## Cofactor Definition:

M O

$$C_{ij} = (-1)^{i+j} \det \begin{vmatrix} a_{11} & \dots & & a_{1n} \\ \vdots & & & \vdots \\ \dots & & a_{ij} & \dots \\ a_{n1} & \dots & & a_{nn} \end{vmatrix}$$

$$A_{ik} C_{ij} = \delta_{kj} |A|$$

$$A_{ki} C_{ji} = \delta_{kj} |A|$$

## Inverse of a $n \times n$ matrix:

Compare Exercise 3.2.24 on p. 113.

Assume determinant $|A| \neq 0$. Then,

$$(A^{-1})_{ij} = \frac{C_{ji}}{|A|}$$

where $C_{ji}$ is the $j$th cofactor of $|A|$.

Proof:

$$\underbrace{A_{ki}\, C_{ji}}_{A_{ki}\,(A^{-1})_{ij}} = \delta_{kj}\, |A| \quad \Rightarrow \quad A A^{-1} = 1$$

$$(A^{-1})_{ij}\, A_{jk} = \frac{C_{ji}\, A_{jk}}{|A|} = \delta_{ik}$$

$$\Rightarrow A^{-1} A = 1$$

---

Note: $\quad |A^{-1} A| = |A^{-1}|\,|A| \qquad (3.49)$

$$\underbrace{|1|}_{=|A^{-1}A|} = 1 \Rightarrow |A^{-1}| = \frac{1}{|A|}.$$

## Orthogonal Matrices: (p. 193)

Application of matrices to vectors:

$$\vec{x}' = A\,\vec{x}$$

$$\vec{x}' = \begin{pmatrix} x_1' \\ \vdots \\ x_n' \end{pmatrix}, \qquad \vec{x} = \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix}$$

$$x_i' = a_{ij}\, x_j$$

Einstein convention.

We are interested in "rotations", which leave the Euclidean norm $|\vec{x}| = \sqrt{\vec{x}^2}$ invariant, i.e., $\underline{\underline{\vec{x}'^2 = \vec{x}^2}}$.

$$x_i' x_i' = a_{ij} x_j \, a_{ik} x_k = x_j x_k \, a_{ij} a_{ik}$$

$$= x_j x_k \, \delta_{jk} \quad \text{for all } x_j, x_k$$

$$\Rightarrow \quad a_{ij}\, a_{ik} = \delta_{jk}$$ {Mutually orthonormal vectors.

Orthogonality condition on matrix A.

<u>Transpose</u> Matrix definition:

$$\tilde{A} = (\tilde{a}_{ij}) \quad \text{with} \quad \tilde{a}_{ij} = a_{ji} .$$

Orthogonality relation: $\tilde{A} A = 1$,

$$\tilde{A} = A^{-1} .$$

Therefore also, $A \tilde{A} = 1$

$$a_{ij} \tilde{a}_{jk} = a_{ij} a_{kj} = \delta_{ik}$$

<u>Determinants:</u> $1 = |A \tilde{A}| = |A| |\tilde{A}|$

$$= |A|^2$$

$$\Rightarrow \quad \underline{|A| = \pm 1.}$$

$\frac{1}{2} n(n+1)$ independet equations.

$\frac{1}{2} n(n-1)$ free parameters left.

**2D:** $\frac{1}{2} n(n-1) = 1$ free parameter

$$\sum_{i=1}^{2} a_{ij} a_{ik} = a_{1j} a_{1k} + a_{2j} a_{2k} = \delta_{jk}$$

$$a_{11} a_{11} + a_{21} a_{21} = 1$$
$$a_{11} a_{12} + a_{21} a_{22} = 0$$
$$a_{12} a_{11} + a_{22} a_{21} = 0$$
$$a_{12} a_{12} + a_{22} a_{22} = 1$$

