Crystals, Symmetry and Tensors

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2D Point Group-l

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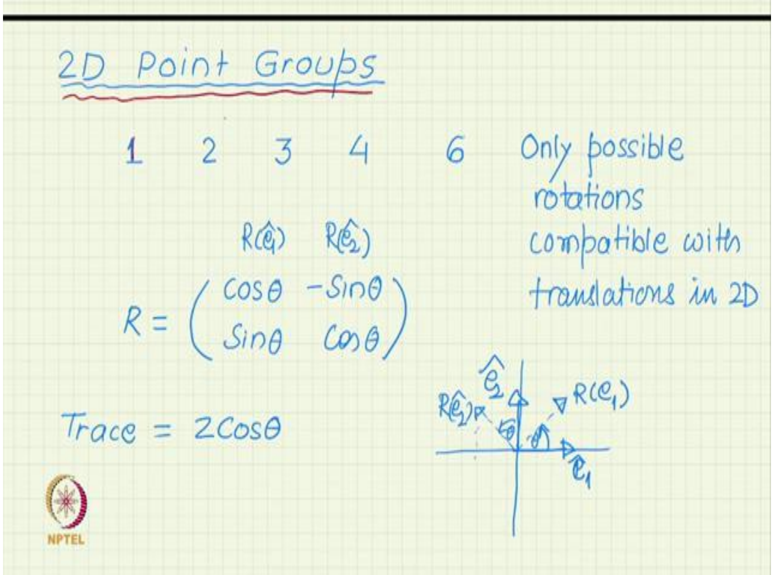

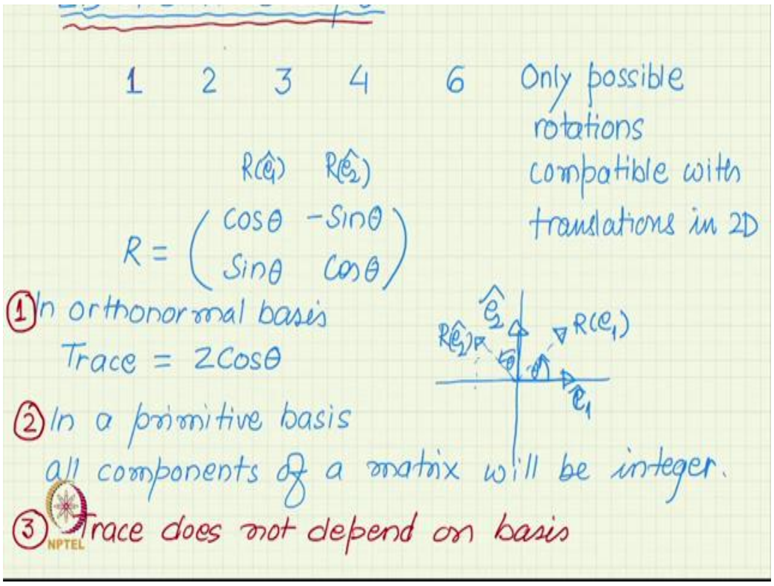

So, 2D point groups just like in 3D we had shown but that proof was for 3D, but it can be easily extended to 2D and you can show that in 2D also you will have only these 5 rotation possible the proof is again through matrix you can get or through a drawing of 2D lattice we had given both the proofs for 3D you can do that proof so the only rotation axis possible.

All you have to do is to write a rotation matrix in 2D rotation matrix in 2D will be cos theta minus sin theta, cos theta in an orthogonal coordinate system if you rotate by theta the first column will be the components of rotated e1, e1 is a unit vector along the x axis, if you rotate it you get R e1 at an angle theta since it is a unit vector its component will be cos theta and sin theta.

Similarly, e2 is rotated into R e2 again since it is a unit vector it is component will be minus sin theta cos theta so that is your rotation matrix. So, again that is all the same philosophy only thing is that there you got the trace as 2 cos theta plus 1 because there was one more column 0, 0, 1. Here the trace will be simply 2 cos theta.

