Crystals, Symmetry and Tensors

Professor Rajesh Prasad
Department of Materials Science and Engineering
Indian Institute of Technology Delhi

Lecture 9d

Coordinate transformation of a matrix representing symmetry operation

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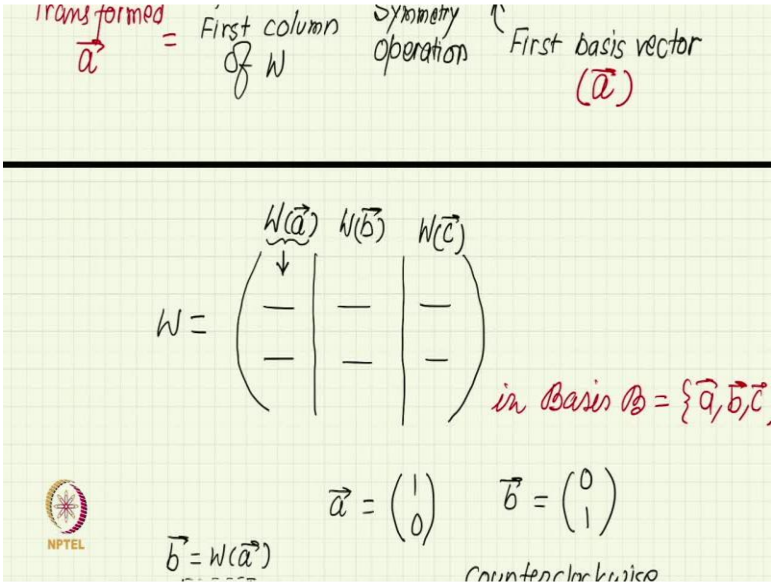

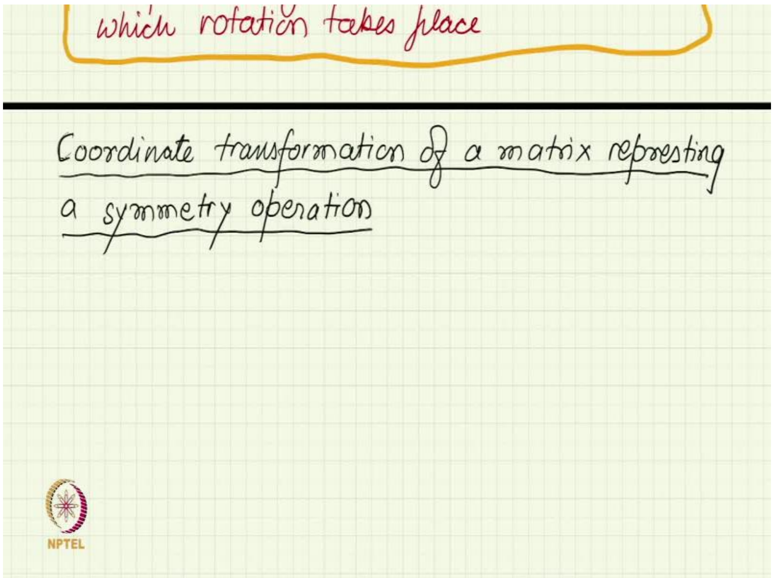

Let us now look at this. We have seen that we are a this we given any basis look at the algorithm of our settings up of the setting up of the transformation matrix that given any basis because all these are in some basis, if you change your basis, if you take a different basis, then you know that vectors transform instead of x, they become x prime through Q, your Q matrix changes the vectors. If the vectors are changing, then the same matrix will not be able to represent the original transformation, so the numbers within the matrix also will change representing the same 90 degree rotation, but now, it will have a different. In the different basis it will have different numbers.

So in a sense the rotation matrix is having a 9 just like a vector is having 3 components and on changing of coordinates, those 3 components changes to other 3 components, the matrix also representing the. So those 3 components, the column vector is representing some physical vector and it is represented by those 3 numbers, but those 3 number representation changes depending on your basis although the vector each same.

Similarly, although your operation is same, your transformation is same, you are still talking about 90 degree rotation, but if you change the basis, why did you get 0, 0, 1, in the third column?

Student: Because the axis was.

Professor: Because the rotation the z axis was along the rotation axis, it was saying that the third axis is not changing. If I still have a 90 degree rotation, but I choose a basis in which z axis is not along the rotation axis, will I get the third column as 0, 0, 1?

Student: No.

