PHY HC 5026: Solid State Physics: Lecture 02

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1 Crystal Structure: Continued

1.1 Symmetry

So far we have introduced the most basic concepts to be used in the study of crystalline solids, today we are going to dive into categorizing various classes or types of lattices that we may expect to find in nature. Apriori, we may expect that there can be hundreds and perhaps thousands of kinds of lattice structures, but it would be really helpful if you could know what exactly are the kinds of lattices that exists in nature. Turns out, symmetry can be used as a guide to predict how many kinds of lattice structure are allowed to exist in nature. For example:
Question: why do we have two hands?
Answer: it's not a complete answer but a hypothesis, most mammals have 4 such limbs, 3 points make up a plane, so one can stand in a stable way, and the `4th` can be used to do be lifted and do other stuffs while one is standing. Symmetry plays a great role here, almost all creatures have a mirror symmetry, if you draw a line through the front, the left and the right side of the body remain symmetrical, therefore, an extra human hand would probably be placed on the chest or the back and should have even number of fingers to maintain the symmetry. Which way the hand will band? To maintain the mirror symmetry, the elbow should band inward or outward, both will be very uncomfortable and less useful. Also, our left-brain operates the right side and vice versa, which part will manage that third hand? Position of our hearts of course breaks the mirror symmetry but it has a lot of efficiency related reasons and it's an involuntary organ that is not consciously commanded by us.

Similarly, spherical symmetry of the gravitational law $1/|\vec{\mathbf{r}}|^2$ dictates that heavenly bodies will tend to be spherical in shape, and therefore, we know why it's crazy to imagine a "flat earth!" and how unstable a "flat planet" will be under gravity and therefore will get deformed pretty soon even if we built one and placed in space. Anyway, what we are trying to establish here is that symmetry is a great tool to guess in what forms we can expect various "objects" to exist. We can guess, why trees will tend to be growing perpendicular to the surface of earth due to gravity, why planets must revolve around a star only in a plane and not in all crazy orbits due to the conservation of angular momentum that again comes due to the rotational symmetry of space. So symmetry alone can explain most of the phenomena around us, in fact "symmetry" lies at the center of physics, most physical laws we have discovered so far, are all due to our understanding of symmetries in nature.

Question: What do we mean by symmetry mathematically speaking or in the language of physics?
Answer: Any operation that leaves the appearance of a system intact is a symmetry of the system.

Example 1: a perfect sphere: take a white (or any single colored) sphere, rotating it around any of its axis by any amount will not change the way it looked before the rotation, you won't be able to detect any difference in its appearance, therefore "rotation by any angle through any of its central axes" is a symmetry of the sphere. Now, take a marker and draw a dot on the sphere, will the sphere still have the same old symmetry? If "yes", give an argument in support, if "no", does the sphere poses any left-over symmetry? Or all symmetries gone? Explain.

Example 2: An isosceles triangle on a plane has 3-fold (a "fold" will be explained later) rotational symmetry, rotation by 60^o along one of its perpendicular bisectors of its bases will leave the triangle looking exactly the same. Taking mirror images along planes passing through those axes will be its symmetries too. Therefore, "rotation by 60 degrees along perpendicular bisectors" of an isosceles triangle is a symmetry of this triangle, "taking mirror images" by mirror planes passing through those same axes will also be its symmetries. Will breaking a corner of the triangle by a tiny amount destroy the above mentioned symmetries? Explain.

1.2 Symmetries of Lattices

There are 3 types of symmetry operations in a lattice, (1) rotation, (2) reflection by a mirror plane, and (3) inversion about a point, about the origin that would be $x \to -x, y \to -y, z \to -z$ or simply $\vec{r} \to -\vec{r}$. You can find any shape that has a lot of symmetries, but that shape may not qualify as a primitive cell of a lattice and therefore cannot build a whole lattice. Remember, a primitive cell is the kind of shape that must have only one enclosed point, when repeated infinitely, there should not be any gaps or overlaps in the resulting lattice. An individual unit cell may have a symmetry but a lattice that is extended up to infinity in all possible directions, might not have that particular symmetry. For example:

A pentagon: consider a regular pentagon (all sides equal) as shown in Fig. (1), if you consider a rotation axis through its center, every $360^o/\mathbf{5}$ angle, it will be back to its original form.

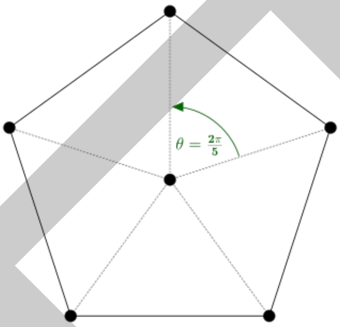

Figure 1: *5-fold* symmetry of a pentagon, every $2\pi/3$ radian rotation around its central axis, it comes back to itself.

