Crystals, Symmetry and Tensors

Professor Rajesh Prasad

Department of Materials Science and Engineering.

Indian Institute of Technology Delhi

Invariance of a Trace of Symmetry Operation during Basis Transformation

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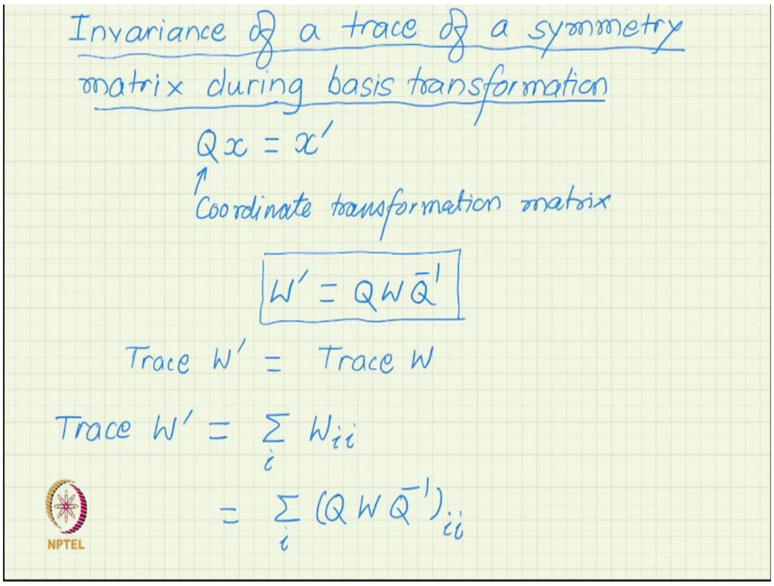

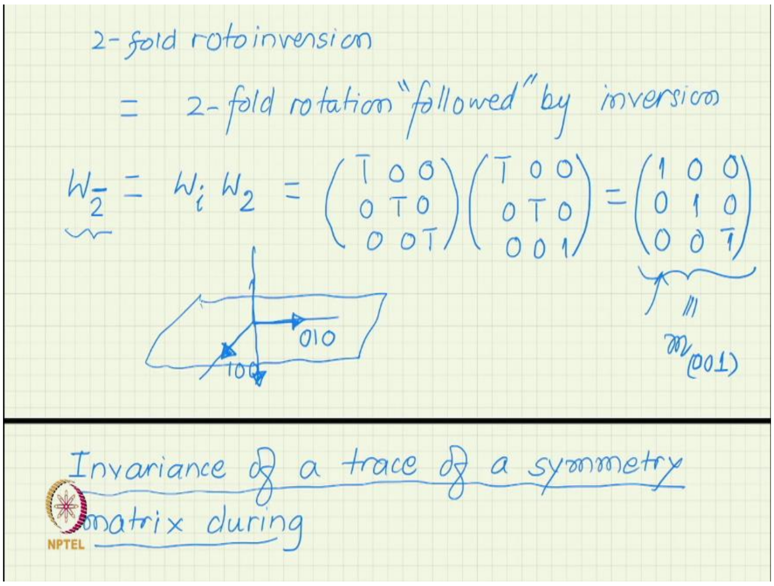

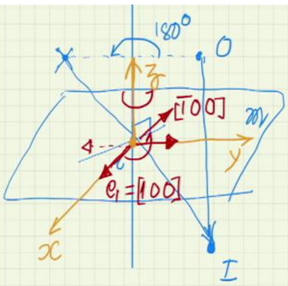

Matrix Method

2-fold rotoinversion

2-fold rotation:

$$W_2 = \begin{pmatrix} -1 & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