Professor: No, having some different number, but that new matrix still will be representing 90 degree rotation. So how did I how do I formulate what is the form of new matrix. So, if I know the vector transformation, if I know the coordinate transformation by matrix Q, what is the proper way of transforming a symmetry transformation W? So that is the problem which we now try to solve.

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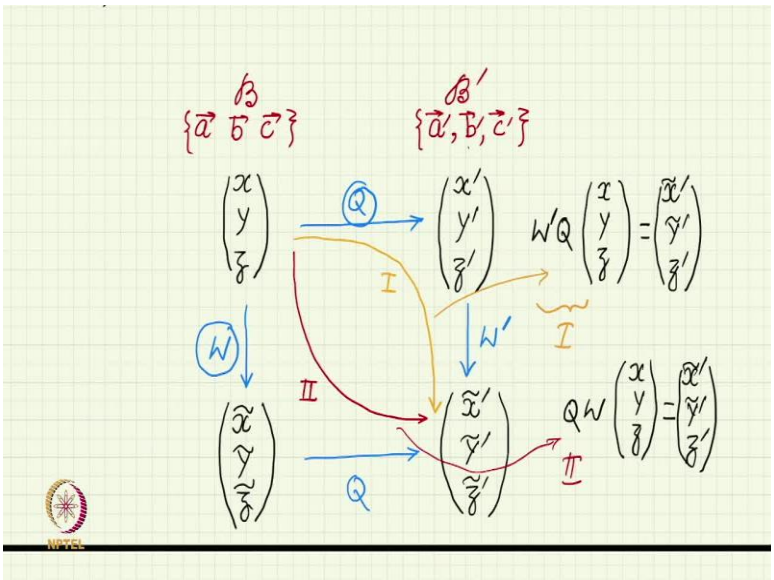

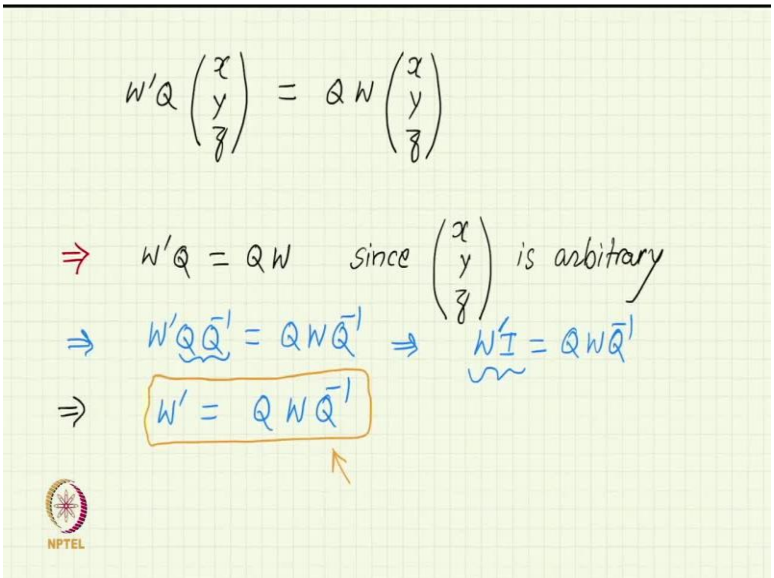

So, we have 2 basis B and B prime, B represented by a, b and c, B prime represented by a prime, b prime and c prime. And we have some vector x which has representation let us say x, y, z in the basis B, it has representation x prime, y prime, z prime in basis B prime so, this is the basis change, and we know how to achieve this is to just multiply by matrix multiply by matrix?

Student: Q.

Professor: Q. So this we have learned. Now there is a symmetry operation which transforms a vector x, y, z, to x tilde, y tilde, I do not particularly like this tilde, but again, in respect to the international tables, they have used this. And I can see some utility, you can throw in x prime or x tilde or whatever notation randomly. But then what they are trying to do in international tables is to keep track of whether it is a coordinate transformation or whether it is a symmetric transformation.

In symmetric transformation coordinates are not transforming vector is transforming, in basis transformation vector is not transforming coordinates are transforming although both are happening by through representation of columns and 3 by 3 matrices.

So algebraically, or mathematically, or numerically, both are representing the same thing, but physically the meaning is different and they want to keep track of that, so that is why they are using this kind of symbolism. So I am also trying to follow that, so that we can communicate with them better, in case we have to read the international table sometime, so and anyway, it is a good practice I feel. So let us look at this. So how do we go from x, y, z to x tilde, y tilde, z tilde? What matrix defines that?

Student: W.

