A Lagrange egyenletek:

általánosított koordináták:

$$\underline{x} = \{\underline{x}_1, \dots, \underline{x}_N\} = x_\nu \quad \text{holonom kényszerek}$$

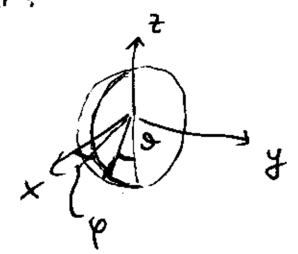
$$\Rightarrow \quad \exists \; \{q_1, \dots, q_f\} \;: \quad \underline{x}_i = \underline{x}_i(\{q_e\})$$

$$\text{v.} \quad = \underline{x}_i(\{q_e\}, t) \qquad e = 1, \dots, f$$

pl.: • merev test $\underline{R}$, $\{\vartheta, \varphi, \psi\}$ $\Leftrightarrow$ $\underline{x}$

• gömbfelületen mozgó tömegpont:

$$\underline{r} = R \begin{pmatrix} \sin\vartheta \cos\varphi \\ \sin\vartheta \sin\varphi \\ -\cos\vartheta \end{pmatrix}$$



sebesség:

$$\dot{\underline{x}}_i = \frac{\partial \underline{x}_i}{\partial q_e} \dot{q}_e + \frac{\partial \underline{x}_i}{\partial t} \qquad \left(\dot{x}_\nu = \frac{\partial x_\nu}{\partial q_e} \dot{q}_e + \frac{\partial x_\nu}{\partial t} \right)$$

gyorsulás:

$$\ddot{\underline{x}} = \frac{\partial \underline{x}}{\partial q_e} \ddot{q}_e + \frac{\partial^2 \underline{x}}{\partial q_e \partial q_m} \dot{q}_e \dot{q}_m + 2 \frac{\partial^2 \underline{x}}{\partial t \partial q_e} \dot{q}_e + \frac{\partial^2 \underline{x}}{\partial t^2}$$

fel tudjuk írni a Newton egyenleteket q_e-re?

D'Alembert:

$$\sum_i (m_i \ddot{\underline{x}}_i - \underline{F}_i)\, \delta \underline{x}_i^* = 0 \qquad \forall \text{ megengedett virtuális elm.-ra..}$$

$$\underline{x}_i(\{q_e\}, t) \quad \Rightarrow \quad \delta \underline{x}_i^* = \sum_e \frac{\partial \underline{x}_i}{\partial q_e} \delta q_e$$

$$\sum_{i,e} m_i \ddot{\underline{x}}_i \frac{\partial \underline{x}_i}{\partial q_e} \delta q_e = \sum_e \Big(\underbrace{\sum_i \underline{F}_i \frac{\partial \underline{x}_i}{\partial q_e}}_{\equiv\, Q_e} \Big) \delta q_e = \sum_e Q_e \delta q_e$$

általánosított erő

$$\sum_i \left\{ \frac{d}{dt}\left(m_i \dot{\underline{x}}_i \frac{\partial \underline{x}_i}{\partial q_e} \right) - m_i \dot{\underline{x}}_i \underbrace{\frac{d}{dt} \frac{\partial \underline{x}_i}{\partial q_e}} \right\}$$

$$= \frac{\partial \dot{\underline{x}}_i}{\partial \dot{q}_e} \qquad \dot{\underline{x}}_i = \dot{\underline{x}}_i(\{q_e\}, \{\dot{q}_e\}, t)$$

első $\Rightarrow \dfrac{d}{dt} \dfrac{\partial}{\partial \dot{q}_e} \left(\sum_i \frac{1}{2} m_i \dot{\underline{x}}_i^2 \right)$

áll.: $$\frac{d}{dt}\frac{\partial \underline{x}_i}{\partial q_e} = \frac{\partial}{\partial q_e}\frac{d}{dt}\underline{x}_i = \frac{\partial \dot{\underline{x}}_i}{\partial q_e}$$

$$\frac{d}{dt}\underbrace{\frac{\partial \underline{x}_i}{\partial q_e}}_{f(\{q_e\},t)} = \left(\frac{\partial}{\partial t} + \dot{q}_k\frac{\partial}{\partial q_k}\right)\frac{\partial}{\partial q_e}\underline{x}_i = \frac{\partial}{\partial q_e}\left(\frac{\partial}{\partial t} + \dot{q}_n\frac{\partial}{\partial q_n}\right)\underline{x}_i = \frac{\partial}{\partial q_e}\frac{d\underline{x}_i}{dt}$$

így $$-\sum_i m_i \dot{\underline{x}}_i \frac{d}{dt}\frac{\partial \underline{x}_i}{\partial q_e} = -\sum_i m_i \dot{\underline{x}}_i \frac{\partial \dot{\underline{x}}_i}{\partial q_e} = -\frac{\partial}{\partial q_e}\sum_i m_i \frac{1}{2}\dot{\underline{x}}_i^2$$

tehát

$$\sum_i \left(m_i \ddot{\underline{x}}_i - \underline{F}_i\right)\delta \underline{x}_i^* = \sum_e \left\{\frac{d}{dt}\frac{\partial K}{\partial \dot{q}_e} - \frac{\partial K}{\partial q_e} - Q_e\right\}\delta q_e \underset{\uparrow}{=} 0$$

$\forall\, \delta q_e$-re!

$$\boxed{\frac{d}{dt}\frac{\partial K}{\partial \dot{q}_e} - \frac{\partial K}{\partial q_e} = Q_e}$$ Lagrange egyenletek

Ha $$\underline{F}_i = -\frac{\partial U}{\partial \underline{x}_i} \Rightarrow Q_e = -\sum_i \frac{\partial U}{\partial \underline{x}_i}\frac{\partial \underline{x}_i}{\partial q_e} = -\frac{\partial U}{\partial q_e}$$

akkor

$$\frac{d}{dt}\frac{\partial K}{\partial \dot{q}_e} - \frac{\partial (K-U)}{\partial q_e} = 0 \qquad \text{de} \quad \frac{\partial U}{\partial \dot{q}_e} = 0$$

$$\Rightarrow \boxed{\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_e} - \frac{\partial L}{\partial q_e} = 0} \qquad \boxed{L = K - U}$$ Lagrange fv.