Now, this was in orthogonal system if you do it in a lattice basis primitive lattice basis all those arguments which we gave for 3D is exactly we are repeating in a primitive basis all components of a matrix will be integer.

So, we are using 2 different basis in orthonormal basis because this matrix which we wrote was the orthonormal basis the first point was this in orthonormal basis, the second point is that in a primitive basis, but the third point is that trace does not we prove that in 3D that proof is applicable to 2D also that trace does not depend on basis when you change the basis, matrix numbers will change, but when you add the diagonal terms you will get the same number.

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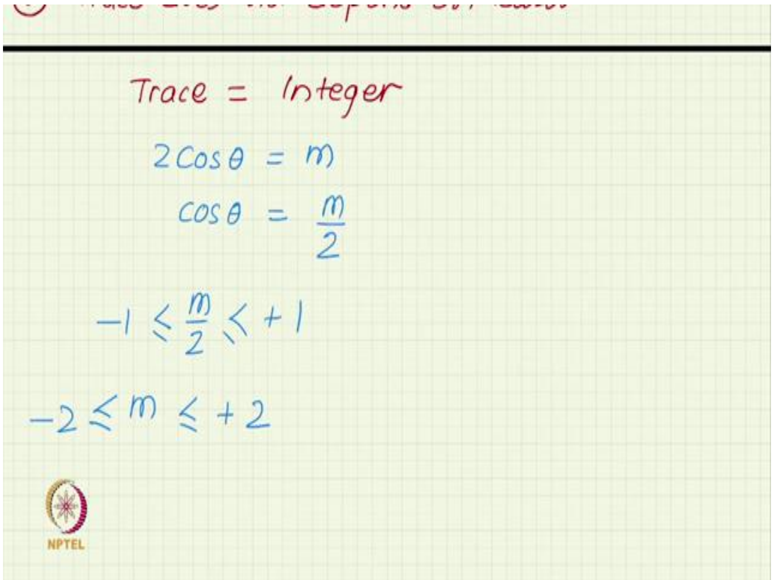