Professor: W. So you are with me, I am very happy. So W. Now, e x tilde, y tilde, z tilde is again a vector, a new vector, a rotated vector or a reflected vector in the basis B, I can transform it to the basis B prime and what matrix do I have to use that for that transformation?

Student: Q.

Professor: Again, Q because the same basis transformation, all vectors will transform by the same matrix, so x tilde, y tilde, and z tilde also transforms by the same, so this is also by Q. But as we have seen, in the new basis, the same symmetric operation will now have a new avatar, it will have a new roop.

So although it is now the same rotation with the same rotation, or the same reflection, which took x, y, z to x tilde, y tilde, z tilde, that same rotation, will take x prime, because x prime, y prime, z prime is just a different name of the same vector and x prime tilde, y prime tilde, z prime tilde is the name of the rotated vector, transformed vector.

So the transformation is the same, but its representation is going to be different, let us call that W prime. So if this picture is clear to you, then the derivation is just a straightforward that how is W prime represented to related to W. All you have to do is to take 2 different paths from going from x, y, z to x tilde prime, y tilde prime, z tilde prime, diagonally opposite.

So let us take one path the golden path, path 1 and the another path, the red path, path 2. What we mean by path 1 and path 2 is I want to transform x, y, z. So, what essentially I am trying to do is, to I want to rotate let us say W is representing a rotation. So I want to rotate a given vector but I have the coordinates of the un-rotated vector in basis 1, I want the coordinates of the rotated vector in basis 2. Un-rotated vector x, y, z is in the unprimed coordinate system B, rotated vector x tilde prime, y tilde prime, and z tilde prime is represented in the new basis B prime, this is what I want to do.

So, I can do it in 2 steps, I can first transform x, y, z by Q to x prime, y prime, z prime, that is I changed the basis and then I apply the rotation in the new basis. So, what will I get? So, I have x, y, and z, I multiplied by Q to get x prime, y prime, z prime. Now, what should I do to get x tilde, y tilde, z tilde?

Student: W dash.

Professor: I have to multiply by W prime, because now I am in basis after multiplying by Q I am in basis B prime. So, if I wish to apply the symmetry operation, I will now apply the matrix W prime. So this product should nothing be but x tilde prime, y tilde prime, z tilde prime. So this is path 1. Now, let us apply path 2, we first do the rotation itself. So, we again have x, y, z we rotate it, how do we rotate? Multiply by W and then do the basis transformation, how do I do that?

Student: Multiply by Q.

Professor: And what do I get out of it?

Student: x tilde prime.

Professor: x tilde, y tilde, z tilde, you can see from these 2 now, R.H.S. is the same so, L.H.S. also has to be the same. So, that means W Prime Q, x, y, z, should be Q W x, y, z. Once we have this what was x, y, z, a special vector or a general vector?

Student: General vector.

Professor: So, if 2 matrices are there and W prime Q and Q W are different matrices, because W prime is different from W an order of multiplication is also different, so they are different matrices at least on the face of it. But 2 matrices if they give you the same product with all the vectors this is only possible if the 2 are actually identical matrices otherwise it will not be possible. So, this implies W prime Q, Q W since this is arbitrary, so we have proved this. What was our goal, what we were looking for?

Student: Relation between W prime.

Professor: W prime. That what is I know this W the symmetry transformation matrix in my original basis, I know Q, how to do basis transformation from B to B prime. So I wanted what is the representation of the same symmetry transformation in the new basis that is W prime. So, I was looking for W prime in terms of W and Q and that is exactly what we have achieved. So, W prime is equal to Q W Q inverse because you have to right multiply by Q inverse on both sides, means I am jumping one step but for sake of clarity.

Let us do that those steps also. I multiply right multiply by Q inverse on both sides still one more step, W I because Q, Q inverse will be the identity matrix I. So and W I sorry W prime I and W prime I is W prime, where identity will not change the matrix, so you get this. So, you can see that this interesting result an important result comes out that how do you relate a given matrix representation of a symmetry operation in a given basis to another basis, if you know the basis transfer.

So, it is not see an important thing is that the vectors were transforming X was transforming as Q X, but W is not transforming as Q W, it is transforming Q W Q inverse physically also you can see that see what you wanted you wanted a transformation in the new basis you wanted W prime in the new basis, but you do not you know the transformation in the old basis W. So, what you first do is to transform your vector x prime, y prime, z prime, back into old basis, so that is the first thing which Q inverse does. So Q inverse brings you back from B prime to B, and then you be you know the transformation and that is W.