$L(\{q_e\},\{\dot{q}_e\},t)$

pl.: gömbinga:

$$\dot{\underline{x}} = R\begin{pmatrix}\cos\vartheta\cos\varphi\\ \cos\vartheta\sin\varphi\\ \sin\vartheta\end{pmatrix}\dot{\vartheta} + R\begin{pmatrix}-\sin\vartheta\sin\varphi\\ \sin\vartheta\cos\varphi\\ 0\end{pmatrix}\dot{\varphi}$$

$$\Rightarrow K = \frac{1}{2}m\dot{\underline{x}}^2 = \frac{mR^2}{2}\left(\dot{\vartheta}^2 + \sin^2\vartheta\,\dot{\varphi}^2\right)$$

$$U = mgz = -mgR\cos\vartheta$$

$$L = K - U = \frac{mR^2}{2}\left(\dot\vartheta^2 + \sin^2\vartheta\,\dot\varphi^2\right) + mgR\cos\vartheta$$

$L(\dot\vartheta, \dot\varphi, \cancel{\varphi}, \vartheta)$ ciklikus vált. $\Rightarrow$

$$\Rightarrow \quad \frac{d}{dt}\frac{\partial L}{\partial\dot\varphi} = \frac{\partial L}{\partial\varphi} = \text{cst} \qquad \frac{d}{dt}\underbrace{\left(mR^2\sin^2\vartheta\,\dot\varphi\right)}_{\text{cst} \,\equiv\, L_z} = \emptyset$$

$$\frac{d}{dt}\frac{\partial L}{\partial\dot\vartheta} = \frac{\partial L}{\partial\vartheta} \quad \Rightarrow \quad mR^2\ddot\vartheta = -mgR\cos\vartheta + mR^2\sin\vartheta\cos\vartheta\,\dot\varphi^2$$

$$mR^2\ddot\vartheta = -mgR\cos\vartheta + \frac{L_z^2}{mR^2}\frac{\cos\vartheta}{\sin^3\vartheta}$$

Ciklikus vált: $\quad q_\ell$ ciklikus, ha $\dfrac{\partial L}{\partial q_\ell} = 0 \Rightarrow \boxed{p_\ell \equiv \dfrac{\partial L}{\partial\dot q_\ell} = \text{cst}}$

ált. impulzus

p_ℓ ált. impulzus ?

tömegpont: $\quad L = \frac{1}{2}m\dot{\underline{x}}^2 - U(\underline{x}) \Rightarrow \underline{p} = m\dot{\underline{x}}$ ✓

Energiamegmaradás: (Jacobi-féle integrál)

$$\frac{dL}{dt} = \frac{dL(q,\dot q,t)}{dt} = \dot q\frac{\partial L}{\partial q} + \ddot q\frac{\partial L}{\partial\dot q} + \frac{\partial L}{\partial t} = \frac{d}{dt}\left(\dot q\frac{\partial L}{\partial\dot q}\right) + \dot q\left(\frac{\partial L}{\partial q} - \dot q\frac{\partial L}{\partial\dot q}\right) + \frac{\partial L}{\partial t}$$

$$\frac{d}{dt}\left(\dot q\frac{\partial L}{\partial\dot q}\right) - \dot q\frac{d}{dt}\frac{\partial L}{\partial\dot q}$$

$$\Rightarrow \quad \frac{d}{dt}\left(\dot q\frac{\partial L}{\partial\dot q} - L\right) = -\frac{\partial L}{\partial t}$$

$$\boxed{E \equiv \dot q\frac{\partial L}{\partial\dot q} - L} \qquad \text{ha } \frac{\partial L}{\partial t} = 0 \Rightarrow \frac{dE}{dt} = 0$$

$$\boxed{\frac{dE}{dt} = -\frac{\partial L}{\partial t}}$$

időben homogén világ

Állítás: $\quad E \Longleftrightarrow$ energia $\quad$ t.f.h. $\quad \underline{x}_i = \underline{x}_i(q, \cancel{t})$

ekkor $\quad K = \frac{1}{2}\sum_i m_i\dot{\underline{x}}_i^2 = \frac{1}{2}\sum_{i,\ell,\ell'} m_i\,\dot q_\ell\,\dot q_{\ell'}\,\frac{\partial\underline{x}_i}{\partial q_\ell}\cdot\frac{\partial\underline{x}_i}{\partial q_{\ell'}}$

$$K = \frac{1}{2} \sum_{e,e'} \dot{q}_e \, M_{ee'}(\underline{q}) \, \dot{q}_{e'} \qquad \text{ahol} \qquad M_{ee'} = \sum_i m_i \frac{\partial \underline{x}_i}{\partial q_e} \frac{\partial \underline{x}_i}{\partial q_{e'}}$$

$M(\underline{q})$ valós, szimmetrikus, poz. def.

$$K(\alpha \dot{\underline{q}}, \underline{q}) = \alpha^2 K(\dot{\underline{q}}, \underline{q}) \qquad K \ \dot{\underline{q}}\text{-nak homogén másodrendű fv.-e}$$

$$\Rightarrow (\text{Euler}) \qquad \dot{\underline{q}} \cdot \frac{\partial K}{\partial \dot{\underline{q}}} = 2K$$