The n-fold symmetry: a “fold” is the number of times a geometrical shape repeats itself if you rotated it around a symmetry axis by 2π radian or 360^o. For example, a **square** has “4-fold” symmetry, because if you rotate it by 2π radian, every $2\pi/4$ radian or 90^o it will come back to itself, or n-times a square will repeat itself within that 360^o.

Question: does a rectangle have “4-fold” symmetry? If not, how many fold symmetry does a rectangle have?
Answer: a rectangle comes back to itself after a rotation of every $2\pi/2$ radian, that is after a 180^o and the final 360^o, therefore, a rectangle or even a parallelogram (oblique) has this exact “2-fold” symmetry.

Question: What else does a rectangle have? Maybe a reflection symmetry? Through which plane? Does an oblique parallelogram has the same mirror symmetry?

Question: Can you build a lattice using a pentagon? In other words, can a 2D lattice have so called “**5-fold**” symmetry?

1.3 Bravais Lattices

Auguste Bravais (1850), using symmetry arguments, first time showed that only **5** types of lattices are possible in **2 dimension** and **14** types (under 7 general categories) possible in **3 dimensional** space. These lattice types are called *Bravais lattices.*

1.3.1 Bravais lattices in 2D:

most general kind of lattice we can consider in 2D will be an *oblique lattice* with two unequal sides (opposite sides are equal) and the angle between them $\neq 90^o$, if you take any axis passing through one of its corner-points (or even through its center), perpendicular to its plane, a rotation by $2\pi/2 = \pi$ and 2π radians will leave the lattice intact, therefore, we say that “an oblique lattice has a *2-fold* rotational symmetry”. In 2D, an oblique lattice can have 4 more special types based on their side-lengths and angles, these types: that is “oblique” plus four of its special types comprise the total

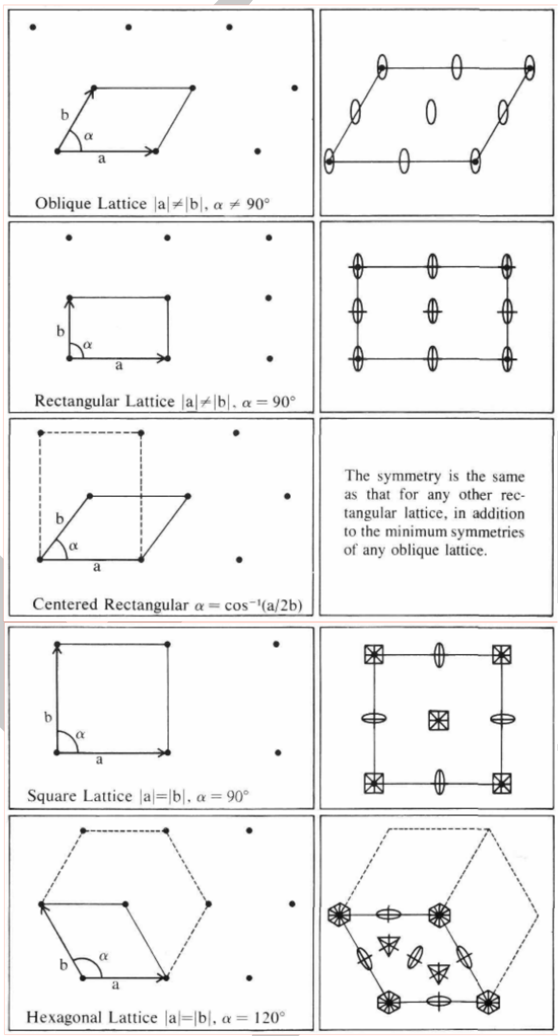

Figure 2: 0 = 2-fold rotation axis. △ = 3-fold rotation axis. □ = 4-fold rotation axis. ⬡ = 6-fold rotation axis. | = mirror symmetry plane. + = orthogonal mirror planes. ✻ = mirror planes every 45^o

"5 types of lattice structures allowed in 2D", they have been listed in Fig. (2). All the rotational-symmetry axes and mirror-symmetry planes have been marked using standard symbols as shown in the figure.

A few more important definitions related to symmetry of a lattice are:

Reflection: If you place a mirror on a plane and a cell under reflection by that mirror, looks exactly the same as that of the cell before reflection, then that plane is a mirror symmetry plane of the cell.

Inversion: If you could find an origin O such that, if you replced all the position vectors of the atoms of a cell $\vec{r}$ by $-\vec{r}$ from that origin, and the resulting new cell looked exactly the same as it did before this *inversion*, then this origin would be an *inversion point* of the cell and the lattice will be said to have an inversion symmetry.

Note: Check that 2D lattices do not have separate *inversion* symmetry, this is because the same result is achievable through a rotation. Check for yourself, draw a square, take one of its corners as an inversion point, then invert every side and the diagonal through this corner, then notice that you could as well take an axis of rotation through the same corner and did just a rotation by 180^o and would have achieved the same result.

