Contents

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1.1 Calculating x' and y' for $\mathbf{R}_z$

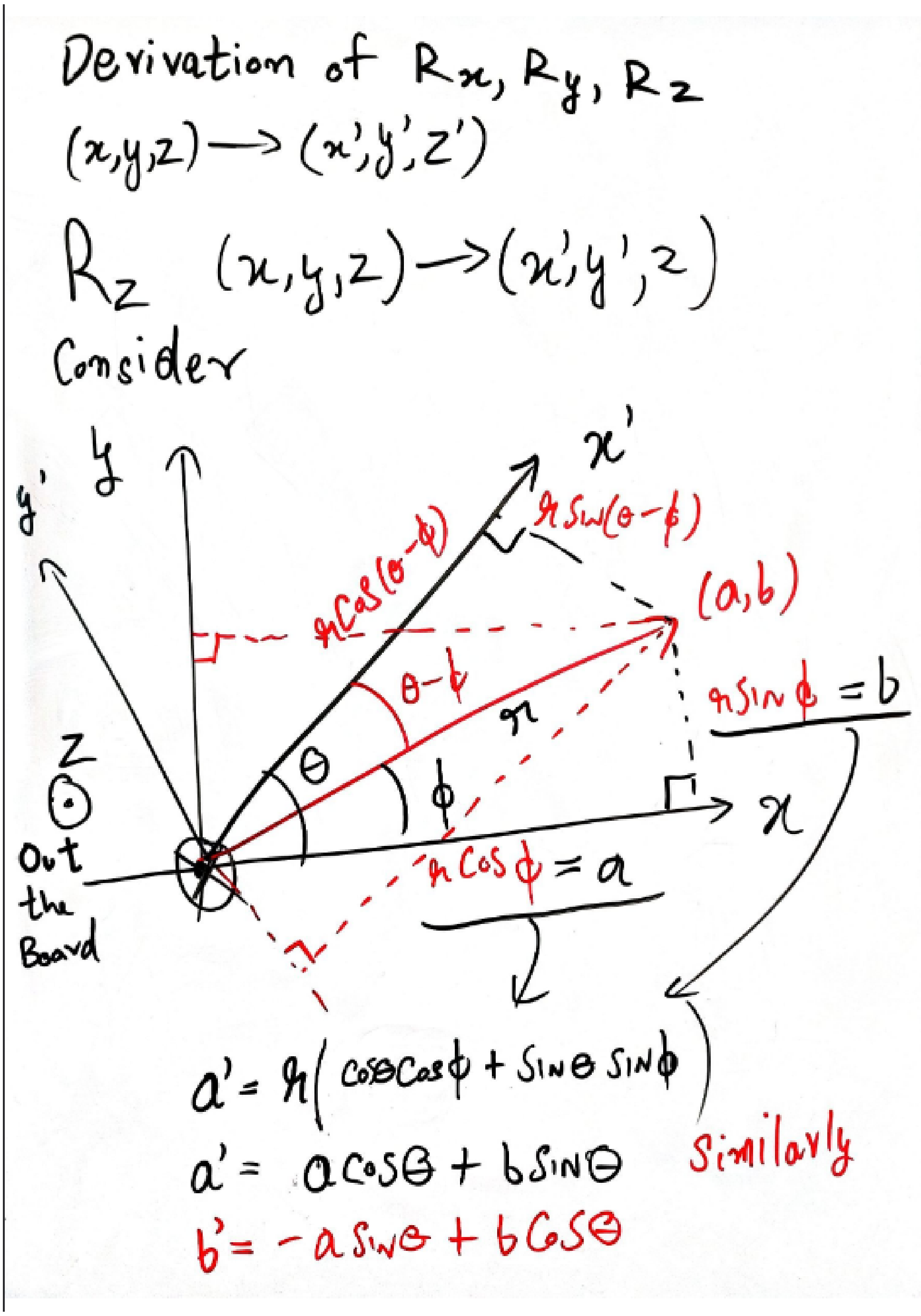


Figure 1: Derivation of R_z

1.2 Calculating x' and z' for R_y

