Crystals, Symmetry and Tensors

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Lecture 15b

The angle between mirrors is half the angle of rotation

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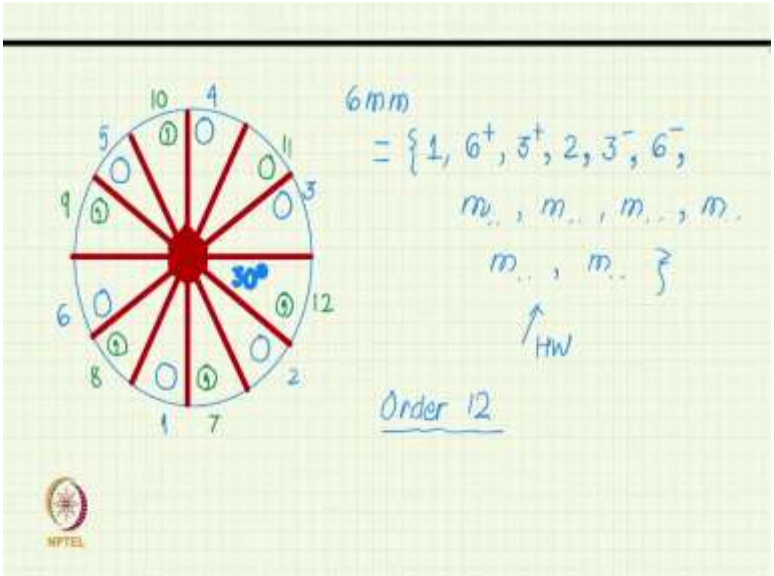

So, everywhere we saw that the mirror has got, mirror comes at an angle of half the angle of rotation. So, is seems like a general result. So, can we prove this?

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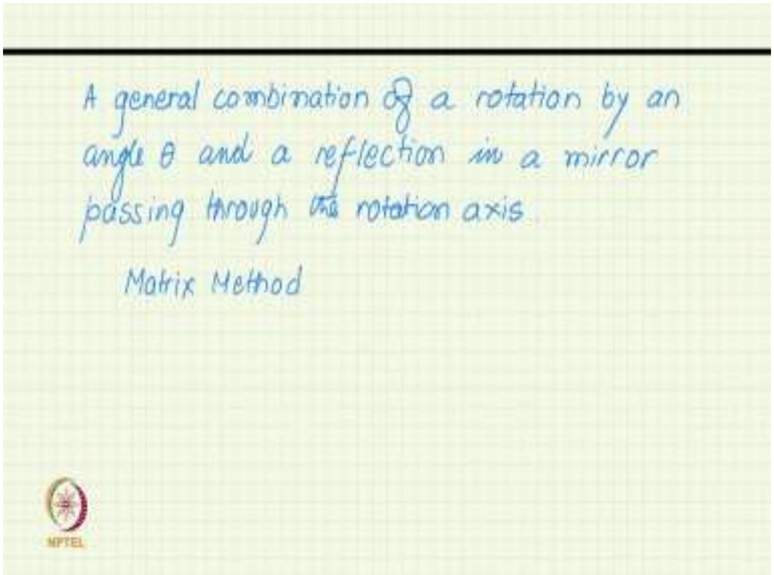

So, let us try this to find out so, a general combination of a rotation by an angle theta and a reflection in a mirror passing through the rotation axis. So, let us do it let us do means in a sense, we have proved it case by case taking all this thing, but, a general proof can be again given geometrically, but we will do it algebraically through not sites operation, but through matrix operation because a translation is not involved we use sites operator when we have the translations.