Euler: $f(\underline{x}, \underline{y})$: ha $f(\alpha \underline{x}, \underline{y}) = \alpha^p f(\underline{x}, \underline{y}) \Rightarrow \underline{x} \frac{\partial f}{\partial \underline{x}} = p f$

akkor $\frac{d}{d\alpha} f(\alpha \underline{x}, \underline{y}) \Big|_{\alpha=1} = \underline{x} \frac{\partial f}{\partial \underline{x}}(\alpha \underline{x}, \underline{y}) \Big|_{\alpha=1} = \underline{x} \cdot \frac{\partial f}{\partial \underline{x}} = p \alpha^{p-1} f(\underline{x}, \underline{y}) \Big|_{\alpha=1}$

$$\Rightarrow \qquad \underline{x} \frac{\partial f}{\partial \underline{x}} = p \, f(\underline{x}, \underline{y})$$

explicit bizonyítás: $\frac{\partial K}{\partial \dot{q}_m} = \sum_e \frac{1}{2} \dot{q}_e M_{em} + \frac{1}{2} \sum_{e'} M_{me'} \dot{q}_{e'} = \sum_{e'} M_{me'} \dot{q}_{e'}$

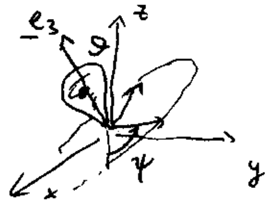
$$\sum_m \dot{q}_m \frac{\partial K}{\partial \dot{q}_m} = \sum_{m,e'} \dot{q}_m M_{me'} \dot{q}_{e'} = 2K$$

ekkor tehát

$$E = \dot{\underline{q}} \cdot \frac{\partial L}{\partial \dot{\underline{q}}} - L = \dot{\underline{q}} \frac{\partial K}{\partial \dot{\underline{q}}} - L = 2K - (K - U) = K + U \ \checkmark$$

Példa: súlyos szimmetrikus pörgettyű

Euler szögek ϑ, φ, ψ ; $I_1 = I_2$; I_3



$$\Rightarrow \Omega_1 = \dot\vartheta \cos\psi + \dot\varphi \sin\vartheta \sin\psi$$
$$\Omega_2 = -\dot\vartheta \sin\psi + \dot\varphi \sin\vartheta \cos\psi$$
$$\Omega_3 = \dot\psi + \dot\varphi \cos\vartheta$$

$$K = \frac{I_1}{2}\left(\Omega_1^2 + \Omega_2^2\right) + \frac{I_3}{2}\Omega_3^2 \quad ; \quad U = mgh\cos\vartheta$$

$$L = K - U = \frac{I_1}{2}\left(\dot\vartheta^2 + \dot\varphi^2 \sin^2\vartheta\right) + \frac{I_3}{2}\left(\dot\psi + \dot\varphi\cos\vartheta\right)^2 - mgh\cos\vartheta$$

φ, ψ ciklikus változók $\Leftrightarrow$ $\underline{e}_z$ ill. $\underline{e}_3$ körüli forg.
(Euler!)

$$p_\psi = I_3\left(\dot\psi + \dot\varphi\cos\vartheta\right) \equiv M_3 = \text{cst}$$

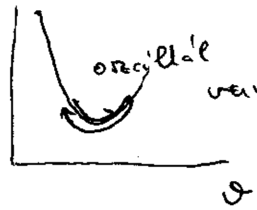
$$p_\varphi = I_1\dot\varphi\sin^2\vartheta + I_3\cos\vartheta\left(\dot\psi + \dot\varphi\cos\vartheta\right) \equiv M_z = \text{cst}$$

energia: $E = K + U$ $\qquad \dot\varphi = \dfrac{M_z - M_3\cos\vartheta}{I_1\sin^2\vartheta}$

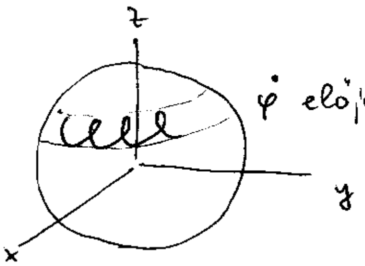
$$\Rightarrow E = \frac{I_1}{2}\dot\vartheta^2 + \underbrace{\frac{1}{2I_1}\frac{\left(M_z - M_3\cos\vartheta\right)^2}{\sin^2\vartheta} + mgh\cos\vartheta}_{U_{eff}(\vartheta)} + \cancel{\frac{M_3^2}{2I_3}}$$

gyors pörg: $\dfrac{M_z^2}{2I_1} \gg mgh$

$\Rightarrow$ általában $M_z \neq M_3$



$\Rightarrow$



„alvó pörgettyű” $\vartheta = 0$: $M_z = M_3$ stabil-e?

$$U_{eff} \approx \text{cst} + \left(\frac{M_3^2}{8I_1} - \frac{mgh}{2}\right)\vartheta^2 + \dots$$

$M_3 < \sqrt{4 I_1 mgh}$ $\Rightarrow$ instabillá válik...

