Lecture 5

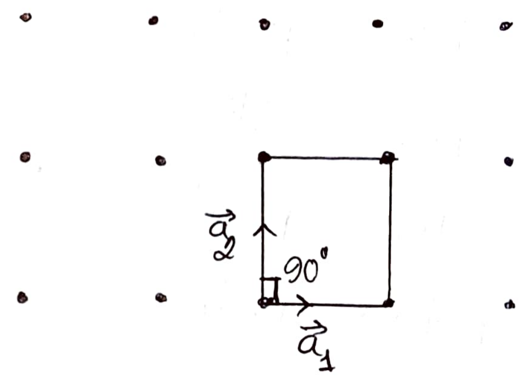
The classification of Bravais lattices

The problem of classifying all possible crystal lattices/ structures is too complex to approach directly. Hence, we will consider first the classification of Bravais lattices. Here, we will consider the Bravais lattice as a crystal structure formed by placing at each point an abstract basis - a sphere centered around a lattice point. This ensures that no symmetry of the Bravais lattice is lost, for example translational symmetry. The operation of the symmetry group will include rotation, reflection, inversion and possible combinations of them. Along with these, we will also consider the translation as another symmetry operation. First, let's talk about two-dimensional lattices.

Two dimensional Bravais lattices

There is an infinite number of possible lattices in two dimension since there is no restriction on the lengths of the lattice basis vectors or the angle between them. However, it turns out that in two dimension we can classify the 2D Bravais lattices into five categories. We will start with a lattice with maximum symmetry and reduce the symmetry by deforming it to find new lattice types.

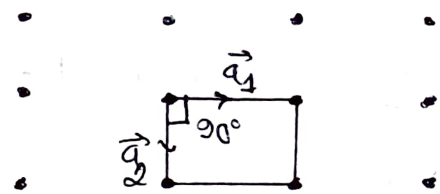
(i) Square lattice: For this type of lattice, $a_1 = a_2$ and $\phi = 90°$. The lattice has a four-fold rotation axis. In addition, it also has four reflection lines.



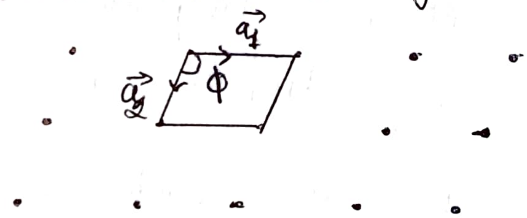
The four fold rotation axis is passing through perpendicular to the lattice plane. One reflection line is parallel to a_1, another to a_2, and the other two are along the body diagonals.

(ii) Rectangular lattice: We can reduce the symmetry by pulling one of the axis such that, $a_1 \neq a_2$, however $\phi = 90°$ still. The resulting lattice is a rectangular lattice. It has a two fold rotation axis and two reflection lines.

The two fold rotation axis is perpendicular to the plane of the paper and the reflection lines are one parallel to a_1 and another parallel to a_2.

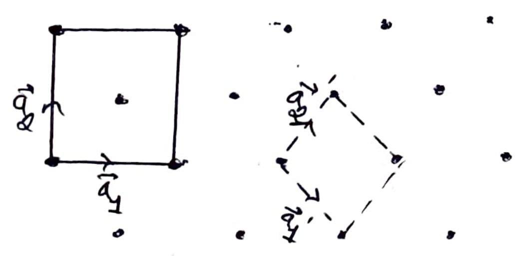


(iii) Oblique lattice: A second attempt to reduce the symmetry even more is to make the lattice such that a_1 and a_2 is arbitrary ($a_1 \neq a_2$) and ϕ is arbitrary as well ($\phi \neq 90°$). The resulting lattice is the oblique lattice. The only symmetry present there is the two-fold rotation axis.



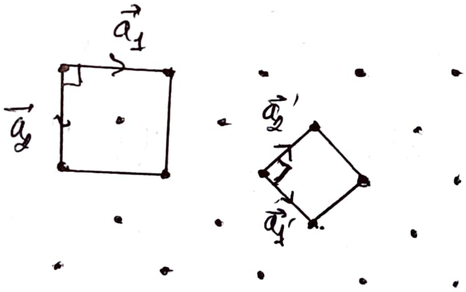
(iv) Centered rectangular lattice: One can construct Bravais lattices with centerings of the lattice points such that the translational symmetry is not broken. In 2D, we can have a lattice point at the midpoint of the rectangular lattice, so that the unit cell has a total of two lattice points.