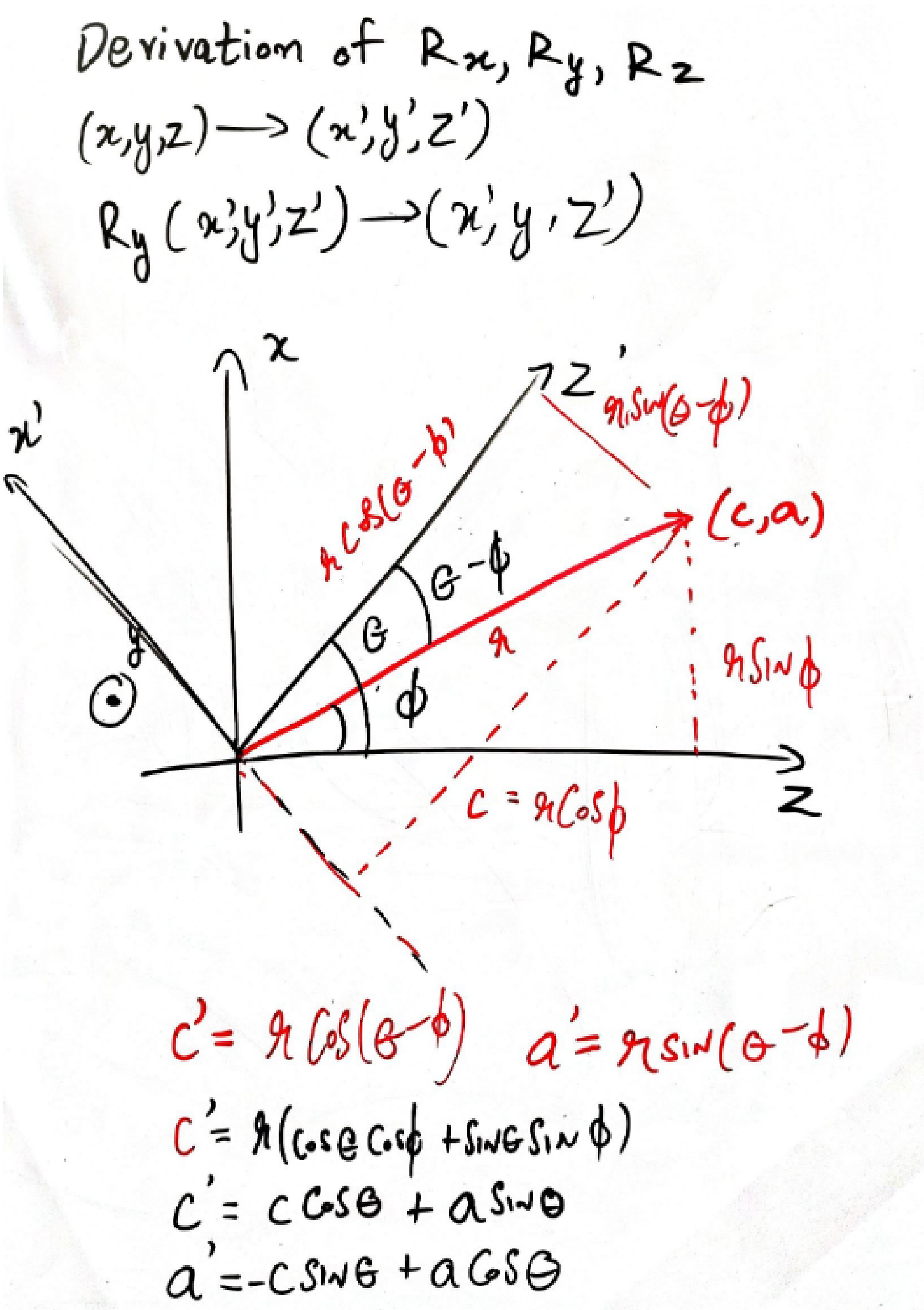


Figure 2: Derivation of R_y

1.3 Setting up the matrix form

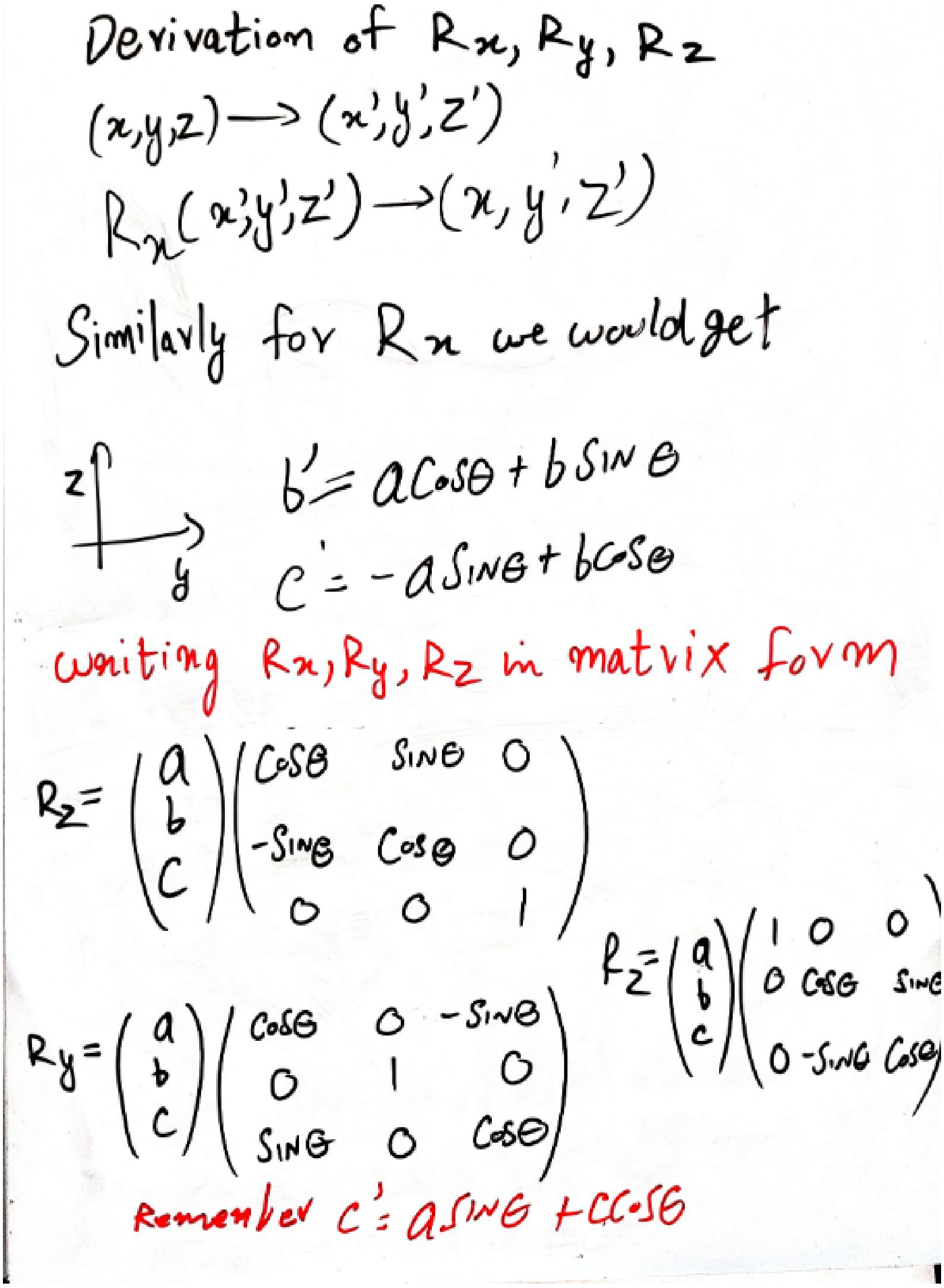


Figure 3: Representation in Matrix form

More formally we can write R_z in the form of unit vectors along the intial and final axes

$$\hat{e_x} = (\hat{e'_x} \cdot \hat{e_x})\hat{e'_y} + (\hat{e'_y} \cdot \hat{e_x})\hat{e'_y}$$

$$\hat{e_y} = (\hat{e'_x} \cdot \hat{e_y})\hat{e'_x} + (\hat{e'_y} \cdot \hat{e_y})\hat{e'_y}$$