Anholonom kényszerek:

s holonom kényszer $\Rightarrow$ $f = 3N - s$ szab. fok

$q_1, \dots, q_f$

további s' kényszerek $\Rightarrow$ q_e-ek nem függetlenek...

$$\sum_i \underline{a}_i^k \delta \underline{x}_i^* = \emptyset \qquad k = 1, \dots, s' \qquad \Rightarrow \sum_e \underbrace{\sum_i \underline{a}_i^k \frac{\partial \underline{x}_i}{\partial q_e}}_{= A_e^k} \delta q_e^*$$

$$\Rightarrow \qquad \underline{A}^k \cdot \delta \underline{q}^* = 0 \qquad k = 1, \dots, s'$$

D'Alembert:

$$\sum_i \left(m_i \ddot{\underline{x}}_i - \underline{F}_i \right) \delta \underline{x}_i^* = 0 \qquad \Rightarrow \qquad \sum_e \left(\frac{d}{dt} \frac{\partial K}{\partial \dot{q}_e} - \frac{\partial K}{\partial q_e} - Q_e \right) \delta q_e^* = \emptyset$$

minden meg. elm.

vektorjel.: $\left(\frac{d}{dt} \frac{\partial K}{\partial \dot{\underline{q}}} - \frac{\partial K}{\partial \underline{q}} - \underline{Q} \right) \delta \underline{q}^* = 0$

$\forall\ \delta \underline{q}^*$-ra, ha $\underline{A}^k \cdot \delta \underline{q}^* = 0$ $\forall\ k$-ra

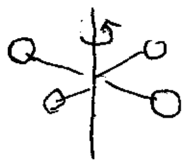
$$\Rightarrow \qquad \frac{d}{dt} \frac{\partial K}{\partial \dot{\underline{q}}} - \frac{\partial K}{\partial \underline{q}} - \underline{Q} \in \underline{A}^k\text{-k által kif. tér}$$

$$\Rightarrow \qquad \boxed{\frac{d}{dt} \frac{\partial K}{\partial \dot{\underline{q}}} - \frac{\partial K}{\partial \underline{q}} = \underline{Q} + \underline{R}}$$

kényszerek

$$\underline{R} = \sum_k \lambda_k \underline{A}^k$$

Disszipáció pl. forgó szélkakas



t.f.h. $\exists\ D(\{\dot{\underline{x}}_i\}, \{\underline{x}_i\}, t) = D(\underline{x}, \dot{\underline{x}}, t)$

$$\underline{S}_i = -\frac{\partial D}{\partial \dot{\underline{x}}_i} \qquad \text{pl.: } \underline{S}_i = -\eta_i(\underline{x}_i) \dot{\underline{x}}_i \Rightarrow D = \sum_i \frac{\eta_i}{2} \dot{\underline{x}}_i^2$$

súrlódási erő

holonom kényszerek $\Rightarrow$ $\underline{x}_i = \underline{x}_i(\underline{q}, t)$ $\qquad \underline{q} = \{q_1, \dots, q_f\}$

D'Alembert: $\sum_i \left(m_i \ddot{\underline{x}}_i - \underline{F}_i - \underline{S}_i \right) \delta \underline{x}_i^* = 0$ $\forall$ megeng. $\delta \underline{x}_i^*$-ra

$$\Rightarrow \qquad \underbrace{\sum_i \left(m_i \ddot{\underline{x}}_i - \underline{F}_i \right) \delta \underline{x}_i^*}_{\rightarrow \left(\frac{d}{dt} \frac{\partial K}{\partial \dot{\underline{q}}} - \frac{\partial K}{\partial \underline{q}} - \underline{Q} \right) \delta \underline{q}} = \sum_i \underline{S}_i \delta \underline{x}_i^*$$

$$\delta \underline{x}_i^* = \sum_e \frac{\partial \underline{x}_i}{\partial q_e} \delta q_e$$

$$\sum_i \underline{s}_i \cdot \delta \underline{x}_i^* = -\sum_{i,e} \frac{\partial D}{\partial \dot{\underline{x}}_i} \underbrace{\frac{\partial \underline{x}_i}{\partial q_e}}_{\frac{\partial \dot{\underline{x}}_i}{\partial \dot{q}_e}} \delta q_e = -\frac{\partial D}{\partial \dot{q}} \cdot \delta q^*$$

$$\Rightarrow \left(\frac{d}{dt} \frac{\partial K}{\partial \dot{q}} - \frac{\partial K}{\partial q} - Q + \frac{\partial D}{\partial \dot{q}} \right) \delta q = 0 \qquad \forall\ \delta q\text{-ra}$$

$$\Rightarrow \boxed{\frac{d}{dt} \frac{\partial K}{\partial \dot{q}} - \frac{\partial K}{\partial q} = Q - \frac{\partial D}{\partial \dot{q}}} \quad (*) \qquad D(\dot{q}, q, t)$$

ált. súrlódási erő

Energiamegmaradás?

t.f.h. $\quad Q = -\frac{\partial U}{\partial q} \qquad L = K - U \qquad$ akkor

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{q}} = \frac{\partial L}{\partial q} - \frac{\partial D}{\partial \dot{q}}$$

$$\Rightarrow \frac{d}{dt}\left(\dot{q} \frac{\partial L}{\partial \dot{q}} - L \right) = \cancel{\ddot{q} \frac{\partial L}{\partial \dot{q}}} + \dot{q} \frac{d}{dt} \frac{\partial L}{\partial \dot{q}} - \frac{\partial L}{\partial t} - \dot{q} \frac{\partial L}{\partial q} - \cancel{\ddot{q} \frac{\partial L}{\partial \dot{q}}} =$$

$$= -\frac{\partial L}{\partial t} - \dot{q} \frac{\partial D}{\partial \dot{q}}$$

$$\boxed{\frac{dE}{dt} = -\frac{\partial L}{\partial t} - \dot{q} \frac{\partial D}{\partial \dot{q}}}$$

disszipatív tag!