2-fold rotation

Coordinate transformation matrix

$$\boxed{W' = Q W Q^{-1}}$$

$$\boxed{\text{Trace } W' = \text{Trace } W}$$

$$\text{Trace } W' = \sum_i W'_{ii}$$

$$= \sum_i (Q W Q^{-1})_{ii}$$

$$= \sum_i \sum_j \sum_k Q_{ij} W_{jk} Q^{-1}_{ki}$$

$$= \sum_i \sum_j \sum_k (Q^{-1}_{ki} Q_{ij}) W_{jk}$$

$$= \sum_i (Q W Q^{-1})_{ii}$$

$$= \sum_i \sum_j \sum_k Q_{ij} W_{jk} Q^{-1}_{ki}$$

$$= \sum_i \sum_j \sum_k (Q^{-1}_{ki} Q_{ij}) W_{jk}$$

$$= \sum_i \sum_j \sum_k (Q^{-1} Q)_{kj} W_{jk}$$

$$= \sum_i \sum_j \sum_k (I_{kj} W_{jk})$$

$$= \sum_i \sum_j \sum_k (Q'Q)_{kj} W_{jk}$$

$$= \sum_i \sum_j \sum_k (I_{kj} W_{jk})$$

$$= \sum_i \sum_j \sum_k W_{kk}$$

$$= \text{Trace } W$$

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Now, let us look at the Invariance of the trace, hardly any complicated matrix comes in what you are seeing for 2-fold roto-inversion, these are the kinds of matrices which comes in crystallography. So, most of the symmetry operations will be represented by the simple combination of 0, 1 sometimes maybe a fraction half or two, but beyond that means, it will not be some sort of complicated numbers, which you have to handle.

So, as such matrix algebra is not complicated, only the interpretation is important. That is why I am going slowly and that is why I am asking you questions. So, that you understand and appreciate what the matrices are doing. And once you have understood that the rest of it will be very simple and straightforward and calculations are hardly difficult, you can always do manually on paper you will not even need a computer.

So, let us see invariance of a trace of a symmetry matrix. What do we mean by this is we saw that an axis system is required to write the symmetry matrix matrices, the same matrix this matrix had a very simple form these matrices had very simple form, because we chose our axis also nice and simple, we kept x and y in the mirror plane z perpendicular to the mirror plane, if we would have chosen an arbitrary set of axis, then the matrix will have a complicated form.

So, suitable choice of axis are essential, but sometimes you need to change from one set of axis to another set of axis. Because for one problem one set of axis may be simple for another problem, another set of axis may be seem simpler, but now, you have to consider both the cases. So, you have to translate from one axis to another axis in that we saw that if there is we can translate from one basis.

So, matrix during basis transformation, basis transformation or coordinate transformation. So, we saw that if there is n vector x, then the new coordinates will be given by Qx equal to x prime, where Q is the coordinate transformation matrix. We also saw that if there is a symmetry operation W in one of the earlier classes we have seen, then that will also transform into new coordinate system by a different matrix.

But now, the relation is not as simple as QW, but the relation is QW Q inverse. This we have established in one of the previous classes please review that and when we say that trace of a matrix does not change, what we are seeing that the numbers of W prime will be different from numbers of W. But when you add the diagonal terms, they will come out to be the same. So, trace W prime should be trace W. Now, how do we prove this?

So, let us start with LHS trace W prime since you have to add diagonal term, it is Wii summed over i going from one to three. So, we replace for W because, we know that W sorry this is W prime. So, since we know W prime is QW Q inverse, we just substituted that, then we use what is meant by matrix product. So, Q Wii i element i i element of a matrix product QW Q prime QW Q inverse can be written as Qij Wjk Q inverse ki and now the summation, since we have summation over j as summation over k.

So, we have two more summations. But written in the component form these numbers are now scalars So, they are not restricted by their position as in the matrix multiplication in matrix multiplication you cannot flip the position. But now, since these are numbers I can flip them. So, I can bring I can write this as Q inverse ki Qij Wjk this is using the property of what will you call for numbers, commutative property of a scalar multiplication we can flip them and bring them like this.

But now, since ki Q inverse ki into Qij with i running from one to three what will that represent? So, let me just write one more step. So, that will be Q inverse Qkj and this as you said becomes dell or you can say identity matrix kj Wjk but, I kj into Wjk is again a matrix product summed over j. So, this can be written as Wkk because summation is over j and Wkk summed over k is equal to 1, 2, 3 is nothing but trace W.

So, this shows this algebra shows that we will not do that, but at least once one should see the proof to convince oneself, but this relation we will use often now, that trace does not change.

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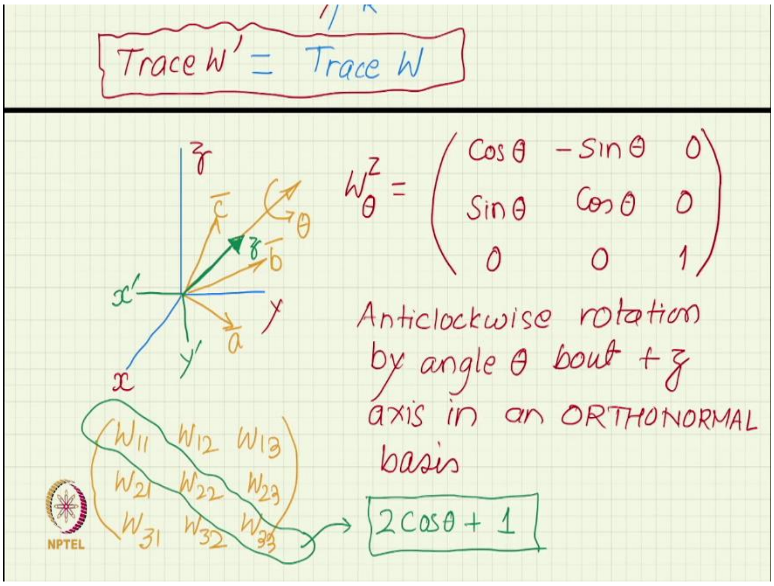