Solutions: $a_{11} = \cos\phi\,, \quad a_{21} = \underset{(+)}{-}\sin\phi$

$$\cos\phi \; a_{12} - \sin\phi \; a_{22} = 0$$
$$a_{12} \cos\phi - a_{22} \sin\phi = 0$$

$$a_{12} = \underset{(-)}{+}\sin\phi\,, \quad a_{22} = \underset{(-)}{+}\cos\phi$$

$$A = \begin{pmatrix} \cos\phi & \sin\phi \\ -\sin\phi & \cos\phi \end{pmatrix}$$

$\uparrow$ Angle

## Complex possibility:

$$a_{11} = \cosh\xi \,, \qquad a_{21} = i\sinh\xi$$

$$\cosh\xi \; a_{12} - i\sinh\xi \; a_{22} = 0$$

$$a_{12} = i\sinh\xi \,, \qquad a_{22} = \cosh\xi$$

$$A = \begin{pmatrix} \cosh\xi & -i\sinh\xi \\ i\sinh\xi & \cosh\xi \end{pmatrix}$$

$S_1 \rightarrow S$

Special Relativit Supplement

Rapidity

---

**3D:** Show and explain Euler Angle

Book p. 200/201.

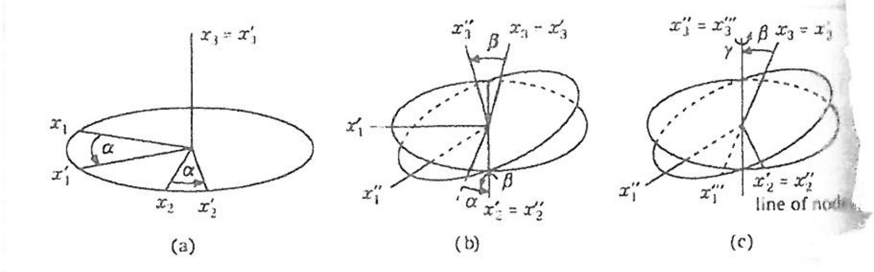


**Figure 3.7**

(a) Rotation About $x_3$ Through Angle $\alpha$,
(b) Rotation About $x'_2$ Through Angle $\beta$, and
(c) Rotation About $x''_3$ Through Angle $\gamma$



The three matrices describing these rotations are

$$\mathsf{R}_z(\alpha) = \begin{pmatrix} \cos\alpha & \sin\alpha & 0 \\ -\sin\alpha & \cos\alpha & 0 \\ 0 & 0 & 1 \end{pmatrix}, \tag{3.98}$$

exactly like Eq. (3.92), but different sign for $\beta$ in

$$\mathsf{R}_y(\beta) = \begin{pmatrix} \cos\beta & 0 & -\sin\beta \\ 0 & 1 & 0 \\ \sin\beta & 0 & \cos\beta \end{pmatrix} \tag{3.99}$$

and

$$\mathsf{R}_z(\gamma) = \begin{pmatrix} \cos\gamma & \sin\gamma & 0 \\ -\sin\gamma & \cos\gamma & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{3.100}$$

The total rotation is described by the triple matrix product:

$$\mathsf{A}(\alpha, \beta, \gamma) = \mathsf{R}_z(\gamma)\mathsf{R}_y(\beta)\mathsf{R}_z(\alpha). \tag{3.101}$$

Note the order: $\mathsf{R}_z(\alpha)$ operates first, then $\mathsf{R}_y(\beta)$, and finally $\mathsf{R}_z(\gamma)$. Direct multiplication gives

$$\mathsf{A}(\alpha, \beta, \gamma) = \begin{pmatrix} \cos\gamma\cos\beta\cos\alpha - \sin\gamma\sin\alpha & \cos\gamma\cos\beta\sin\alpha + \sin\gamma\cos\alpha & -\cos\gamma\sin\beta \\ -\sin\gamma\cos\beta\cos\alpha - \cos\gamma\sin\alpha & -\sin\gamma\cos\beta\sin\alpha + \cos\gamma\cos\alpha & \sin\gamma\sin\beta \\ \sin\beta\cos\alpha & \sin\beta\sin\alpha & \cos\beta \end{pmatrix}. \tag{3.102}$$

## Hermitian and Unitary Matrices

QM: Complex Variables.