a fenti példában $\quad D(\alpha \dot{q}, q, t) = \alpha^2 D(\dot{q}, q, t)$

$$q \rightarrow \underline{x}_i(q, \cancel{t})$$

$$\Rightarrow \quad \dot{q} \frac{\partial D}{\partial \dot{q}} = 2D \geq 0$$

• Sebességfüggő erők ~ néha beépíthetők L-be

töltött részecske elektromágneses térben

$$\boxed{m\ddot{\underline{x}} = q\underline{E} + q\underline{v}\times\underline{B}}$$

$\underline{E}(\underline{r},t)$ $\underline{B}(\underline{r},t)$

Maxwell : $\mathrm{div}\,\underline{E} = \frac{1}{\epsilon_0}\varrho$; $\mathrm{div}\,\underline{B} = 0$

$\mathrm{rot}\,\underline{E} = -\frac{\partial \underline{B}}{\partial t}$ $\mathrm{rot}\,\underline{B} = \mu_0 \underline{j} + \mu_0\epsilon_0\frac{\partial \underline{E}}{\partial t}$

$\mathrm{div}\,\underline{B} = 0 \Rightarrow \underline{B} = \mathrm{rot}\,\underline{A} \Rightarrow \mathrm{rot}(\underline{E} + \dot{\underline{A}}) = 0 \Rightarrow$

$\Rightarrow \underline{E} + \dot{\underline{A}} = -\mathrm{grad}\,\phi \Rightarrow \underline{E} = -\mathrm{grad}\,\phi - \frac{\partial \underline{A}}{\partial t}$

Áll.: $$\boxed{L = \frac{m}{2}\dot{\underline{x}}^2 - q\,\phi(\underline{x},t) + q\,\dot{\underline{x}}\cdot\underline{A}(\underline{x},t)}$$

nézzük az x koordinátát

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{x}} = \frac{\partial L}{\partial x} \Rightarrow \frac{d}{dt}\left(m\dot{x} + q\,A_x(\underline{x},t)\right) = -q\frac{\partial\phi}{\partial x} + q\dot{x}\frac{\partial A_x}{\partial x} + q\dot{y}\frac{\partial A_y}{\partial x} + q\dot{z}\frac{\partial A_z}{\partial x}$$

$$m\ddot{x} + q\left(\frac{\partial A_x}{\partial t} + \dot{x}\frac{\partial A_x}{\partial x} + \dot{y}\frac{\partial A_x}{\partial y} + \dot{z}\frac{\partial A_x}{\partial z}\right) = -q\frac{\partial\phi}{\partial x} + q\left(\dot{x}\frac{\partial A_x}{\partial x} + \ldots\right)$$

$$m\ddot{x} = \underbrace{\left(-\partial_x\phi - \dot{A}_x\right)}_{E_x} q + q\left\{\dot{y}\underbrace{\left(\partial_x A_y - \partial_y A_x\right)}_{(\mathrm{rot}\,\underline{A})_z = B_z} - \dot{z}\underbrace{\left(\partial_z A_x - \partial_x A_z\right)}_{(\mathrm{rot}\,\underline{A})_y = B_y}\right\}$$

$$m\ddot{x} = E_x q + q\underbrace{\left(\dot{y}B_z - \dot{z}B_y\right)}_{(\dot{\underline{x}}\times\underline{B})_x}$$

$$m\ddot{\underline{x}} = \underline{E}q + q\,\dot{\underline{x}}\times\underline{B} \quad \checkmark$$

$\Rightarrow$ • impulzus $\boxed{\underline{p} = \frac{\partial L}{\partial \dot{\underline{x}}} = m\dot{\underline{x}} + q\underline{A}}$

kinetikus vektorpot...

• energia: $E \overset{?}{=} \dot{\underline{x}}\frac{\partial L}{\partial \dot{\underline{x}}} - L = \frac{1}{2}m\dot{\underline{x}}^2 + q\phi$

nem marad meg ált. ... $\frac{dE}{dt} = -\frac{\partial L}{\partial t} = -q\partial_t\phi + q\underline{v}\,\partial_t\underline{A}$

• $\underline{A}$, ϕ nem rögzíthető (mérték) $\Rightarrow$ L nem egyért.

Rezgések:

molekula ~ hogyan rezeg?

vagy

q_ℓ ált. koordináták ; $q = \{q_1, \dots, q_f\}$

$$K = \frac{1}{2} \sum_{\ell,m} \dot{q}_\ell \, G_{\ell m}(q) \, \dot{q}_m = \frac{1}{2} \dot{q} M \dot{q}$$

$$\boxed{L = \frac{1}{2} \dot{q} \underbrace{G(q)}_{\text{"tömegmátrix"}} \dot{q} - V(q)}$$

$$G_{\ell m}(q) = \sum_i m_i \frac{\partial x_i}{\partial q_\ell} \frac{\partial x_i}{\partial q_m}$$

egyensúly: $\frac{\partial V}{\partial q} = 0 \quad \Rightarrow \quad q = q_0 + \eta \ ; \ \dot{q} = \dot{\eta}$

$$V(q) = V(q_0) + \underbrace{\frac{\partial V(q_0)}{\partial q}}_{= \emptyset} \eta + \frac{1}{2} \eta \underbrace{\frac{\partial^2 V(q_0)}{\partial q \, \partial q}}_{D} \eta + \dots$$

$$D_{\ell m} \equiv \frac{\partial^2 V}{\partial q_\ell \partial q_m}(q_0)$$

$$L \approx \frac{1}{2} \dot{\eta} \overbrace{G(q_0)}^{M} \dot{\eta} - \frac{1}{2} \eta D \eta + cst + \mathcal{O}(\eta^3)$$

$$\boxed{L \approx \frac{1}{2} \dot{\eta} G \dot{\eta} - \frac{1}{2} \eta D \eta}$$