1.3.2 Bravais Lattices in 3D:

Studying all the 3 kinds of symmetries (rotations, reflections, and inversions), it can be shown that lattices in 3 dimensions can exist in total 14 types, but they come under 6 main broad classes as shown below:

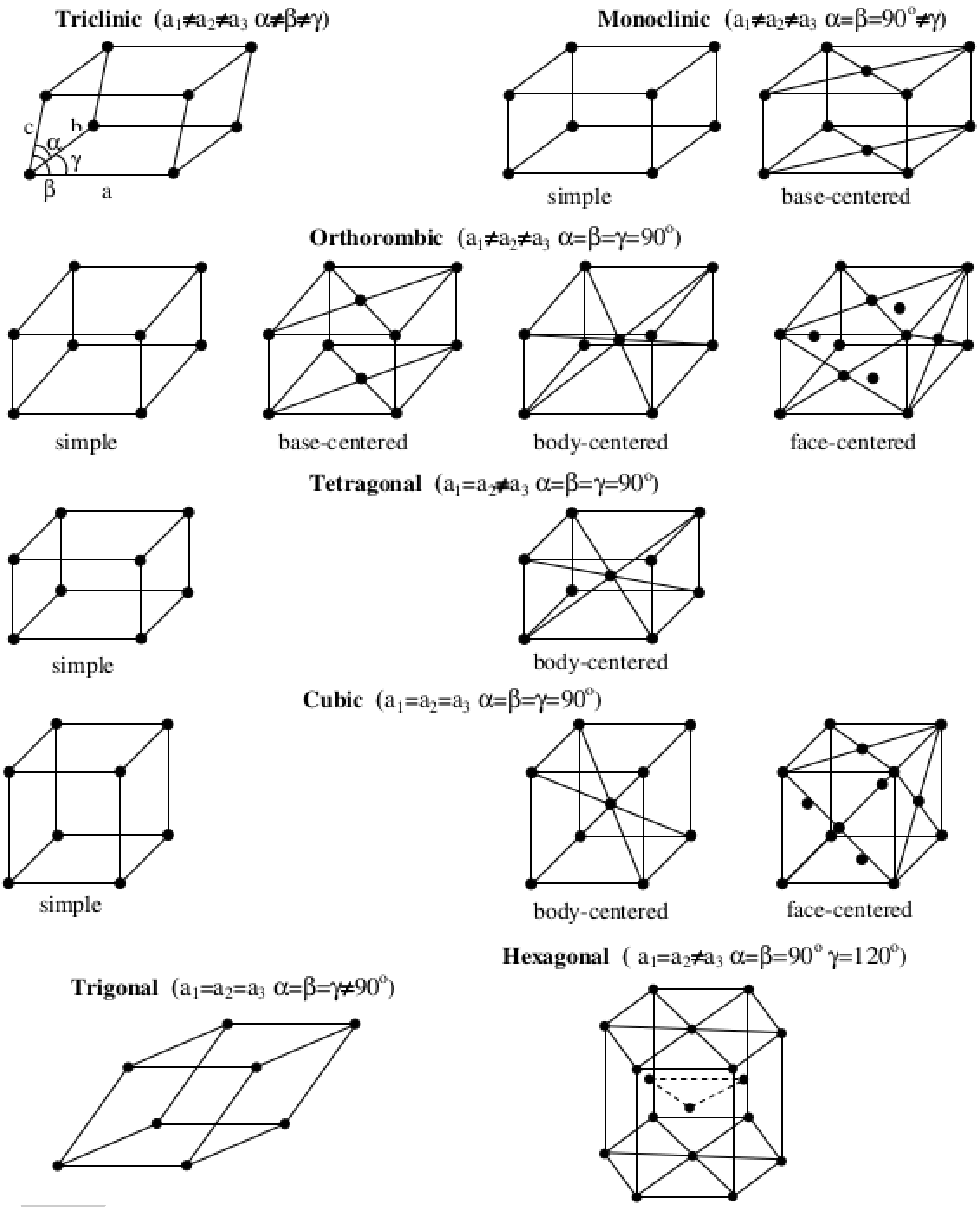

Figure 3: All possible Bravais lattices in three dimensions.

1.3.3 Symmetries of a cubic cell

1. **4-*fold* axes:** this is the axis through which you have a 4-fold rotational symmetry. We know that a square has a 4-fold symmetry, therefore, if you look from above this axis, the cube should look like a square! In other words, an axis passing through the middle of any face and perpendicular to that face will be a 4-fold axis. A cube has 6 faces, but an axis will pass through two opposite faces, therefore, 2 opposite faces will correspond to a single such axis, hence there will be three 4-*fold* rotational-symmetry axes for a cube, as shown in Fig. 4.