$z = x + iy$ , $i = \sqrt{-1}$

$z^* = x - iy$ complex conjugate.

Matrix: $A^* = (a^*_{ij})$

Adjoint matrix: $A^\dagger = (a_{ik})^\dagger = (\tilde{a}^*_{ik}) = (a^*_{ki})$.

Hermitian matrix: $A^\dagger = A$

also called self-adjoint.

If A is real: real symmetric matrix.

Unitary matrix: $U^\dagger = U^{-1}$

U real: $U^\dagger = \tilde{U} = U^{-1}$

orthogonal matrices back.

Leave length of complex vector unchanged. Conservation of Probability in QM.

$$\vec{x} = \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix}, \quad \vec{x}^{\dagger} = (x_1^*, \ldots, x_n^*)$$

$$\vec{x}^{\dagger} \cdot \vec{x} = \vec{x}^{\dagger} \vec{x} = \sum_i x_i^* x_i = \sum_i |x_i|^2 \geq 0$$

Let $\vec{y} = U \vec{x}$:

$$\vec{y}^{\dagger} \vec{y} = (U\vec{x})^{\dagger} U\vec{x} = \vec{x}^{\dagger} U^{\dagger} U \vec{x}$$

$$= \vec{x}^{\dagger} U^{-1} U \vec{x} = \vec{x}^{\dagger} \vec{x}$$

Transformation of an operator $A$:

Let $\vec{y} = A\vec{x}$, $\vec{x}' = U\vec{x}$, $\vec{y}' = U\vec{y}$.

We want: $\quad \vec{y}' = A' \vec{x}'$. $\quad (*)$

Solution: $\quad A' = U A U^{\dagger}$.

$$A'\vec{x}' = UAU^{\dagger}U\vec{x} = UA\vec{x} = U\vec{y} = \vec{y}'. \ \square$$

$(*)$ is called Similarity Transformation.

# Diagonalization of Matrices by Similarity Transformation.

Example: Moments of Inertia Matrix

$$\vec{L} = I\,\vec{\omega}$$

with $I_{ij} = \sum_k m_k \left(\delta_{ij}\,\vec{r}^{\,2} - x_i x_j\right).$

By rotation of axis we can bring $I$ into diagonal form: Principal Axis. In these coordinates

$$I' = \begin{pmatrix} I'_1 & & 0 \\ & I'_2 & \\ 0 & & I'_3 \end{pmatrix} = \begin{pmatrix} \lambda_1 & & 0 \\ & \lambda_2 & \\ 0 & & \lambda_3 \end{pmatrix}$$

with orthonormal eigenvectors $\quad \hat{v}'_i\,\hat{v}'_j = \delta_{ij}$

$$\hat{v}'_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix},\quad \hat{v}'_2 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix},\quad \hat{v}'_3 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

$$I'\,\hat{v}'_i = \lambda_i\,\hat{v}'_i$$

(No summation on r.h.s.!)

<u>Orthogonal</u>

Transformation from the original frame:
$$I' = R I \tilde{R}, \quad \hat{V}_i' = R \hat{V}_i,$$

$$I = \begin{pmatrix} I_{11} & I_{12} & I_{13} \\ I_{21} & I_{22} & I_{23} \\ I_{31} & I_{32} & I_{33} \end{pmatrix}, \quad R^{-1} = \tilde{R}$$

$$I' \hat{V}_i' = \lambda_i \hat{V}_i' = \lambda_i R \hat{V}_i$$

$$R I R^{-1} R \hat{V}_i = R I \hat{V}_i$$

$$\Rightarrow I \hat{V}_i = \lambda_i \hat{V}_i$$

Eigenvalues Eigenvectors

So, we are looking for <u>solutions</u> of the <u>homogeneous linear equation</u>

$$(I - \lambda_i 1_3) \hat{V}_i = 0$$

3x3 unit matrix.