G : szimmetrikus, valós, poz. definit

D : " , " , poz. szemidefinit

mozgásegyenlet:

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{\eta}} - \frac{\partial L}{\partial \eta} = 0 \quad \Rightarrow \quad M \ddot{\eta} + D \eta = 0$$

keressük a megoldást $\eta = \psi \, \mathrm{Re}\{e^{-i\omega t}\}$ alakban

$$\Rightarrow \quad (\omega^2 M - D) \psi = 0 \quad \Rightarrow \quad \boxed{\det\{\omega^2 M - D\} = \emptyset}$$

M, D valós, szimm, poz. def. $\Rightarrow$ $\omega_\mu^2 \geq 0$ valós ✓

ω_μ^2 : $\det(\omega_\mu^2 M - D) = 0 \Rightarrow \exists \, \psi_\mu$ valós, $\boxed{(\omega_\mu^2 M - D)\psi_\mu = 0}$

állítás: $\omega_\mu^2 \neq \omega_\nu^2 \Rightarrow \psi_\mu M \psi_\nu = \emptyset$

biz.: $\psi_\mu (\omega_\nu^2 M - D) \psi_\nu = 0$

$\psi_\nu (\omega_\mu^2 M - D) \psi_\mu = 0$ $\Rightarrow$ $(\omega_\mu^2 - \omega_\nu^2) \psi_\nu M \psi_\mu = 0$ ✓

↑ D, M szimmetrikus ~ $\psi_\mu D \psi_\nu = \psi_\nu D \psi_\mu$

így ψ_μ normálható : $\boxed{\psi_\mu M \psi_\nu = \delta_{\mu\nu}}$ $\left(\frac{\psi_\nu}{\sqrt{\psi_\nu M \psi_\nu}} \to \psi_\nu \right)$

ekkor $\Psi_\mu\left(\omega_\mu^2 M \Psi_\mu - D\Psi_\mu\right) = 0 = \omega_\mu^2 - \Psi_\mu D \Psi_\mu$

tehát $\underline{\Psi_\mu D \Psi_\mu = \omega_\mu^2}$; és hasonlóan $\Psi_\mu D \Psi_\nu = \emptyset$
ha $\mu \neq \nu$

$$\eta \equiv \sum_\mu \Psi_\mu \Theta_\mu$$

$$\Rightarrow \quad L = \frac{1}{2}\sum_{\mu,\nu} \overbrace{\underbrace{\dot\Theta_\mu \Psi_\mu}_{\dot\eta} M \underbrace{\Psi_\nu \dot\Theta_\nu}_{\dot\eta}}^{\delta_{\mu\nu}} - \frac{1}{2}\sum_{\mu,\nu} \overbrace{\underbrace{\Theta_\mu \Psi_\mu}_{\eta} D \underbrace{\Psi_\nu \Theta_\nu}_{\eta}}^{\delta_{\mu\nu}\cdot\omega_\mu^2}$$

$$\boxed{L = \frac{1}{2}\sum_\mu \left(\dot\Theta_\mu^2 - \omega_\mu^2 \Theta_\mu^2\right)}$$

Θ_μ : normálkoordináta , $\boxed{\ddot\Theta_\mu + \omega_\mu^2 \Theta_\mu = 0}$

Ψ_μ : normálmódus

$$\Rightarrow \quad \boxed{\eta(t) = \sum_\mu \Psi_\mu \, \mathrm{Re}\left\{\Theta_\mu(0) e^{-i\omega_\mu t}\right\}}$$

komplex

ω_μ : rezgés frekvenciája

<u>Egyszerű példa:</u>

$$L = \frac{m_1}{2}\dot\eta_1^2 + \frac{m_2}{2}\dot\eta_2^2 - \frac{D_0}{2}(\eta_1 - \eta_2)^2$$

$$\det\left|M\omega^2 - D\right| = \begin{vmatrix} m_1\omega^2 - D_0 & D_0 \\ D_0 & m_2\omega^2 - D_0 \end{vmatrix} = m_1 m_2 \omega^4 - (m_1+m_2) D_0 \omega^2$$

$$D = \begin{pmatrix} D_0 & -D_0 \\ -D_0 & D_0 \end{pmatrix}$$

$\underline{\omega_1^2 = 0} \Rightarrow \Psi_1 := \begin{pmatrix} 1 \\ 1 \end{pmatrix} \xrightarrow{\text{norm}} \Psi_1 M \Psi_1 = m_1 + m_2 \Rightarrow \underline{\Psi_1 = \frac{1}{\sqrt{m_1+m_2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}}$

$\underline{\omega_2} = \left(\frac{m_1+m_2}{m_1 m_2} D_0\right)^{1/2} \Rightarrow \left(\frac{m_1}{m_2}, 1\right)\cdot\Psi_2 = \emptyset \Rightarrow \Psi_2 = \frac{1}{\sqrt{m_1 m_2 (m_1+m_2)}}\begin{pmatrix} m_2 \\ -m_1 \end{pmatrix}$

redukált tömeg

ellenőrzés $\Psi_1 M \Psi_2 = \emptyset$ ✓

$$\boxed{\eta(t) = \Psi_1 \overbrace{\Theta_1(t)}^{a+bt} + \Psi_2 \overbrace{\Theta_2(t)}^{A\cos(\omega_2 t + \delta)}}$$

transzláció rezgés

Molekulák rezg. spektruma

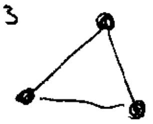
transzláció - rotáció $\Rightarrow$ 0 - módusok

pl.: H_2

5 db 0 - módus (6 szab. fok)

1 db rezgés

O_3



6 db 0 - módus

2 +1 rezg módus

$\uparrow$ degenerácio szimmetriából köv.! (D_{3v}) $\Longleftrightarrow$ csoportelm.

hogyan látjuk ezeket?