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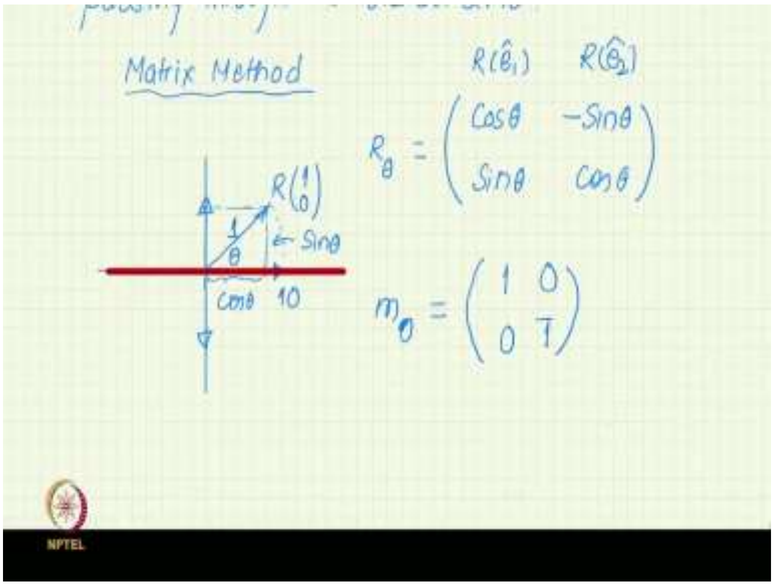

So, through let us use an orthonormal basis we go because that is convenient to write the rotation matrix. So, rotation by an angle theta about an origin we had done that if you remember. So, we start with the unit vector 1 0. So, and that will rotate by theta, so, its component so, this is a rotated 1 0 vector and its components are cos theta and sin theta.

So, the matrix first column is the rotated 1 0 whatever happens to on rotation, you write it as the first column and you are seeing that the vector it is going to is cos theta sin theta. And similarly, R e2 goes to minus sin theta cos theta. So, that is the rotation matrix. The reflection matrix mirror plane now mirror plane you can take in any orientation, but it is convenient to choose it along your x axis or y axis. Since x axis is a better reference line.

Let us call that that is our mirror and I am calling this a mirror at 0 degrees. So, mirror is being characterized by its tilt with respect to the x axis. So, this is m 0 and what will be x columns first column 1 0 because that is where it takes e1, e1 is now along the mirror. So, it does not go anywhere it reflects into itself the second vector will reflect downwards will become 0 bar 1.

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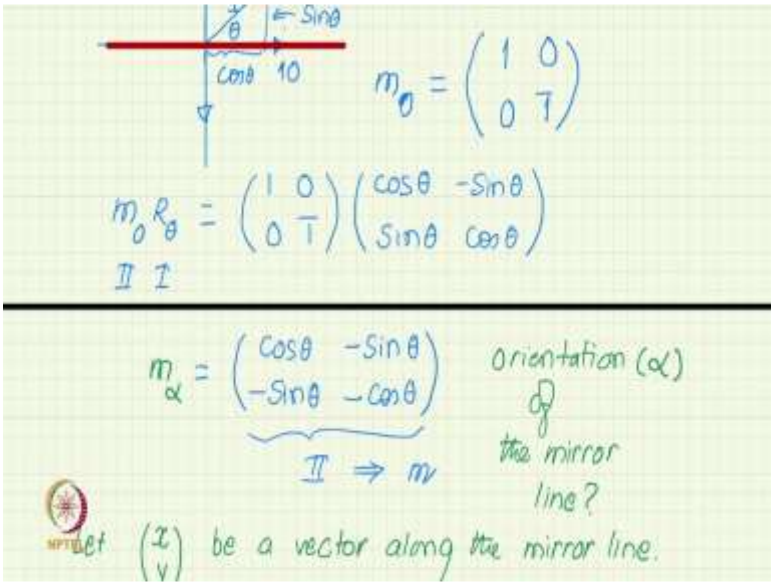

So, all you have to do is now to combine these two, these two operations. So, let us say we first apply R theta and then we reflect that is how we were doing in stereogram also. So, what is rotation by theta by combined with a mirror reflection which is inclined at 0 degree to the x axis. So, that is what we are trying to find. So, 1 0, 0 bar 1 multiplied by cos theta it is a simple matrix multiplication.

Remember, we are combining a reflection type 2 with a rotation type 1, so, the resulting operation has to be type 2. And we know that type 2 operation in 2d is a mirror. So, it is a mirror but which mirror, so, to see which mirror we have to find the line of mirror orientation of the mirror. So, how do we find orientation of the mirror line? So, let x y be the vector along the line. So, then what will this mirror do? Let us call since we know that it is a mirror.

So, it will be some mirror passing through the origin, so, it will have some inclination So, let us call this m alpha. So, orientation means what is that angle alpha this is what we want to find out.