Required:

$$0 = \det \begin{vmatrix} I_{11}-\lambda & I_{12} & I_{13} \\ I_{21}-\lambda & I_{22}-\lambda & I_{23} \\ I_{31} & I_{32} & I_{33}-\lambda \end{vmatrix}$$

$\Rightarrow$ Polynomial $\lambda^3 + a_2\lambda^2 + a_1\lambda + a_0 = 0$

which will have three (possibly degenerate) root $\lambda_1, \lambda_2, \lambda_3$.

Once the roots are known, the eigenvectors follow from the equations

$$A_i \hat{v}_i = (I - \lambda_i)\hat{v}_i = 0.$$

Example: $\rightarrow$ Classwork 14.

$$\hat{v}_i = \begin{pmatrix} v_i^1 \\ v_i^2 \\ v_i^3 \end{pmatrix}, \qquad \hat{v}_i' = R\hat{v}_i$$

$$\delta_{ij} = \hat{v}_i \tilde{R} \cdot R \hat{v}_j = \hat{v}_i \hat{v}_j.$$

## Calculation of the matrix R:

$$\hat{V}_i = \tilde{R}\,\hat{V}_i' \quad \text{implies}$$

$$\begin{pmatrix} V_1^1 \\ V_1^2 \\ V_1^3 \end{pmatrix} = \begin{pmatrix} \tilde{r}_{11} \\ \tilde{r}_{21} \\ \tilde{r}_{31} \end{pmatrix}, \quad \begin{pmatrix} V_2^1 \\ V_2^2 \\ V_2^3 \end{pmatrix} = \begin{pmatrix} \tilde{r}_{12} \\ \tilde{r}_{22} \\ \tilde{r}_{32} \end{pmatrix}$$

First eigenvector $\hat{V}_i$

$$\begin{pmatrix} V_3^1 \\ V_3^2 \\ V_3^3 \end{pmatrix} = \begin{pmatrix} \tilde{r}_{13} \\ \tilde{r}_{23} \\ \tilde{r}_{33} \end{pmatrix}$$

$$\tilde{R} = \begin{pmatrix} V_1^1 & V_2^1 & V_3^1 \\ V_1^2 & V_2^2 & V_3^2 \\ V_1^3 & V_2^3 & V_3^3 \end{pmatrix}$$

$$R = \begin{pmatrix} V_1^1 & V_1^2 & V_1^3 \\ V_2^1 & V_2^2 & V_2^3 \\ V_3^1 & V_3^2 & V_3^3 \end{pmatrix}$$

# Normal Modes of Vibration (Molecules)

Double Oscillator → ~~Fig 3.10,~~ p.219.

$$\ddot{x}_1 = +\frac{K}{M}(x_2 - x_1)$$

$$\ddot{x}_2 = +\frac{K}{m}(x_1 - x_2) + \frac{K}{m}(x_3 - x_2)$$

$$\ddot{x}_3 = +\frac{K}{M}(x_2 - x_3)$$

$x_j$ are displacements from zero position.

Ansatz:

$$x_j = a_j e^{i\omega t}, \quad j = 1, 2, 3.$$

$$\ddot{x}_j = -\omega^2 a_j e^{i\omega t} = -\omega^2 x_j$$

Matrix form of eqns:

$$\begin{pmatrix} \frac{K}{M} - \omega^2 & -\frac{K}{M} & 0 \\ -\frac{K}{m} & \frac{2K}{m} - \omega^2 & -\frac{K}{m} \\ 0 & -\frac{K}{M} & \frac{K}{M} - \omega^2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = 0$$