- fajhő
- fényszórás (Raman, infra ..)

nehéz: $\hbar \omega_{f\acute{e}ny} \gg \hbar \omega_r$

Noether - tétel köv. (köv oldal folyt.

$$\boxed{L = \sum_i \frac{m_i}{2} \dot{\underline{x}}_i^2 - U(\{\underline{x}_i\})}$$

① transzláció $\underline{x}_i \to \underline{x}_i + s\,\underline{n}$

$$\sum_i \frac{\partial L}{\partial \dot{\underline{x}}_i} \frac{\partial \underline{x}_i}{\partial s} = \left(\sum_i m_i \dot{\underline{x}}_i \right) \cdot \underline{n} = \text{cst} \qquad \boxed{\underline{P} \cdot \underline{n} = \text{cst}}$$

② forgásinvariancia:

$$\underline{x}_i \to \underline{x}_i + ds\, \underline{n} \times \underline{x}_i$$

$$\Rightarrow \sum_i m_i \dot{\underline{x}}_i \cdot (\underline{n} \times \underline{x}_i) = \sum_i m_i (\dot{\underline{x}}_i, \underline{n}, \underline{x}_i) = \sum_i \underline{n} \cdot (\underline{x}_i \times m_i \dot{\underline{x}}_i) = \underbrace{\underline{n} \cdot \underline{L}}_{= \text{cst}}$$

$$\boxed{\underline{n} \cdot \underline{L} = \text{cst}}$$

- térelméletek (kiterjesztés ..)
- akkor is működik, ha $L(Q, \dot{Q}, t) = L(q, \dot{q}, t) + \frac{df(q)}{dt}$

A Lagrange-fv. szimmetriái, Noether tétel

tegyük fel, hogy van egy leképezésünk:

$$Q : \underset{\uparrow\,\text{paraméter}}{s}, q \to Q(q,s) \qquad Q(q,0) = q$$

ez $\forall$ pályához hozzárendel egy másikat

$Q(t) = Q(q(t),s)$

$q(t),\ \dot q(t)$

$$q(t) \to Q(t) = Q(q(t),s)$$

$$\dot q(t) \to \dot Q(t) = \frac{\partial Q}{\partial q}\cdot \dot q$$

tegyük fel, hogy $\boxed{L(Q,\dot Q,t) = L(q,\dot q,t)}$ $\forall$ s-re, q-ra, $\dot q$-ra

Áll: ekkor $Q(t)$ is megoldása a Lagrange egyenleteknek

biz.: (1) érezzük...

(2) $Q(t) = Q(q(t),s)$; $\dot Q(t) = \dot Q(q(t),\dot q(t),s)$

$$(*) \quad \frac{\partial L}{\partial q_k} = \frac{\partial L(Q,\dot Q,t)}{\partial q_k} = \frac{\partial L}{\partial Q}\frac{\partial Q}{\partial q_k} + \frac{\partial L}{\partial \dot Q}\frac{\partial \dot Q}{\partial q_k}$$

$$(**) \quad \frac{d}{dt}\frac{\partial L}{\partial \dot q_k} = \frac{d}{dt}\frac{\partial L(Q,\dot Q,t)}{\partial \dot q_k} = \frac{d}{dt}\frac{\partial L}{\partial \dot Q}\underbrace{\frac{\partial \dot Q}{\partial \dot q_k}}_{\frac{\partial Q}{\partial q_k}} = \left(\frac{d}{dt}\frac{\partial L}{\partial \dot Q}\right)\cdot\frac{\partial Q}{\partial q_k} + \frac{\partial L}{\partial \dot Q}\underbrace{\frac{d}{dt}\frac{\partial Q(q,s)}{\partial q_k}}_{\text{áll.}\ = \frac{\partial}{\partial q_k}\frac{dQ}{dt}}$$

$$-(*) + (**) = \quad 0 \quad = \left(\frac{d}{dt}\frac{\partial L}{\partial \dot Q} - \frac{\partial L}{\partial Q}\right)\frac{\partial Q}{\partial q_k} \qquad \forall\ k\text{-ra}$$

$$\Rightarrow \quad \frac{d}{dt}\frac{\partial L}{\partial \dot Q} = \frac{\partial L}{\partial Q} \qquad \square$$

Áll. $\boxed{\frac{d}{dt}\left(\frac{\partial L}{\partial \dot q}\cdot\frac{\partial Q}{\partial s}\right)\Bigg|_{s=0} = 0}$ Noether-tétel

biz.: $L(t,s) \equiv L(\underset{\uparrow}{Q(t)}, \underset{\uparrow}{\dot Q(t)}, t) = L(Q(q(t),s), \dot Q(q,\dot q,s), t)$
impl. függvények