In such a Bravais lattice, $a_1 \neq a_2$ and $\phi = 90°$. However, one could also define the lattice by a primitive cell (shown by the dashed line) with $a_1' = a_2'$ and $\phi \neq 90°$.

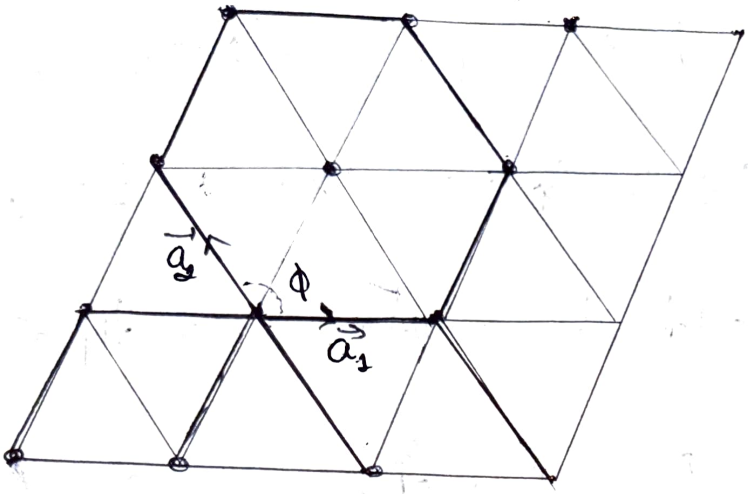


One might wonder whether we can have a cetered square lattice or not. It might seem that we can have such a lattice. However, a closer inspection reveals that redundancy occurs when we try to do so.

For the centered square lattice, the primitive cell is also a square. Defining the lattice with the smaller square then can span the whole lattice. It is redundant to use the same shape for defining a new lattice.



(iv) Hexagonal lattice: Finally, we can consider a different Bravais lattice than the others. We consider the hexagonal structure to form this lattice type. The lattice has a six-fold rotation axis of symmetry. It also has two mirror reflection lines. Here, $a_1 = a_2$ and $\phi = 120°$. This can be viewed as the Wigner-Seitz primitive cell. However, the parameters a_1 and a_2 are defined by a regular primitive cell (dotted one) which can guide the translation vectors.



$a_1 = a_2 = a$

$\phi = 120°$

So, the 2D hexagonal structure is made up from the triangular nets. A 3D hexagonal lattice then can be made up by stacking up these triangular nets.

Three dimensional lattice types

When a symmetry operation has a locus (a point for inversion, ax axis for rotation, a plane for reflection) that is unchanged by the symmetry operation, then the locus is called the symmetry element. Symmetry elements in a group have at least one common point, and as a result, the symmetry operations at least leave a point of an object unmoved.

A group of such point symmetry operations (whose operation leaves at least a point unmoved) is referred to as a point group. Lattice translation is not included in any point group, since the operation does not leave any point unmoved.

When examining nontranslational symmetries, one often considers only those operations that leave a particular point fixed. This subset of full symmetry group is called the point group of the Bravais lattice. There turn out to be only seven distinct point groups that a Bravais lattice can have. Any crystal structure belongs to one of seven crystal systems, depending on which of the seven point groups the underlying Bravais lattice have. When one relaxes the restriction to point operations and considers the full symmetry including the translation, there turn out to be fourteen distinct space groups that a Bravais lattice can have. What we mean by this is, we places lattice points in the Bravais lattice such that, the lattice structure becomes invariant under a translation from one lattice point to another. One can then involve symmetry operations called "screw axes" and "glide plane", and involve the symmetry of the basis as well as the Bravais lattice (meaning we relax the condition that basis is just a sphere which ensures maximum symmetry of the basis). The total number of space groups then greatly increases. In total, there are a total of 32 distinct crystallographic point groups and 230 space groups. We will talk about these later.

How we classify crystal systems and Bravai lattices

From the point of view of symmetry, a Bravais lattice is characterized by the specifications of all rigid operations (operations that preserve the distance between ~~two point~~ all lattice points) that take the lattice into itself. The set of operations is known as the symmetry group or space group of the lattice.

The operations in a symmetry group of a Bravais lattice include all translation through lattice vectors. In addition, there are rotations, reflections and inversion that take the lattice into itself.