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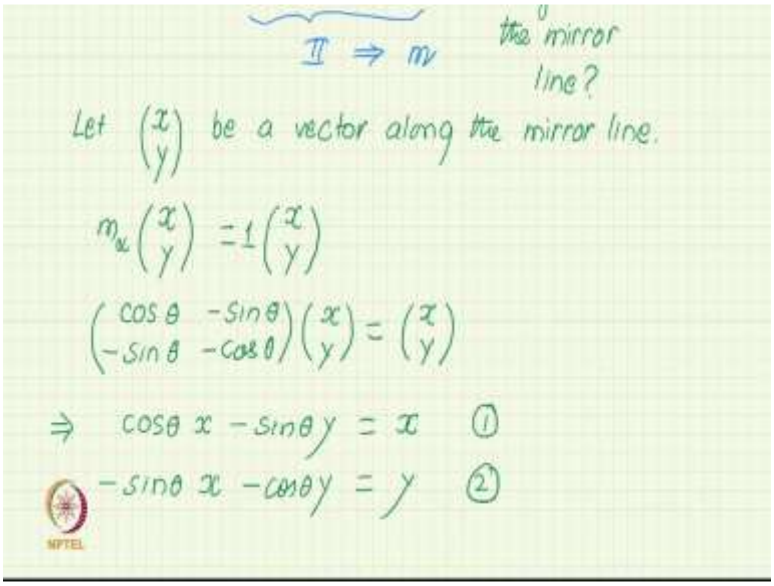

So, if x y is a vector on the mirror line then what will m alpha x y be it will remain x y. So, essentially in terms of your matrix jargon, you can say that x y is an Eigen vector with an Eigen value 1 of this matrix m alpha.

That is not important, what is important here to try to solve this equation. So, try to solve this equation. So, we write the matrix in full. This is our m alpha matrix multiplied by x y and we want it to be equal to x y.

Student: m alpha should be identically matrix, cannot we say that? Because…

Professor: Identity, yeah. See, if matrix was unknown, and there was this equation that a matrix times a vector is the same vector, then one possible solution for the matrix was identity, here matrix is known, this theta, because I am combining it with some rotation theta is known. So, now matrix is an identity is not a possibility, which you are considering. Although if matrix was an identity, the equation would have been satisfied.

But I am my unknown is not the matrix, but the vector matrix is given, but what is the vector which will not be moved by this matrix will not be disturbed by this matrix. It is a very calm vector. The matrix is trying to disturb it, but it is constant. So, we get these 2 equations, if we multiply out the matrix.

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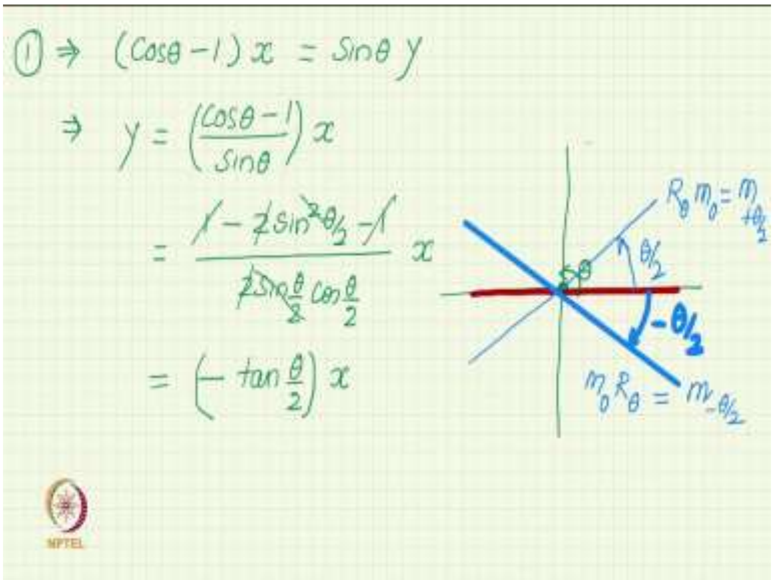

So, cos theta minus 1 x from 1. Cos theta minus 1 x is equal to sin theta y or y is equal to can you do some trigonometric simplification of this cos theta minus 1 is?

Student: minus tan theta by 2.