So after Q inverse you multiply W reading from the right, right to left. So, Q inverse brings you from new basis to the old basis, in the old basis you are happy with W, so you rotate by W, but then you wanted the final result in the new basis. So that W Q prime again you change into their new basis by multiplying by Q. So, Q W Q inverse very-very nice and happy result. So this is a good place to break.

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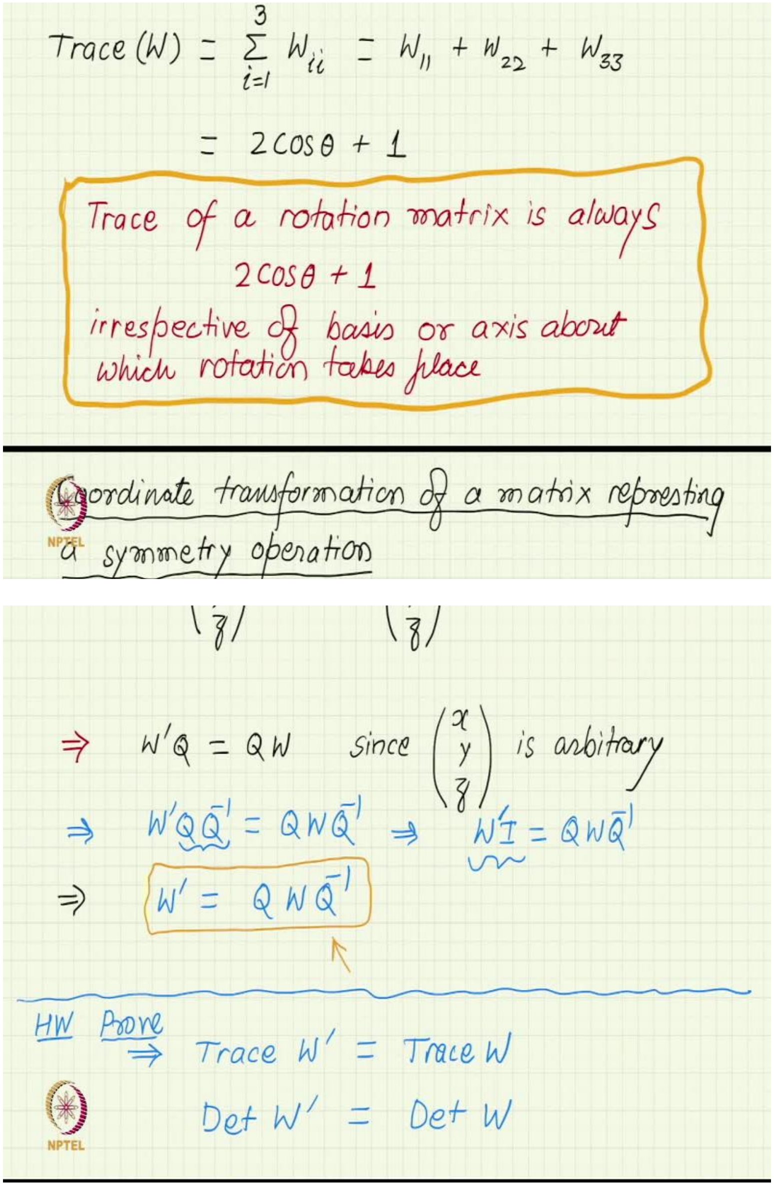

Now, do this exercise a left as a homework using this result? Now, you can easily see the claim which I made here that trace of a rotation matrix is always invariant you can actually show that this implies in general not only for rotation matrix, that trace will not change, you try as homework but we will prove it in the next class anyway.

So that trace W prime is equal to trace W irrespective of whatever basis transformation Q is. So Q will have no effect on trace it will cancel. Determinant W prime is determinant W is obvious by I, because determinant of any product matrix is product of determinants and determinant of an inverse matrix is 1 by the determinant.

So, if you write it as determinant you can also see this is also obvious, trace is not always you will have to work a little bit. But determinant is just too obvious but we can still write that that also follows from that relation that determine and W prime with determinant W.

So that is why both trace and determine and if you read any text in linear algebra or something, the trace and determinant are always called invariants of a matrix, invariant with respect to what? Invariant with respect to such basis transformations, that matrix is representing something physical, matrix is not just a set of numbers, matrix is representing something physical, it is representing rotation or a deformation if you are doing elastic or plastic deformation.

So it is always representing something physical, but that representation is basis dependent if you choose different coordinate system, you will get different numbers. But whatever different numbers they are represented by the sum of diagonal elements is not going to change. So thank you very much for your attention.