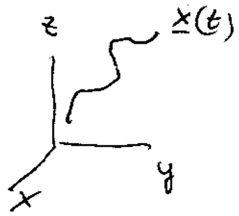
$$0 = \frac{\partial L}{\partial s} = \frac{\partial L}{\partial Q}\frac{\partial Q}{\partial s} + \frac{\partial L}{\partial \dot Q}\underbrace{\frac{\partial \dot Q}{\partial s}}_{\frac{d}{dt}\frac{\partial Q}{\partial s}} = \frac{\partial L}{\partial Q}\frac{\partial Q}{\partial s} + \frac{d}{dt}\left(\frac{\partial L}{\partial \dot Q}\frac{\partial Q}{\partial s}\right) - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot Q}\right)\frac{\partial Q}{\partial s}$$

$$= \left(\frac{\partial L}{\partial Q} - \frac{d}{dt}\frac{\partial L}{\partial \dot Q}\right)\frac{\partial Q}{\partial s} + \frac{d}{dt}\left(\frac{\partial L}{\partial \dot Q}\frac{\partial Q}{\partial s}\right)$$

$$s \to \quad \underbrace{\left(\frac{\partial L}{\partial q} - \frac{d}{dt}\frac{\partial L}{\partial \dot q}\right)}_{0}\frac{\partial Q}{\partial s} + \frac{d}{dt}\left(\frac{\partial L}{\partial \dot Q}\frac{\partial Q}{\partial s}\right)\Bigg|_{s=0} = 0 \qquad \square$$

Hamilton-elv; a legkisebb hatás elve

Funkcionál: $F[q(t)] \to \mathbb{R}$



példa: görbe hossza

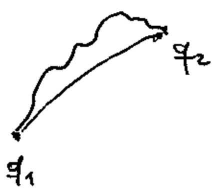
$\underline{x}(t)$ $\uparrow$ param $\quad t \in [0,1]$ $\Longrightarrow$ $\displaystyle\int_0^1 \sqrt{\left(\frac{dx}{dt}\right)^2} \cdot dt$

melyik két pont között a legrövidebb út?

Hatás: $$\boxed{S = S[q(t), t_1, t_2] \equiv \int_{t_1}^{t_2} dt \; L(q(t), \dot{q}(t), t)}$$

Áll.: S extremális arra a pályára mely megoldása a mozgásegy.-nek (legkisebb hatás elve! v. Hamilton elv)

biz.: legyen $q(t)$ tetsz. $q(t_1) = q_1$, $q(t_2) = q_2$



$Q(t) \equiv q(t) + \delta q(t)$

$\uparrow$ inf. pici tetsz. fv. $\qquad \delta q(t_1) = \delta q(t_2) = 0$

$$\delta S = S[Q] - S[q] = \int_{t_1}^{t_2} dt \left\{ L\left(q(t) + \delta q(t), \dot{q}(t) + \delta\dot{q}, t\right) - L(\ldots) \right\}$$

$$= \int_{t_1}^{t_2} dt \left\{ \cancel{L(q(t), \dot{q}(t), t)} + \frac{\partial L}{\partial q}(q(t), \dot{q}(t), t) \cdot \delta q(t) + \frac{\partial L}{\partial \dot{q}}(q(t), \dot{q}(t), t) \cdot \delta \dot{q} + \mathcal{O}(\delta q^2) - \cancel{L(q, \dot{q}, t)} \right\}$$

$\uparrow$ parc. integrál

$$= \underbrace{\left[\frac{\partial L}{\partial \dot{q}} \delta q \right]_{t_1}^{t_2}}_{= \varnothing} + \int_{t_1}^{t_2} dt \left(\frac{\partial L}{\partial q} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}} \right) \cdot \delta q$$

S extremális $\Rightarrow$ $\displaystyle\int dt (\ldots) \delta q = 0$ $\forall\, \delta q$-ra $\Rightarrow$ $$\boxed{\frac{\partial L}{\partial q} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}} = \varnothing}$$

visszafelé triviális

$$\boxed{\delta S = 0} \Leftrightarrow \boxed{\frac{d}{dt}\frac{\partial L}{\partial \dot q} = \frac{\partial L}{\partial q}}$$

• következmény: L nem egyértelmű...

$$L' \equiv L + \frac{d f(q,t)}{dt}$$

$$S'[q] = S[q] + f(2) - f(1) \quad \Rightarrow \quad \delta S' = \delta S \;\ldots$$

• példa:

$$L = \frac{m}{2}\underline{v}^2 - q\phi + q\underline{v}\cdot\underline{A}$$

E.M. invariáns az ún. mértékhajóra:

$$\phi' \equiv \phi + \frac{\partial f(\underline{x},t)}{\partial t} \; ; \quad \underline{A}' \equiv \underline{A} - \frac{\partial f}{\partial \underline{x}}$$

$\Rightarrow$ $\underline{E}, \underline{B}$ változatlan! $\Rightarrow$ L megvált.

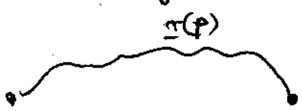
$$L' = \frac{m}{2}\underline{v}^2 - q\phi + q\cdot\underline{v}\cdot\underline{A} \underbrace{- q\frac{\partial f}{\partial t} - q\dot{\underline{x}}\,\mathrm{grad} f}_{-q\frac{df}{dt}\ \checkmark}$$

<u>Kapcsolat</u> a <u>hullámoptikával</u>:

<u>Fény</u>: Fermat-elv: $t_{1\to 2} = \int_{r_1}^{r_2} \frac{ds}{c(\underline{r})} = \min$

$\Rightarrow$ Snellius-Descartes törvény

mögötte: interferencia



$\Rightarrow$ fázis $\varphi[\underline{r}] = \omega\cdot t_{1\to 2}[\underline{r}]$

fény frekvenciája

$\varphi[\underline{r}] \cong \varphi[\underline{r}+\delta\underline{r}]$ $\forall$ $\delta\underline{r}$-re

$\Leftrightarrow$ konstruktív interferencia!

<u>Q.M.</u>: Feynman: $A_{1\to 2} = \sum_{\text{útvonalak}} e^{\frac{i}{\hbar}S[\underline{r}(t), t_1, t_2]}$

konstruktív interferencia $\Leftrightarrow$ $\delta S = 0$!