Professor: Minus tan theta by 2. So, cos theta can be written as 1, 1 minus 2 sin square theta by 2, is not it? Minus 1 and sin theta can be written as 2 sin theta by 2 cos theta by 2. So, it is a line y is equal to mx and m is the slope and what is the slope? So, how is the line incline? So, I had some sort of an enfold rotation there whose throw angle was theta.

So, there was a rotation of theta about this and I had a mirror plane which was lying along the x axis. And now I am finding that the combination of this theta rotation and this mirror is actually another mirror which is that minus theta by 2 which is exactly what was happening in your stereographic projection way of looking at it also.

The 2 operations are non-commutative that is, what we calculated was what we calculated was m 0 R theta. So, m 0 R theta turned out to be m minus theta by 2 if instead you would have calculated the other way round, you can do that as your homework, then you will see that if you apply m first. So, if you have R. R theta followed by m 0, you will again have a mirror at theta by 2, but this time plus theta by 2.

So, when some of you will find this as more convincing than growing the silly stereographic projections, but, the 2 R in 1 to 1 correspondence means, when you have developed enough geometrical intuition the stereographic projection in a sense helps you in working out what the matrix will also give you but tediously and through algebra and as you can see some trigonometry and one by one of course, we have found only 1 mirror at the moment.

So, you will have to and you saw that there are many more mirrors, So, you will have to start combining other operations, 6 with mirror will give you another mirror, 3 plus is also there in the group. So, 3 plus with the same mirror will give you yet another mirror and so on.

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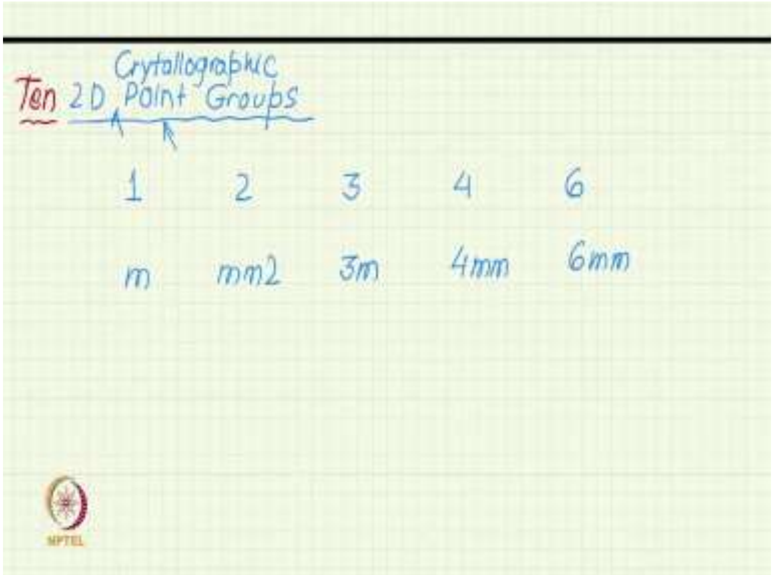

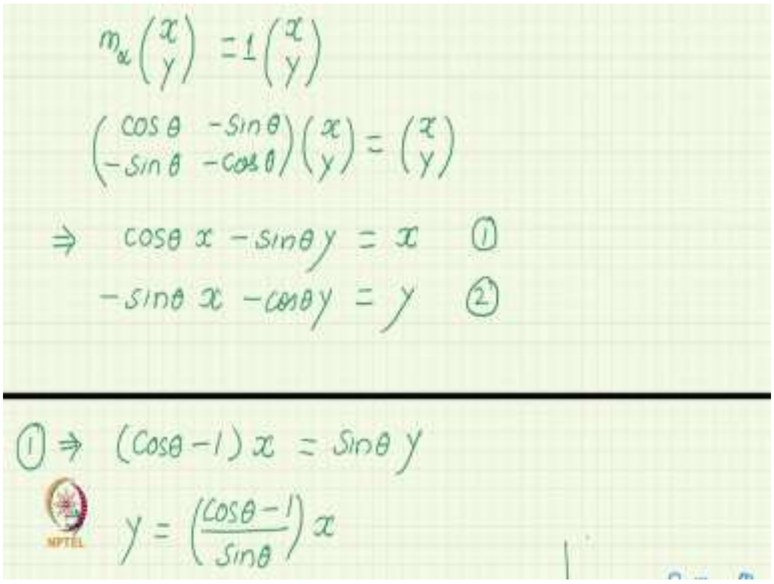

So, we are now convinced and we have completed the list of 2d point groups when we say 2d point groups 2d crystallographic point groups because this restriction from 1 to 6 with 5 not being present is because of the crystallographic requirement of periodicity otherwise, you can have 8 mm, 7 mm point group, pentagon symmetries 5 mm any polygon n gone polygon has a symmetry n mm. So, arbitrary objects can have all these point groups, but crystals cannot have.