This can be rewritten in the form of an orthagonal matrix

$$S = \begin{pmatrix} \hat{e'_x} \cdot \hat{e_x} & \hat{e'_x} \cdot \hat{e_y} \\ \\ \hat{e'_y} \cdot \hat{e_x} & \hat{e'_y} \cdot \hat{e_y} \end{pmatrix}$$

The transformation from one orthogonal Cartesian Coordinate System to another Cartesian Coordinate system is described by an Orthogonal Matrix

2 Rotation in $\mathbb{R}^3$

We can write the 3D rotation matrix matrix just like we did in 2D

$$S = \begin{pmatrix} \hat{e}'_1 \cdot \hat{e}_1 & \hat{e}'_1 \cdot \hat{e}_2 & \hat{e}'_1 \cdot \hat{e}_3 \\ \hat{e}'_2 \cdot \hat{e}_1 & \hat{e}'_2 \cdot \hat{e}_2 & \hat{e}'_2 \cdot \hat{e}_3 \\ \hat{e}'_3 \cdot \hat{e}_1 & \hat{e}'_3 \cdot \hat{e}_2 & \hat{e}'_3 \cdot \hat{e}_3 \end{pmatrix}$$

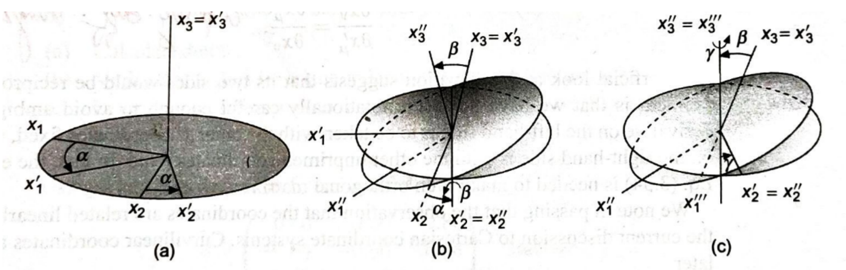
But we still need to find the relations between the elements of S and the angles of rotation.
The number of parameters needed to specify a rotation is 3
I will use **Euler Angles** to define these parameters.

2.1 Euler Angles

Eulers Theorem: Any 3D rotation is equivalent to rotation by some arbitrary amount θ about some axis $\hat{n}$ in the 3D space.
Euler Angles describe $\mathbb{R}^3$ rotation in 3 steps
first 2 rotations ($S_1(\alpha)$ and $S_2(\beta)$) specify the orientation of the new $\hat{e}_3$ The third determining the rotation about that axis.

Note: What we want to achieve is find the rotation matrix for rotating a water molecule by ϕ degrees about an arbitrary axis Euler angles describe the rotation of an axis. We will use the fact that rotation of axis by θ in the counterclockwise direction is the same as rotating the water molecule by θ in the clockwise direction (This is also called the notion of active rotation or passive rotation).

We will find the rotation matrix for each of the steps and the total rotation will be the right hand product of all of those matrices



Euler angle rotations: (a) about $\hat{\mathbf{e}}_3$ through angle α; (b) about $\hat{\mathbf{e}}'_2$ through angle β; (c) about $\hat{\mathbf{e}}''_3$ through angle γ.

