Crystals, Symmetry and Tensors Professor Rajesh Prasad Department of Material Science and Engineering Indian Institute of Technology Delhi Lecture 9c Trace of a rotation matrix

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Trace of a Rotation Matrix by θ ccw rotation in a cubic system about z - axis. $\vec{c} \rightarrow \vec{b} \qquad w(\vec{a}) = \alpha \cos\theta. \vec{a} + \beta \sin\theta. \vec{b} + \alpha$ $\vec{a} \rightarrow w\vec{a}) = \cos\theta. \vec{a} + \beta \sin\theta. \vec{b} + \alpha$ $\vec{a} \rightarrow w\vec{a}) = \cos\theta. \vec{a} + \sin\theta. \vec{b} + \alpha$ $w(u) = \mu \cos \theta \cdot \frac{u}{2} + \mu \sin \theta \cdot \frac{0}{2} + \alpha$ $= \cos \theta \cdot \overline{a} + \sin \theta \cdot \overline{b} + 0$ $W = \begin{pmatrix} \cos\theta & -\sin\theta & 0\\ \sin\theta & \cos\theta & 0\\ 0 & 0 & 1 \end{pmatrix} \xrightarrow{\theta = q\theta'} \begin{pmatrix} 0 & \overline{1} & 0\\ 1 & 0 & 0\\ 0 & 0 & 1 \end{pmatrix}$ Det(W) = + 1 (check this)

Professor: Another interesting quantity is trace. Let us again write 90 degrees counterclockwise rotation in a cubic system. So we saw that that W was so, no I do not want 90 degree you have written CCW rotation by some general angle, let us look at it by a general angle, by theta, let us formulate the matrix for this, this will be interesting. So what are the component of W a?

Student: W a cos theta and W a sin theta.

Professor: Now W is transformed a and a has a length a, so you mean W will also have the same length and then the components are a cos theta,

Student: Cos theta.

Professor: And a sine theta, So W a, so a cos theta is the length, length times the unit vector in the a direction so what will that be? a by a. And similarly, the b component is a sin theta times the unit vector along b, this is again b by a, because length is same, length of a and b is the same, this is cos theta times a plus sin theta times b and plus let us write three dimensionally, so plus 0, the third component is 0, because if it is rotated about the z axis counter claw in a cubic system about z axis, axis has to be specified only angular specification is not sufficient for rotation in 3d.

So we get back so, the components of the transformed vectors are cos theta, sin theta and 0. So you have the first column of your matrix as cos theta, sin theta 0, what about W b?

Student: Minus sin theta cos theta.

Professor: Now, this will go theta this way, b is also of length a, so x component is now on the negative side and that component will be minus sin theta, the y component will be cos theta and 0. And what about the z components?

Student: (()) (5:16)

Professor: Because that is on the rotation axis, so that is the invariant axis, so a vector along the rotation axis do not change, so we have 0, 0, 1. So we have little bit generalized the problem from writing a 90 degree rotation about z axis, we have written a theta degree rotation about z axis, if we put theta is equal to 90 degree, we should be able to recover the original matrix. If you put theta is equal to 90 degree then it becomes.

Student: 0, 1, 0.

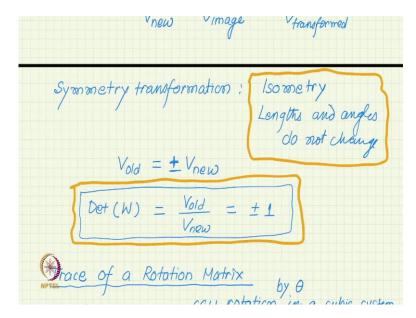
Professor: It becomes 0, 1, 0 minus 1, 0, 0 and 0, 0, 1, which is exactly the matrix we just found for 90 degree rotation, so this is fine. Now, you can check I leave this as an exercise let us not do the algebra, but it is not very difficult you can check that even with this cos theta sin theta this determinant W will still come out to be plus 1.

Student: It will give sin square theta plus cos square theta.

Professor: Sin square theta plus cos square theta. Determinant W is plus 1 as we have assured you that if it is symmetric transformation it has to be like this.

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 $W = \begin{pmatrix} \cos \theta & -\sin \theta & 0 \\ \sin \theta & \cos \theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \xrightarrow{\theta = q\theta'} \begin{pmatrix} 0 & \overline{1} & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ $Det(W) = + 1 \quad (check \ this)$ Trace (W) = $\sum_{i=1}^{3} W_{ii} = W_{ii} + W_{22} + W_{33}$ $= 2\cos\theta + 1$ ۲ Trace (W) = $\sum_{i=1}^{3} W_{ii} = W_{ii} + W_{22} + W_{33}$ = 2 COS 0 + 1 Trace of a rotation matrix is always $2\cos\theta + 1$ pirrespective of basis or axis about which rotation takes place



Professor: But now, let us write the trace, what is a trace of a matrix?

Student: Some of the diagonal elements.

Professor: Yes, some of the elements, this is the definition of trace. In this particular case if we apply what do we get? 2 cos theta plus 1. Now, we are going to show, so this is a very special case, special case in terms of rotation, we have taken a cubic system, where a, b and c are equal, alpha, beta, gamma are 90 degree, we have taken a very simple rotation that is about z axis and we have found the trace, but the surprising and the interesting result.

So, the trace was this sum, the surprising and interesting result is that trace of a rotation matrix always will be 2 cos theta plus 1, even if we would have chosen some arbitrary a b, a c and alpha if you are rotating in a tri clinic system, the trace will still be and you are rotating about some arbitrary axis not about 0, 0, 1, but about 1, 1, 1, in a tri clinic system, trace will remain, we will prove this I am just writing the result first.

So if a rotation matrix is given to you, whether you know what basis it is being referred to whether it is tri clinic crystal or hexagonal crystal or cubic crystal and you do not know that in that crystal about which axis we are talking about the rotation, but you can still confidently say confidently give what is the rotation angle, that this matrix represent a rotation of this much angle because you can only have to add the three terms along the diagonal equated to 2 cos theta plus 1, solve for theta, is always 2 cos theta plus 1 irrespective of the basis in which the matrix is represented and irrespective of axis about which the rotation happens, very-very interestingly result, let us put it in the golden box.

Similarly, the determinant result also we found the determinant for 2 specific matrices and we jump but the determinant of course, determinant you have already proved there you do not need any further proof, because the determinant result is related to the isometric. So, there the key thing was isometric because isometric cannot change volume. It has to be one in magnitude, but depending upon whether the isometric is of type 1 or type 2, whether the handedness is changing or not, it can be either plus 1 or minus 1. So, that was the property of the determinant.