So, we call this 2d crystallographic point groups. So, they are 10 of them. So, 10 crystallographic point groups and those we have now worked out as 1, 2, 3, 4 and 6 and m, m m 2, 3 m, 4 mm, 6 mm these are the only possible symmetries only possible symmetries in 2 dimensional crystals which will leave a point fixed and that is why the point because all these were being represented by let us say matrix and matrix will never take 00 vector anywhere.

Whatever the matrix 00 multiplied by it will only give you 00. So, all these operations leave the whenever you are representing them by matrix you mean that origin is the fixed point of that operation.

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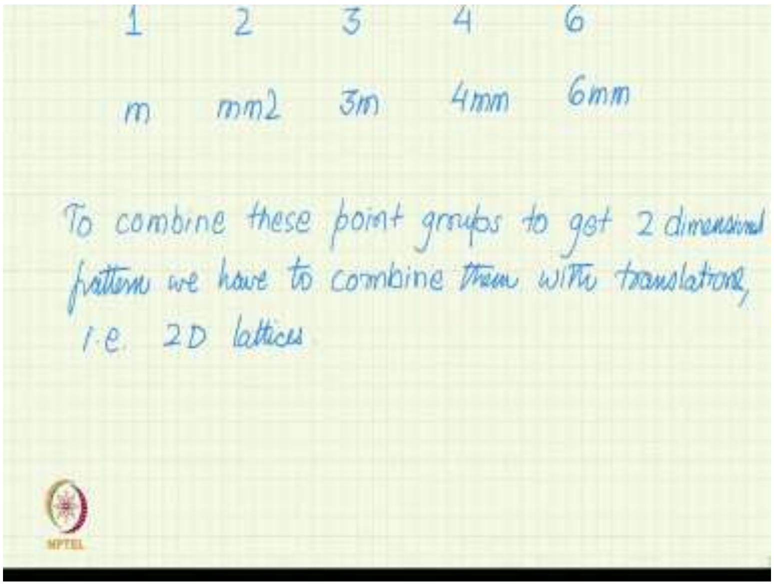

Now, let us bring the translations.

Student: (())(15:14).

Professor: It is a good question, let us look at.

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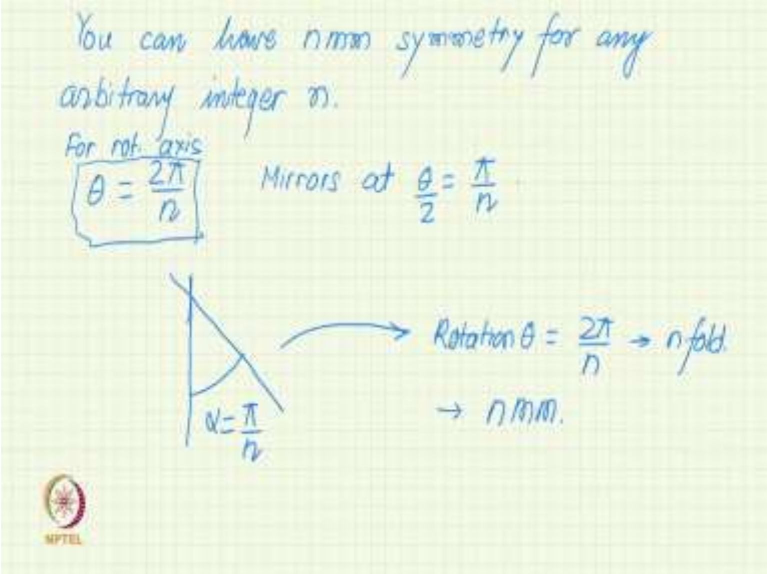