Figure 4: Referring from Arfken and Weber

2.2 Calculating the 3 subrotation Matrices

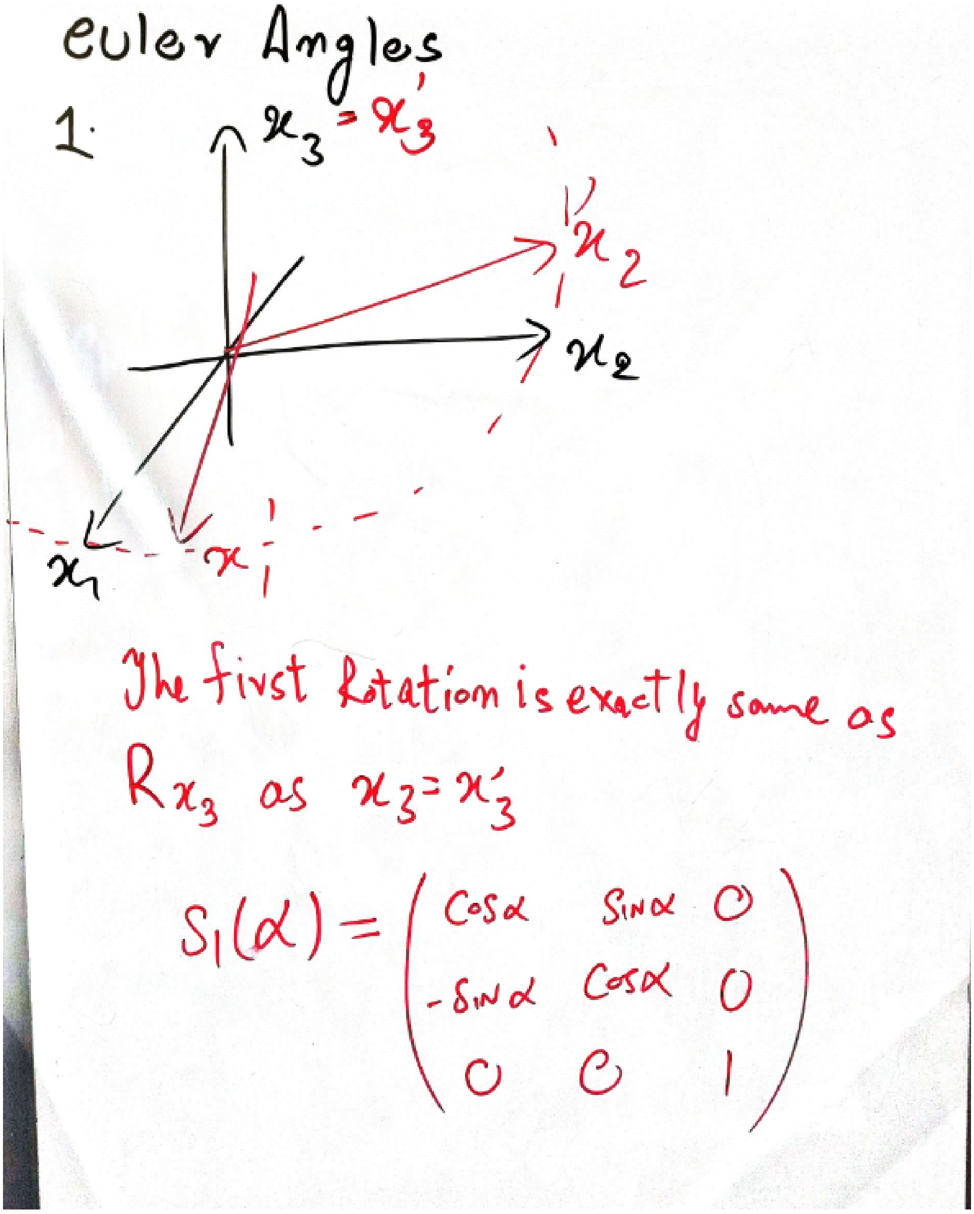