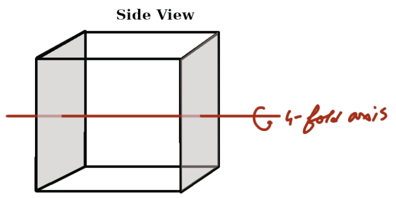

Figure 4: One of the three 4-fold rotational-symmetry axis shown in two different views. Top view makes it clear that you have a square and hence every 45^o the cell will be back to itself.

2. **3-*fold* axes: Q:** What does have a 3-*fold* symmetry? **A:** An isosceles triangle, or a 3-evenly-legged object! **Q:** From which angle a cube looks like it has 3 evenly spaced legs? **A:** if you look from the top of a corner, a cube looks like 3 legs are diverging from that corner, therefore, if you let an axis pass through it that diagonally passes through the opposite corners, it will be a 3-fold axis, as shown in Fig. 5. As there are 4 pairs of corners, at most 4 such axes can be drawn.

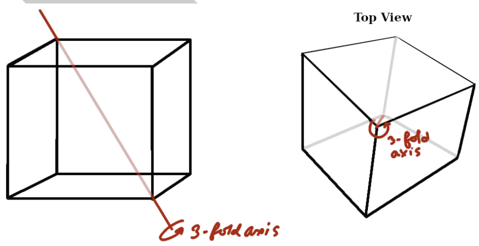

Figure 5: One of the three 3-fold rotational-symmetry axis shown in two different views. Top view makes it clear that you have a 3 lines diverging from the corner and hence every 60^o the cell will be back to itself viewed from this corner angle.

3. **2-*fold* axes:** a very simple example of a shape with a 2-fold symmetry is just a line, or a rod. What part of a cube looks like a line? If you looked at any sides (not faces) of a cube from directly above, it will look like a line dividing the cube into a lower and a upper half, therefore, rotating by 180^o and 360^o (2-fold) will leave the cube intact, as shown in Fig. 6. Therefore, an axis passing through the middle of any of the two opposite sides of a cube is a 2-fold rotational-symmetry axis. One face of a cube has 4 sides, let's start with the *top face*, at first

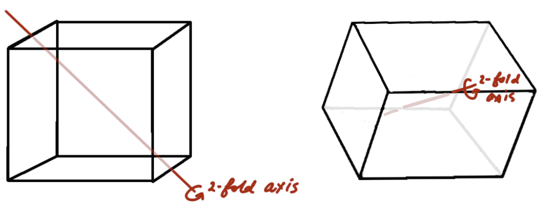

Figure 6: One of the three 2-fold rotational-symmetry axis shown in two different views.

we can draw four 2-fold axes passing through those sides, that means we are also done with the exact opposite face, that is the *bottom face* of the cube. We are now left with only the 4 side-faces of the cube, take one of them, let's take the face directly facing us, upper and lower sides of this face has been already considered while we chose the top face, therefore, we only have left and right sides (2 sides) to draw axes. Therefore, so far $4 + 2 = 6$ axes. Obviously the face in the back, opposite to the one facing us has already been taken care of. Only faces remain are the right and the left faces, but then they share sides with top, bottom, front, and back faces of the cube, which have already been taken care of, therefore, no more axes remain to be drawn. Therefore, there are only six 2-*fold* rotational-symmetry axes in a cube.

4. **All the mirror-symmetry planes of a cube:** Fig. 7 displays all the possible *mirror*-symmetry planes of a cube.

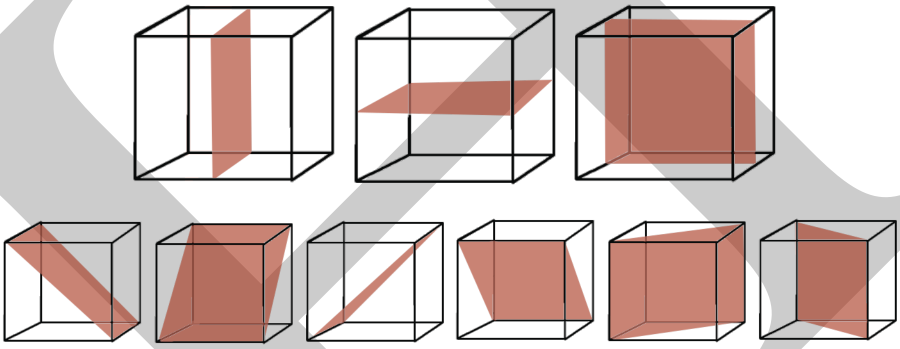

Figure 7: All the mirror planes of a cube are painted in red.

References

Charles, K. (2005), *Introduction to Solid State Physics*, Wiley.

Tsymbal, E. Y. (n.d.), 'Lecture notes: Introduction to solid state physics'.