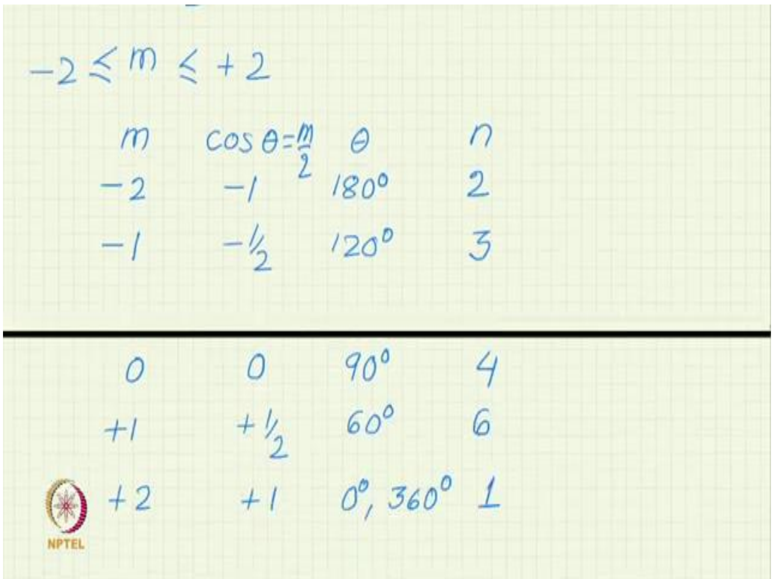

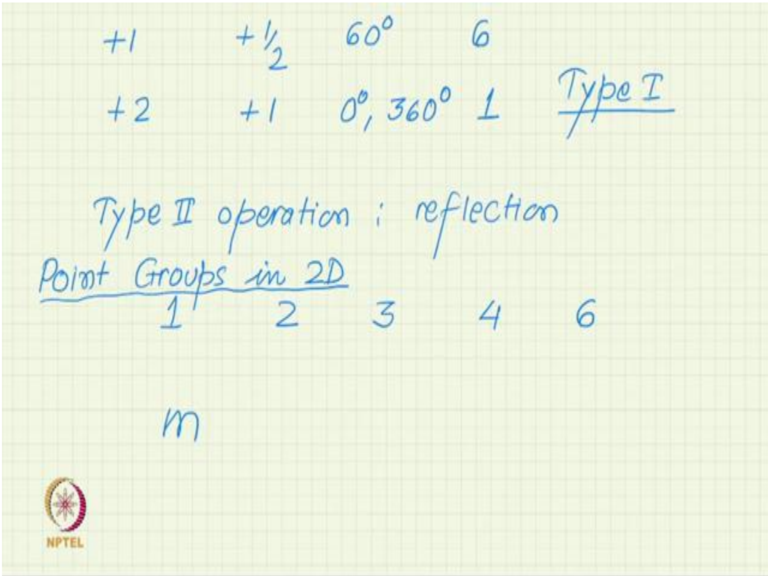

So, in the primitive basis also there is the same trace but in the primitive basis the matrix is integer components of the matrix are integer. So, the trace is an integer sum of integers will be integers or trace is integers so 2 cos theta is an integer you solve for this again you will get the same values. So, 2 cos theta is an integer so cos theta is m by 2 so m by 2 has to be between minus 1 and plus 1 so m is between minus 2 and plus 2.

So, if you take m is equal to minus 2 we start with the lowest value then the corresponding cos theta which is m by 2 is minus 1. So, theta becomes 180 degree. So, it is a 2-fold rotation axis minus 1 becomes a 3-fold rotation axis so these are the only possible rotation axis just like in 3D, 2D also has the same limitation. These are all type 1.

What is a type two operation in 2D reflection? So we have 6 point groups now in 2D 1, 2, 3, 4 and 6 and then we have m as another point group so 6 point groups we have found there are other point groups, which can be obtained by combining and we have met some of them combining m with these rotation axes? In fact, m itself can be considered as combination of 1 and m.

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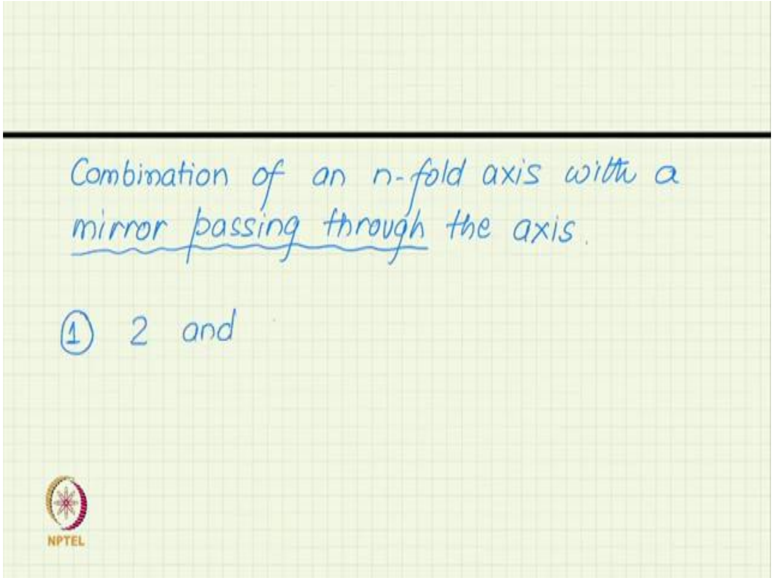
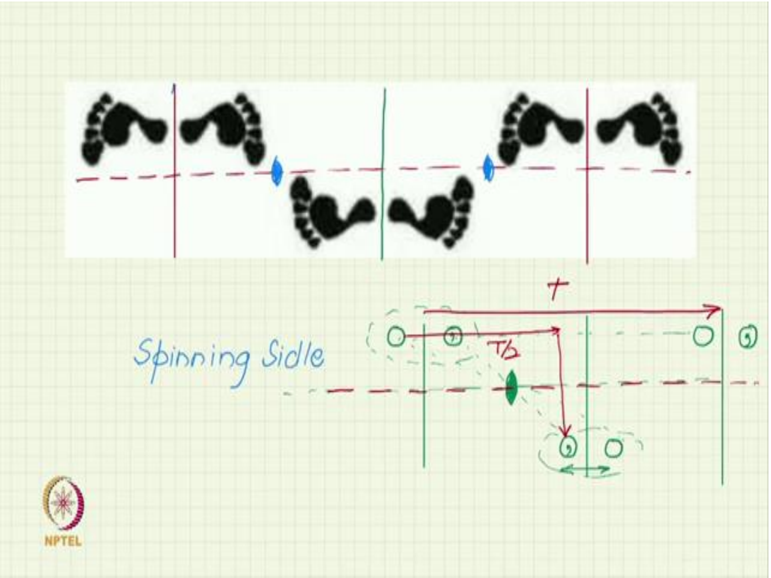