Figure 5: $\mathrm{S}_1(\alpha)$

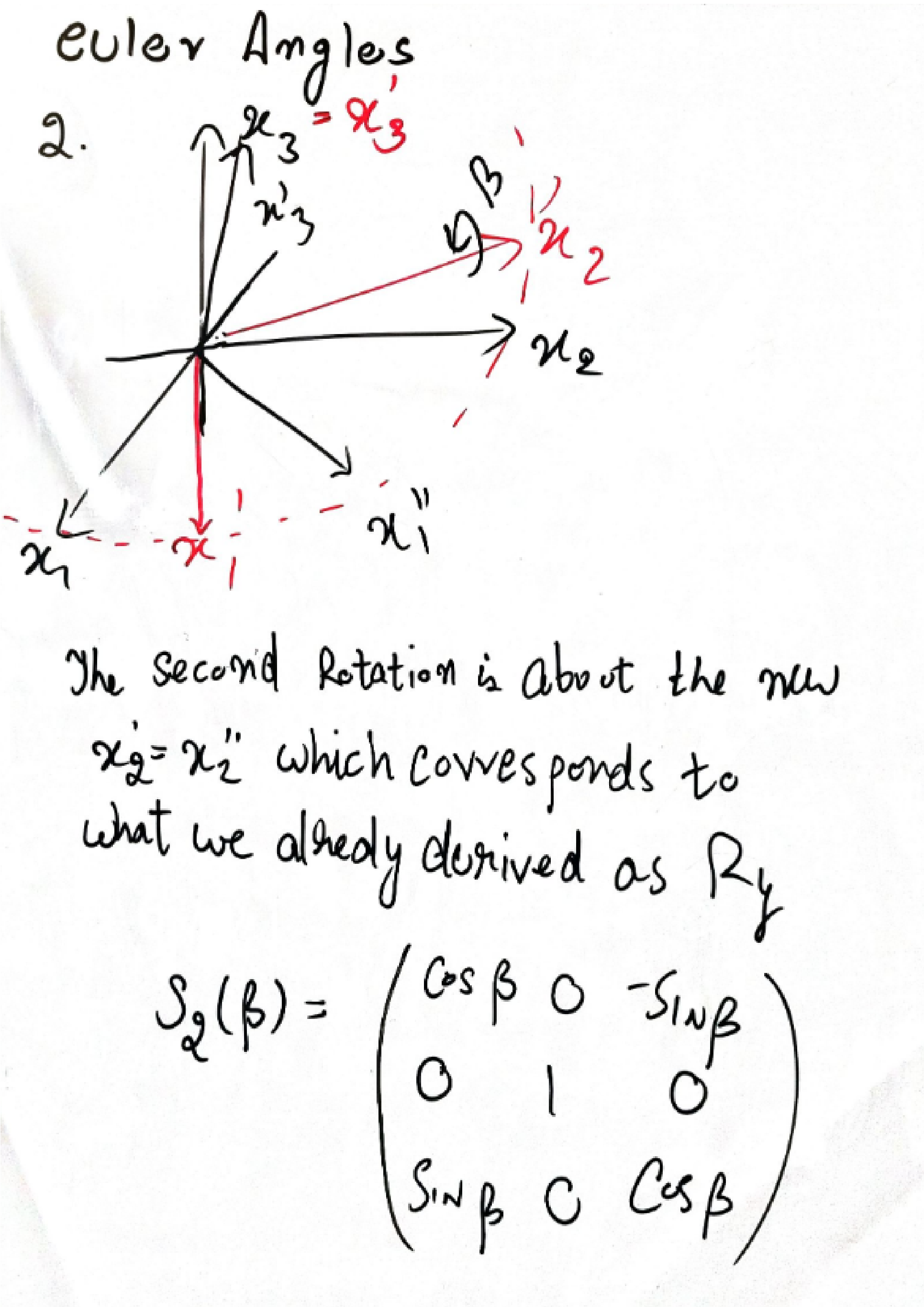


Figure 6: $S_2(\beta)$

[H]