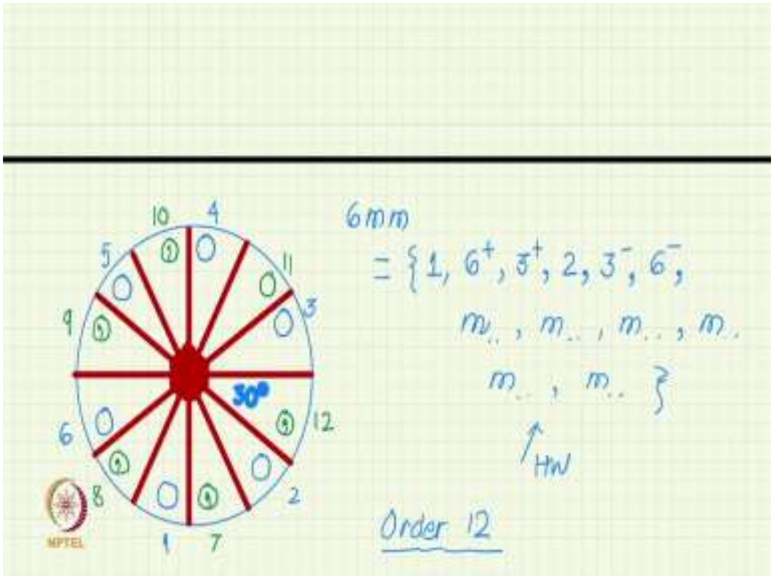

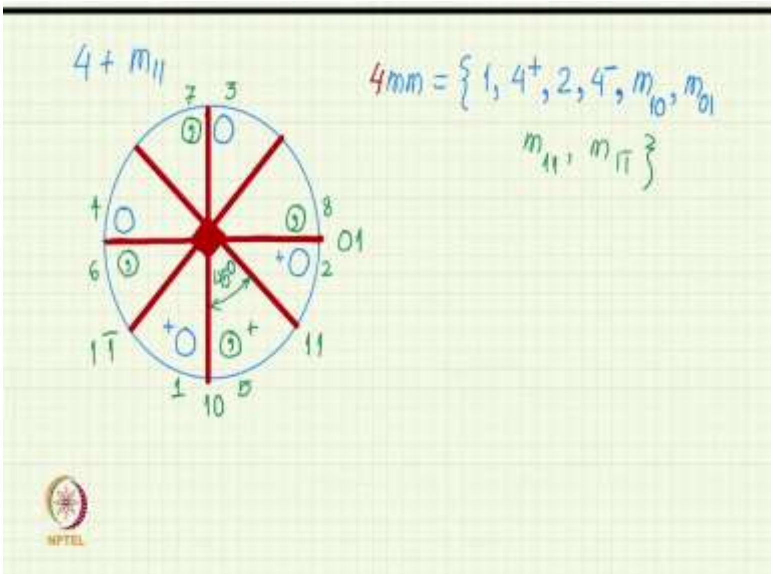

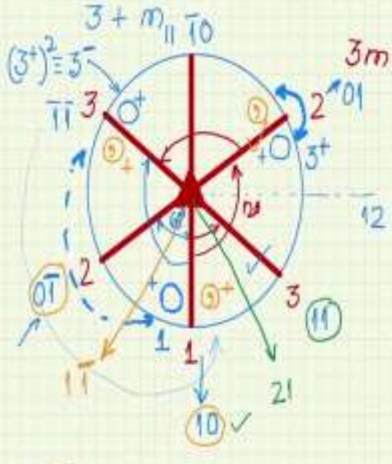

$3m = \{1, 3^+, 3^-, m_{12}, m_{1\bar{1}}, m_{21}\}$

Order 6

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2D Point Groups (Contd)

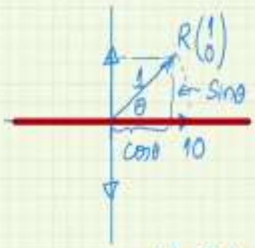
1 2 3 4 6

m 2mm

2mm $= \{1, 2, m_{10}, m_{01}\}$

Matrix Method

$R(\hat{e}_1) \quad R(\hat{e}_2)$



$$R_\theta = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \quad \left(\frac{2\pi}{n}\right)$$

$$m_0 = \begin{pmatrix} 1 & 0 \\ 0 & \bar{1} \end{pmatrix}$$

$$m_0 R_\theta = \begin{pmatrix} 1 & 0 \\ 0 & \bar{1} \end{pmatrix} \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}$$

II I

So, we will take this up, but before let us consider Pryansika's question that what will happen if we were combining a rotation axis with a mirror plane, what if we combined 2 mirror planes themselves at some arbitrary angle if you take these nice angles which we are getting, then you will get back to these point groups. So, if you combine two mirror planes at 30 degree you will get 6 mm, at 45 degree you will get 4 mm, 60 degree you will get 3m, 90 degree 2 mm.