2D Point Groups

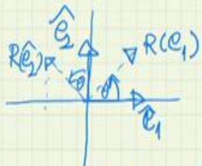
1 2 3 4 6 Only possible rotations compatible with translations in 2D

$$R = \begin{array}{cc} R(\hat{e}_1) & R(\hat{e}_2) \\ \end{array}$$

$$R = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}$$

1. In orthonormal basis

   Trace $= 2\cos\theta$

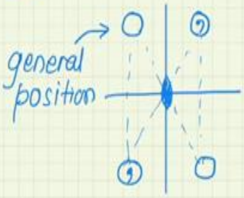


2. In a primitive basis

   all components of a matrix will be integer.

mirror passing through the axis.

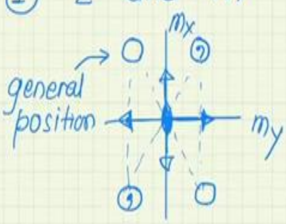
1. 2 and m



$2m_y =$

mirror passing through the axis.

1. 2 and m



$$2m_x = \underbrace{\begin{pmatrix} \bar{1} & 0 \\ 0 & \bar{1} \end{pmatrix}}_{2} \underbrace{\begin{pmatrix} \bar{1} & 0 \\ 0 & 1 \end{pmatrix}}_{m_x} = \begin{pmatrix} 1 & 0 \\ 0 & \bar{1} \end{pmatrix}$$

But what will be combination of 2 and m? We are seeing mirror passing through the axis that is not required for space group we have already seen in our combination that we let the mirror and the 2-fold axis be separated, but then this generated a glide line and it generated a space group we want to generate currently a point group our focus is on point group. So, we want one point to be left fixed we want one point to be left fixed the mirror and the rotation axis will pass through the same point otherwise no point will be left fixed.

So, you have already combined 2 and m many times by now I think you are familiar with this case. So, if you have 2 and you have m what do you get start with a point neither on the mirror nor on the 2 fold. So, that is a general point. So, I reflect in the vertical mirror. So, I get the reflected motif but then I have 2 folds also the 2 fold will bring it here without change handedness 2 fold we will bring it here without changing handedness but now these 2 motif we see are automatically related by a reflection in the horizontal plane is created.

Here we are seeing geometrically if geometry is looking a little fishy to you or not so convincing you can do by matrix multiplication you can write the matrix for 2-fold rotation and write the matrix for a vertical mirror you will find that outcomes are horizontal mirror. So, let us do that way also. So, what will be the matrix for let us call the vertical mirror m y mirror along y axis or actually should we call the mx by international convention.

Because mirrors are denoted in the international table mirrors are denoted not by the line or plane along which there but by the normal to the plane. So, the vertical mirrors normal is x axis. So, let me call that mx. So, this is my this is my m y what will be the matrix what 2 fold it will change the x axis to minus x axis and y axis to minus y axis so that is 2 fold what about the mx mirror the vertical mirror it will reflect 1 to minus 1 to minus 1 is 0 it will not do anything to 0, 1 because 0,1 is along the mirror that will remain write the product or do you get.