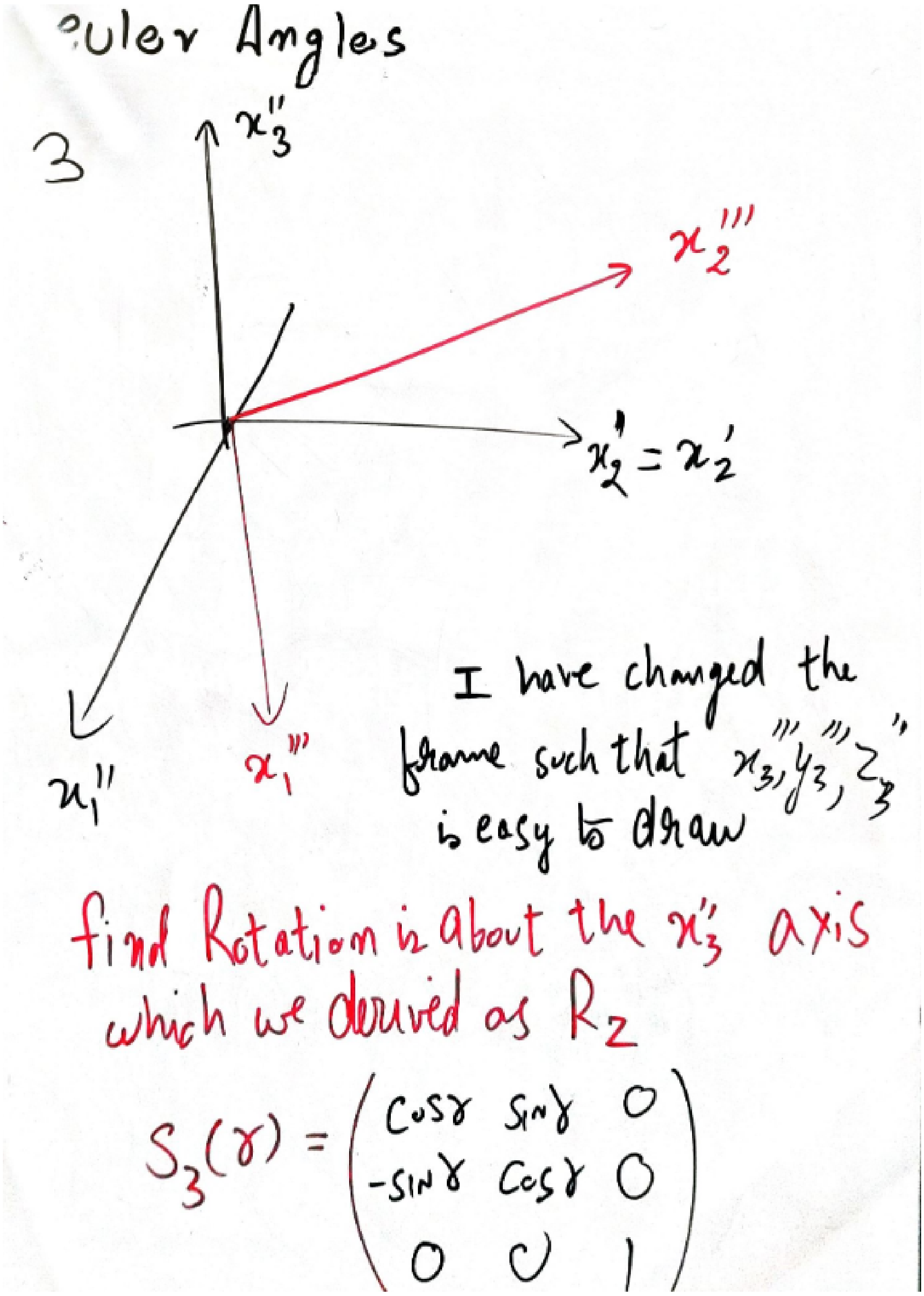


Figure 7: $S_3(\gamma)$

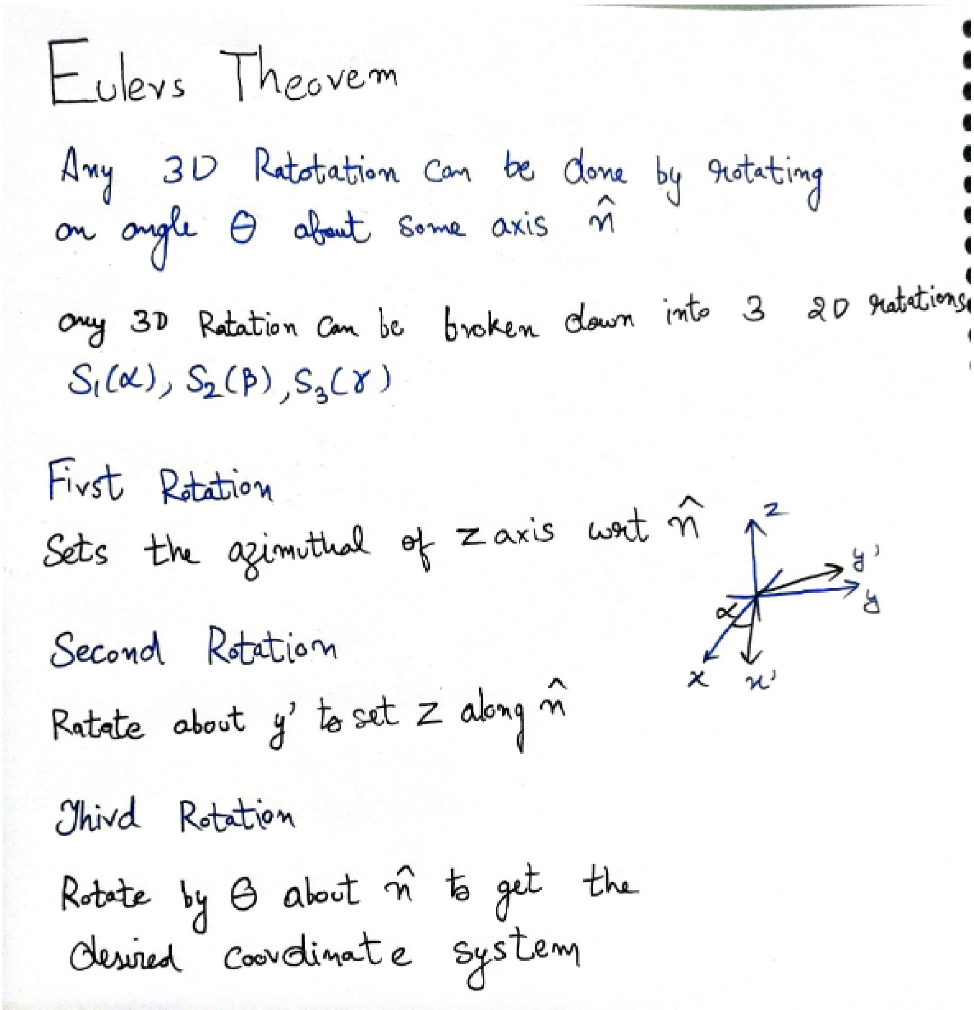


Figure 8: Eulers Theorem

2.3 Results

after obtaining $S_1(\alpha), S_2(\beta), S_3(\gamma)$ now we will calculate the final rotation matrix

$$\mathrm{S}(\alpha,\beta,\gamma) = S_3(\gamma)S_2(\beta)S_1(\alpha) = \begin{pmatrix} \cos\gamma\cos\beta\cos\alpha - \sin\gamma\sin\alpha & \cos\gamma\cos\beta\sin\alpha + \sin\gamma\cos\alpha & -\cos\gamma\sin\beta \\ -\sin\gamma\cos\beta\cos\alpha - \cos\gamma\sin\alpha & -\sin\gamma\cos\beta\sin\alpha + \cos\gamma\cos\alpha & \sin\gamma\sin\beta \\ \sin\beta\cos\alpha & \sin\beta\sin\alpha & \cos\beta \end{pmatrix}$$

Since this was the rotation of axis now we must take the transpose of this matrix to obtain the final result.

$$\mathrm{S}^T(\alpha,\beta,\gamma) = \begin{pmatrix} \cos\gamma\cos\beta\cos\alpha - \sin\gamma\sin\alpha & -\sin\gamma\cos\beta\cos\alpha - \cos\gamma\sin\alpha & \sin\beta\cos\alpha \\ \cos\gamma\cos\beta\sin\alpha + \sin\gamma\cos\alpha & -\sin\gamma\cos\beta\sin\alpha + \cos\gamma\cos\alpha & \sin\beta\sin\alpha \\ -\cos\gamma\sin\beta & \sin\gamma\sin\beta & \cos\beta \end{pmatrix}$$

Hence, we have shown that any rotation in a 3D dimensional space can be expressed as the consequence of 3 successive rotations using **z-y-z Euler Rotation**.
Note that we have taken a right hand coordinate system so the matrix multiplication is also done in such a way to preserve this ann in a right handed system the determinant of an orthogonal matrix is 1 $|S(\alpha,\beta,\gamma)| = 1$