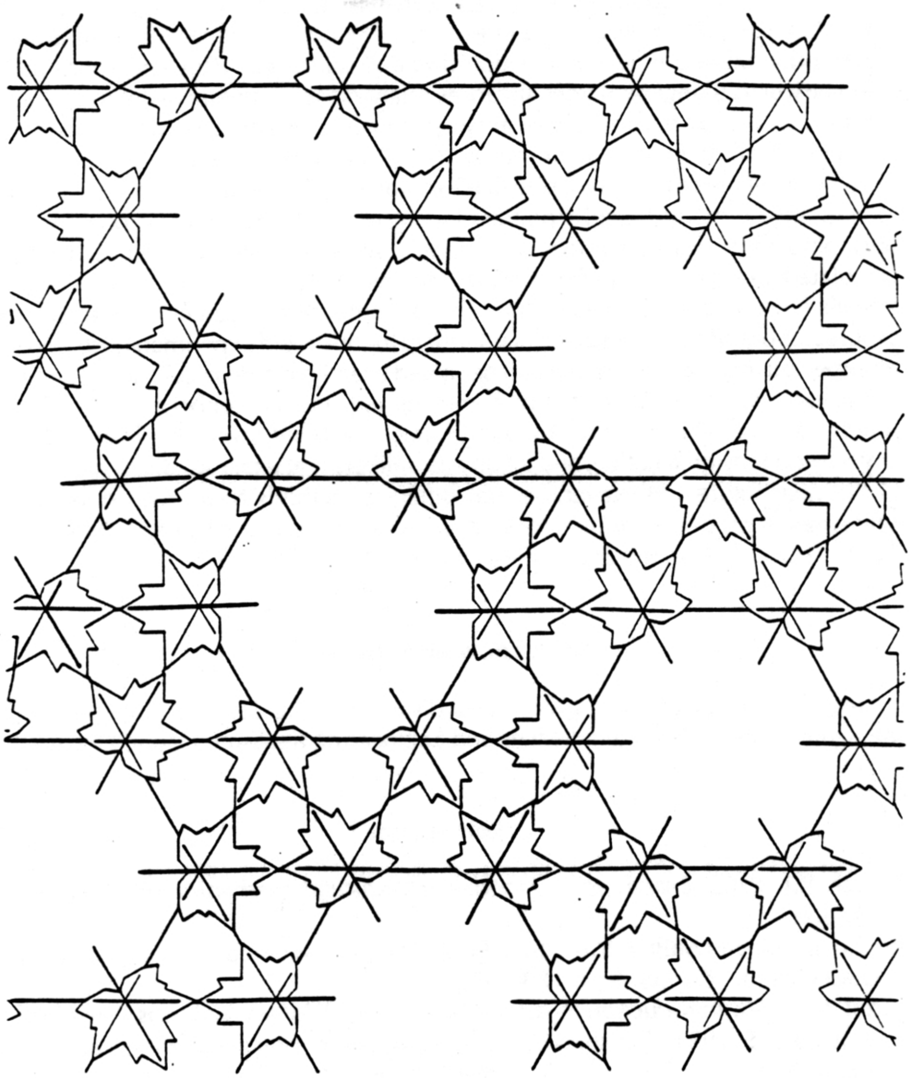

Fig 5 The new lattices decorated with stylized maple leaves. All leaves on each sublattice point in the same direction, but the leaf orientations on different sublattices differ in direction by a multiple of 60°.

Discussion

In this paper it has been shown that the honeycomb (Fig 2a) and kagome (Fig 2b) lattices can be derived from the triangular lattice by deleting sublattices. This led to the derivation of a new lattice by first regarding the triangular lattice as being composed of 7 sublattices and then deleting one of the latter. The remarkable feature of this new lattice is that it is a regular lattice with coordination number five. The symmetry of this lattice has been described in part by decorating the lattice vertices with stylized maple leaves oriented in a different direction on each sublattice. This lattice has half the symmetry of its triangular parent and three quarters the symmetry of the square lattice.

One may predict that real physical systems having the structure of the coordination five lattice will be found and/or made. The physical properties of such systems are likely to be of interest and two possible examples in the field of magnetism are worth mentioning. The Ising model of nonconducting ferromagnets or antiferromagnets is the only physically realistic model of magnetic systems whose properties have been calculated exactly on two-dimensional lattices (the properties of several magnetic models have been calculated exactly on one dimensional lattices or chains). These exact solutions (Baxter, 1982) are of interest to theorists and experimentalists and it can be expected that the Ising model will be solved exactly on the coordination five lattice.

The properties of other magnetic models e.g. the Heisenberg model, that are somewhat more complex than the Ising model, have not been calculated exactly on any two-dimensional lattice, and it appears unlikely that exact solutions will be found in the near future. However, several different methods have been developed to calculate the properties of such models to high precision on standard lattices and the same methods are applicable to these models on the new lattice.

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