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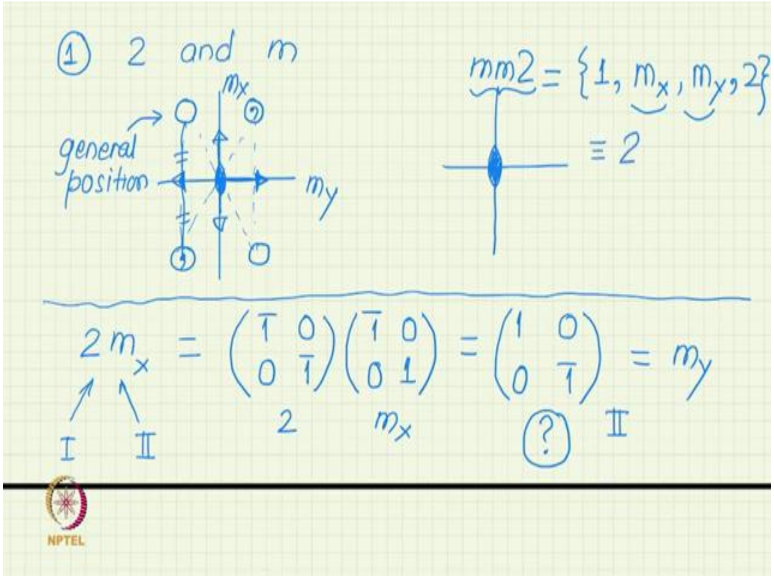

Now, the question is what is this? What is the product? You can see from the behavior itself that it is leaving first of all 2 is which type? Type 1, m is what type? Type 2, now 1 changing the handedness 1 does not change the handedness. So, the combination will change the handedness. So, the product of type 1 and type 2 will always be type 2 product of type 1 and type 1 will remain type 1 product of type 2 and type 2 will be type 1 because change in handedness followed by another change in handedness. So, you will get the original handedness.

So, this is a type 2 operation only type 2 operation in 2D we said was a reflection so it has to be a reflection now looking at the structure of this, we can quickly see that it is a reflection which is not changing in the x axis because1, 0 is remaining 1,0 but it is changing the y axis vector 0,1 to 0 bar 1 so this m y.

So, depending on your taste either you like the algebra? Algebra is obviously a little bit more convincing because drawing although I drew you again require a little bit more proof because you have to make some triangles show their congruence because you have to show that to prove that this is a reflection of this you have to show that this distance is equal to this distance and things like that.

So, geometrically I was being lazy and I was not giving you the full proof only on some sort of faith we were saying that it will appear to be reflected but now algebraically you are more convinced that this product is a reflection. So, we have a group. So, we have a 2 dimensional group in which there are 3 operations in fact 4 operations because identity is always operation so my group consists of identity x mirror, y mirror sorry I am giving subscript to 2-fold x mirror y mirror and a 2 fold 4 operations are there it forms a group and this group is what we are we give a name and that is mm 2.

So, x mirror and y mirror both we denote as in the symbol as m and m and 2 fold. Why will you not both as a mirror? See this 90 degree mirror. Although we have proved it geometrically and algebraically 90 degree mirror is not work was expected from a 2 fold. Because if you say that I am combining a mirror with a 2 fold, what will the 2 fold do to the mirror will rotate by 180 degree.

So, the mirror plane will come into itself it will not rotate a mirror a 2-fold axis is not supposed to rotate the mirror by 90 degree. But the effect is that if you combine the 2 fold with a mirror the mirror does go get rotated by 90 degree and a new mirror generate. So, that generation of the new mirror or a mirror which is not equivalent to the original mirror by 2-fold symmetry, 90 degree is not a 2-fold symmetry.

So, this new mirror is considered to be a distinct mirror. Although it is coming from 2 fold it is the product of 2 fold but still it is not equivalent by the 2-fold symmetry. It is not symmetry equivalent to the 2-fold axis. So, you put both the mirrors in the symbol and call the point to mm 2 or sometimes it is also called 2 mm.