If you combine them with any other angle other than this then the question is what should that angle be to give you a symmetry. So, if actually you can have as I was telling that you can have any n mm symmetry for any arbitrary integer n we have already in our in our proof we were not fixing theta. So, all in our in our proof if we are considering n fold which is outside this 1 to 6.

Then all we have to do is to set theta is equal to 2 pi by n, so if we set theta is equal to 2 pi by n. I will get n fold axis, and that will then tell you that mirrors are at half this angle that is mirrors are at pi by n, theta is 2 pi by n for rotation. So, for a consistent symmetric operation, you want to come back after n operation you want to come back to your original position.

Otherwise, if you take some arbitrary angle by which after n operations you do not get back to your original position, but let us say slightly instead of 360 you go to 361 that will happen if your angle was some arbitrary fraction or any rational number let us say. So, any rational number any mult, integer multiple will not bring it back to an integer.

So, one constraint for symmetry operation is that the angle theta has to be a sub multiple of 2 Pi okay, it has to be 360 degree divided by some integer if it is 360 degree divided by some integer then you are happy and you can combine mirrors. So, you can combine mirrors by, so if you have 2 mirrors at theta let us say you will have let us say alpha you are combining mirrors at alpha.

So, alpha should be the angle between mirror should be some sub multiple of pi and this combination by the reverse operation what we have seen will give you a point group with a rotation theta 2 pi by n that is n-fold and is giving you a mirror at half that angle. So, you will get a point group n mm.

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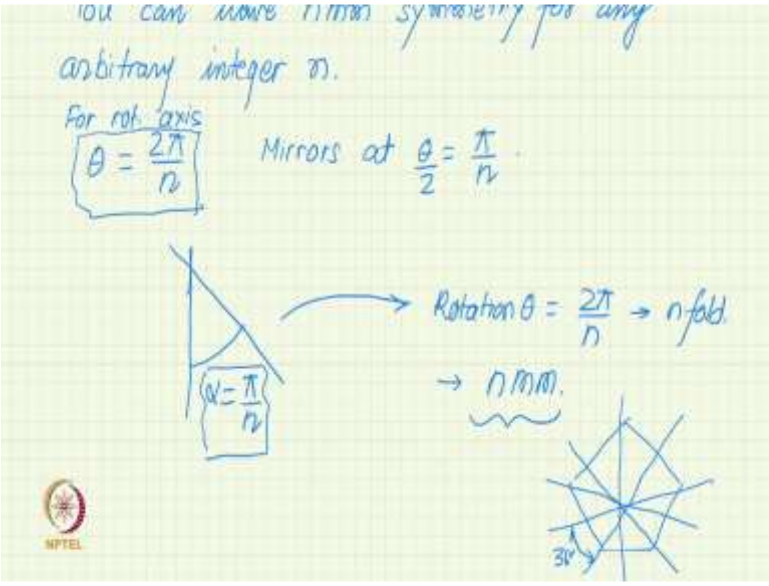

So, answer to your question is that you can select arbitrary angle but not be, not more arbitrary than pi by n, if you want a symmetry and depending on what n you select, you will always get a point group n mm if you set your mirror set pi by n, but unless and until n is equal to 1, 2, 3, 4 and 6 those point groups will not be consistent with translation and cannot be used for crystallography or crystal symmetry.

But, I have 5 mm and I can have a nice Pentagon which is having a 5-fold symmetry but, Pentagon's rotation angle is, the Pentagon's rotation angle is 360 by 5 is equal to 72 degree. So, the mirrors are at 36 degrees. So, mirrors are at 36 degree. If you take theta is equal to 37 degree and combine your mirrors you will get and in you will keep getting an inconsistent set of mirrors. Means you will never come back to an original mirrors you will keep generating newer mirrors.