Normalkoordinaten

$$\cdot a_k^{(i)} \Big| \quad K_{kj}\, a_j^{(l)} = \omega_{(l)}^2 M_{kj}\, a_j^{(l)}$$

$$\cdot a_j^{(l)} \Big| \quad K_{kj}\, a_k^{(i)} = \omega_{(i)}^2 M_{kj}\, a_k^{(i)}$$

$k \leftrightarrow j$
$K_{jk} = K_{kj}$, (M)
$l \to i$

$$\Rightarrow \left(\omega_{(l)}^2 - \omega_{(i)}^2\right) a_k^{(i)} M_{kj}\, a_j^{(l)} = 0$$

$$\Rightarrow a_k^{(i)} M_{kj}\, a_j^{(l)} = A_{ki} M_{kj} A_{jl} = A^T_{ik} M_{kj} A_{jl} = \delta_{il} \quad (\Delta)$$

falls $\omega_{(l)}^2$ nicht entartet — bei geeigneter Normierung

- bei Entartung, z.B. $\omega_1 = \omega_2 \to \alpha \vec{a}^{(1)} + \beta \vec{a}^{(2)}$ Eigenvektor
  α, β so wählen, dass (Δ) erfüllt ist

(Δ): (verallgemeinerte) Orthogonalitätsrelation

$\Leftrightarrow A^T M A = 1$, d.h. A diagonalisiert M

A diagonalisiert auch K:

$$A^T_{ik} K_{kj} A_{jl} = A^T_{ik}\left(\omega_{(l)}^2 M_{kj} A_{jl}\right) = \omega_{(l)}^2 \delta_{il} = \begin{pmatrix} \omega_1^2 & & & \\ & \omega_2^2 & & \\ & & \ddots & \\ & & & \omega_n^2 \end{pmatrix}$$

Normalkoordinaten Q_j:

$$x_i \equiv A_{ij} Q_j \quad \Leftrightarrow \quad Q_l = A^T_{lk} M_{ki}\, x_i$$
$$\left(= A^T_{lk} M_{ki} A_{ij} Q_j = \delta_{lj} Q_j = Q_l \checkmark\right)$$

$$2L = M_{ij}\dot{x}_i \dot{x}_j - K_{ij} x_i x_j = M_{ij} A_{ik} \dot{Q}_k A_{jl} \dot{Q}_l - K_{ij} A_{ik} Q_k A_{jl} Q_l =$$
$$= \delta_{kl} \dot{Q}_k \dot{Q}_l - \omega_{(k)}^2 \delta_{kl} Q_k Q_l = \sum_{k=1}^{n} \left(\dot{Q}_k^2 - \omega_{(k)}^2 Q_k^2\right)$$

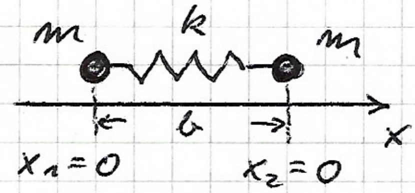
n entkoppelte Oszillatoren!

$\to$ Problem reduziert auf eindim. Schwingungen

Lsg. $Q_l = c_l \cos(\omega_l t + \alpha_l) \Rightarrow \underline{x_j = A_{jl} Q_l = \sum_l a_j^{(l)} c_l \cos(\omega_l t + \alpha_l)}$

- falls $\omega_\ell = 0 \Rightarrow \ddot{Q}_\ell = 0 \Rightarrow Q_\ell(t) = v_\ell t + c_\ell$

<u>Beispiel</u> 2-atomiges Molekül (1 dim)



$$L = \frac{m}{2}(\dot{x}_1^2 + \dot{x}_2^2) - \frac{k}{2}(x_1 - x_2)^2$$

$$= \frac{1}{2}(\dot{x}_1, \dot{x}_2)\underbrace{\begin{pmatrix} m & \\ & m \end{pmatrix}}_{M}\begin{pmatrix} \dot{x}_1 \\ \dot{x}_2 \end{pmatrix} - \frac{1}{2}(x_1, x_2)\underbrace{\begin{pmatrix} k & -k \\ -k & k \end{pmatrix}}_{K}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$$

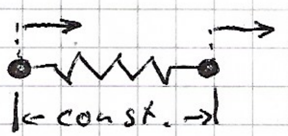
Eigenwertproblem: $(K - \omega^2 M)\vec{a} = 0$

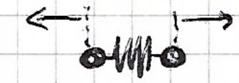
$$\det(K - \omega^2 M) = \det\begin{pmatrix} k - m\omega^2 & -k \\ -k & k - m\omega^2 \end{pmatrix} = (k - m\omega^2)^2 - k^2 =$$

$$= -2mk\omega^2 + m^2\omega^4 = m^2\omega^2\left(\omega^2 - \frac{2k}{m}\right) \stackrel{!}{=} 0$$

$$\Rightarrow \quad \underline{\omega_1 = 0, \qquad \omega_2 = \sqrt{\frac{2k}{m}}}$$

Feder k, reduzierte Masse $m/2$

Translation 

Schwingung 

Eigenvektoren: zu $\omega_1^2 = 0$ $\begin{pmatrix} k & -k \\ -k & k \end{pmatrix}\vec{a}^{(1)} = 0 \Rightarrow \vec{a}^{(1)} \sim \begin{pmatrix} 1 \\ 1 \end{pmatrix}$

zu $\omega_2^2 = \frac{2k}{m}$ $\begin{pmatrix} -k & -k \\ -k & -k \end{pmatrix}\vec{a}^{(2)} = 0 \Rightarrow \vec{a}^{(2)} \sim \begin{pmatrix} 1 \\ -1 \end{pmatrix}$

$$A := \frac{1}{\sqrt{2m}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = A^T \Rightarrow A^T M A = m A^T A = \frac{m}{2m}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}^2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \checkmark$$

Normalkoordinaten: $\vec{Q} = A^T M \vec{x} = \frac{m}{\sqrt{2m}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \sqrt{\frac{m}{2}}\begin{pmatrix} x_1 + x_2 \\ x_1 - x_2 \end{pmatrix}$

$Q_1 \sim$ Schwerpunktskoord. $\qquad Q_2 \sim$ Relativkoord.

$$L = \frac{1}{2}\sum_{i=1,2}(\dot{Q}_i^2 - \omega_i^2 Q_i^2); \quad \underline{Q_1 = v_1 t + c_1, \quad Q_2 = c_2\cos(\omega_2 t + \alpha_2)}$$

$$\vec{x} = A\vec{Q} = \frac{1}{\sqrt{2m}}\begin{pmatrix} Q_1 + Q_2 \\ Q_1 - Q_2 \end{pmatrix}$$