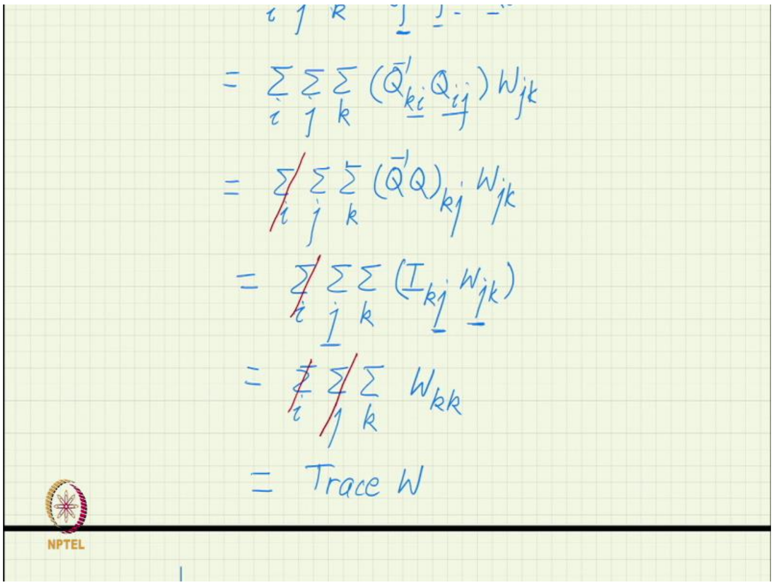

Trace does not change helps us in formulating a very powerful result because we saw that if we have a rotation matrix a very special rotation matrix, we used it effectively what you will see that we have already used this j here i was already used here. So, maybe I should have dropped. So, you are right means now, it is not really required.

We have done that summation effectively means, if you write it in full, you will you will find that yes you have done that summation. So, I will not be in the equation and in the last step we have done the summation over j. So, that also will not be there. So, we are summing only over k in the end. So, we have used those sigmas.

So, now, a rotation matrix we wrote a rotation matrix for by angle theta about z axis what was then cos theta sine theta 0 minus sine theta cos theta 0, 0, 0, 1. So, this is a very simple and very special rotation matrix a rotation matrix. So, let us write that anticlockwise rotation by angle theta about plus z axis in an orthonormal that is Cartesian, in an orthonormal basis.

But now, this is where our this theorem is coming to our, strengthens our hand that not only for this rotation matrix suppose, suppose there was some other rotation matrix, you are not rotating about z axis, let us say you are rotating about some arbitrary axis and suppose you are referring this to some coordinate system which is not even Cartesian.

Some crystallography coordinate system, abc, triclinic system, a not equal, b not equal, c alpha beta gamma not 90 degrees, some arbitrary axis, but the rotation is by an angle theta anticlockwise about this. What will be the trace of that matrix? You can always set up a green coordinate system in which your z axis is parallel to the rotation axis and x and y are orthonormal.

What will be the form of the matrix in the green coordinate system, we have written this in the green coordinate system it has to be cos theta sine theta 0 and this form. Now, in the golden system or whatever that colour is. So, in the crystallographic system the numbers will all change it will not be this simple, but despite that changing when we will add up.

So, in the golden system, the matrix will take the most general form W11, W12, W13. So, W13 will not be 0 like in this matrix W21 and W22, W23 again will not be 0 W31 will not be 0, W32 will not be 0, W33 will not be 1. So, this will be the rotation matrix in this crystallographic coordinate system, but when we will add the theorem is giving us the confidence that when we will add these three numbers, it has to be 2 cos theta plus 1.

So, trace of a rotation matrix, irrespective of the coordinate system. If the rotation is by an angle theta about whatever axis the matrix will matrix will keep changing form depending on which way, the axis is oriented. But if the angle is theta, the trace has to be 2 cos theta plus 1.