Not symmetric! Eigenvectors not orthogonal! ✓

# Computer assisted calculation

```
FORM by J.Vermaseren,version 3.3(Jun 10 2009) Run at: Wed Apr 17 07:20:58
2013
    * PHZ 3113 Weber & Arfken, p.219:
    * 3x3 determinant for normal modes.
    * kM=k/M, km=k/m, la=omega^2 eigenvalues wanted.
        Symbols kM,km,la;
        Off stat;
        Local det=(kM-la)*(2*km-la)*(kM-la)+0+0
                 -(kM-la)*(-km)*(-kM)
                 -(-kM)*(-km)*(kM-la)-0;
    * Reduction by eigenvalue 1: la=0.
        Local dla=-det/la;
    * Remaining eigenvalues la2,3=km+kM-/+Sqrt[(km+kM)^2-2*kM*km-kM^2].
    * Sqrt=-/+km: la2=kM, la3=kM+2*km. Check:
        Local Zero=dla-(la-kM)*(la-kM-2*km);
        Bracket la;
        Print;
        .sort

  det =
     + la * (  - 2*kM*km - kM^2 )

     + la^2 * ( 2*km + 2*kM )

     + la^3 * (  - 1 );

  dla =
     + la * (  - 2*km - 2*kM )

     + la^2 * ( 1 )

     + 2*kM*km + kM^2;

  Zero = 0;

        .end
 0.00 sec out of 0.00 sec
```

$\det|\cdots| = 0 \Rightarrow$ Eigenvalues

$$\omega^2 = 0,\quad K/M,\quad \frac{K}{M} + 2\frac{K}{m}$$

by computer-assisted calculation.

---

Eigenvectors: Substitute eigenvalues into equs.

$\omega^2 = 0$:

$$\left.\begin{array}{l} 1.\ X_2 - X_1 = 0 \\ 3.\ X_2 - X_3 = 0 \end{array}\right\} X_1 = X_2 = X_3$$

Translation.

$\omega^2 = \frac{K}{M}$:

$$1.\ \cancel{-\frac{K}{M}X_1} = \frac{K}{M}X_2 \cancel{-\frac{K}{M}X_1}$$

$$\Rightarrow \quad \underline{X_2 = 0}$$

$$2.\ -\frac{K}{M}X_2 = 0 = \frac{K}{m}X_1 + \frac{K}{m}X_3$$

$$\underline{X_1 = -X_3}$$

Center stationary. Asymmetric $x_1, x_3$ motion.

$$\omega^2 = \frac{k}{M} + 2\frac{k}{m}:$$

1. $$\cancel{-\frac{k}{M}x_1} - 2\frac{k}{m}x_1 = \frac{k}{M}x_2 \cancel{- \frac{k}{M}x_1}$$

$$\underline{\underline{x_2 = -2\frac{M}{m}x_1}}$$

3. $$\cancel{-\frac{k}{M}x_3} - 2\frac{k}{m}x_3 = -2\frac{k}{m}x_1 \cancel{- \frac{k}{M}x_2}$$

$$\underline{\underline{x_3 = x_1}}$$

The outer masses moving together. The center mass is moving opposite to them.

## Numerical calculations:

Be carefull about "ill-conditioned" systems. Rounding error may be multiplied by

$$K_{Turing} = n \, |A_{ij}|_{max} \, |A^{-1}_{ij}|_{max}$$

order of matrix Largest element

Largest element of inverse matrix.

---

## Functions of matrices:

Defined by series expansions. E.g.,

$$\exp(A) = \sum_{n=0}^{\infty} \frac{A^n}{n!}$$

Example: $\sigma_k$ Pauli matrix.

$$\exp(i\sigma_k \theta) = \sum_{n=0}^{\infty} (i)^n \frac{(\sigma_k\theta)^n}{n!}$$

$$(\sigma^k)^n = \begin{cases} \sigma^k & \text{for } n \text{ odd} \\ 1_2 & \text{for } n \text{ even} \end{cases}$$

$$\Rightarrow \quad \exp(i\sigma_k\theta) = \begin{cases} 1_2 \cos\theta \\ \sigma_k \sin\theta \end{cases}$$