Any symmetry operation ~~in~~ of a Bravais lattice can be compounded out of a translation T_R through a lattice translation vector $\vec{R}$ and a rigid operation leaving at least one lattice point fixed. Translation through a lattice vector leave no point fixed. The fact that we stated is not immediately obvious. Consider an ~~exap~~ example. The following figure shows a cubic

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Bravais lattice, where the view is along the c - axis. If one rotates the lattice about an axis going through P perpendicular to the plane of the paper. Although the lattice comes back

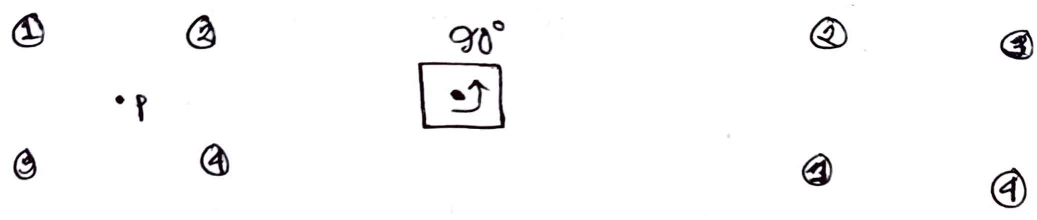

Fig. (a)

to itself, this rigid operation leaves no lattice point fixed. However it can be compounded out of a translation through a Bravais lattice vector and a rotation about an axis that passes through a lattice point as shown in the following figure.

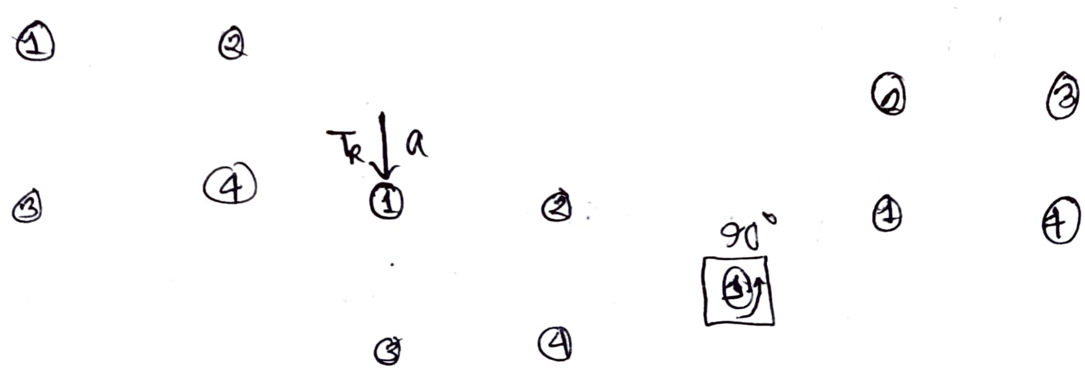

Fig. (b)

This clearly shows how our claim works. This fact is possible in general, which can be seen from the following arguments:

Consider an operation S that takes the lattice onto itself, but leaves no lattice points fixed. Suppose, it takes the origin of the lattice $\vec{0}$ into the point $\vec{R}$. Consider the next case, when after applying the operation S, one apply a translation through $-\vec{R}$, which is denoted by T_{-R}. The composite operation is given by $T_{-R}S$, which is also a symmetry of the lattice, but it leaves at least one point of the lattice (origin in this case fixed). Here, S transports the origin to $\vec{R}$, while T_{R} brings $\vec{R}$ back to the origin. If however, after performing the operation $T_{R}S$ one performs T_{R}, the result is equivalent to performing S alone, since the final application of T_{R} just cancels the effect of T_{R}." Therefore, S can be compounded of $T_{-R}S$, which leaves a lattice point fixed, and the T_{R}, which is a pure ~~transfall~~ translation."

Thus, the full symmetry group of a Bravais lattice contains only ~~two~~ operations of the following form:

1. Translation through Bravais lattice vectors.
2. Operations that leave a particular point on the lattice fixed.

~~3. Successive applications of type 1 and~~
~~or 2 that constitutes other operations.~~

3. Operations that can be constructed by successive applications of 1 or 2.

When one considers the point group (that is made of point symmetry operations), there turns out to be seven distinct crystal system a Bravais lattice can be in. Two point groups are identical if they contain precisely the same operations.

When one relaxes the restriction of point operation and consider the full symmetry group of the Bravais lattice, there turns out to be fourteen distinct space groups that a Bravais lattice can be in.