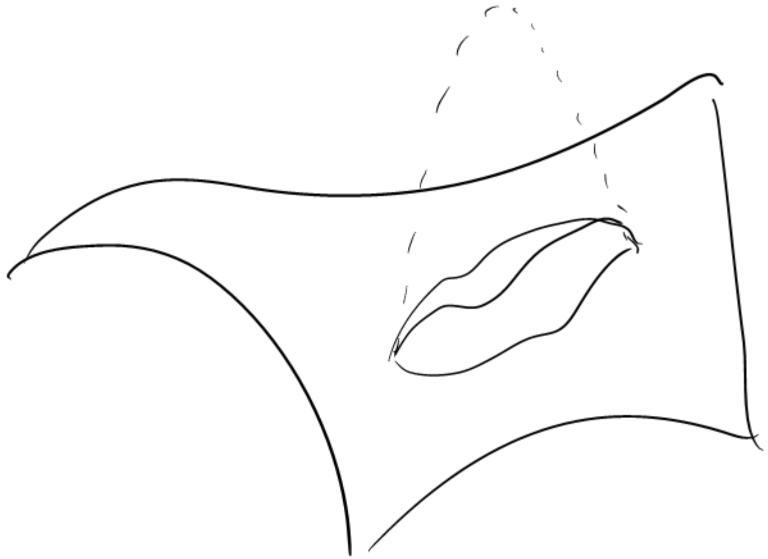
$$\frac{\partial L}{\partial q_i} = \frac{d}{dt} \frac{\partial L}{\partial \dot{q}_i} \qquad L = L(\{q_i\}, \{\dot{q}_i\})$$



constr. surf. $G = 0$

Lagrange multipliers: First for simple calculus, $f(x_1, x_2, \ldots, x_N) \overset{!}{=}$ Min. with

CONSTRAINT $G(x_1, x_2, \dots, x_N) = 0$

$$d\vec{x} = \underbrace{d\vec{x}_{\parallel}}_{\text{\underline{in} the surface}} + \underbrace{dx_{\perp}}$$

perpendic. to the surface

$$df = \sum_i \frac{\partial f}{\partial x_i} dx_i = (\vec{\nabla} f) \cdot d\vec{x} = (\vec{\nabla} f) \cdot [d\vec{x}_{\parallel} + d\vec{x}_{\perp}]$$

$d\vec{x}$ should ONLY live within the surface!

$d\vec{x}_{\perp} = 0$ that means: $df = 0$

$$= (\vec{\nabla} f) \cdot d\vec{x}_{\parallel} = 0$$

$\vec{\nabla} f \perp$ surface. We know: $\vec{\nabla} G \perp$ surface!

$$\vec{\nabla} f = \lambda \vec{\nabla} G$$ Lagrange multiplier

$$\phi(x_1, x_2, \dots, x_N, \lambda) = f(x_1, \dots, x_N) - \lambda G(x_1, \dots, x_N)$$

$$\frac{\partial \phi}{\partial x_i} = \frac{\partial f}{\partial x_i} - \lambda \frac{\partial G}{\partial x_i} \overset{!}{=} 0 \quad \Rightarrow \vec{\nabla} f = \lambda \vec{\nabla} G \checkmark$$

$$\frac{\partial \phi}{\partial \lambda} = -G(x_1, \dots, x_N) \overset{!}{=} 0 \quad \Rightarrow G = 0$$

Calculus of variations:

$$S = \int_{t_1}^{t_2} dt\, L(\{q_i\}, \{\dot{q}_i\}) \stackrel{!}{=} \text{Min.}$$

$$G(\{q_i\}) = 0 \qquad \delta S = \sum_i \int_{t_1}^{t_2} dt \left[\frac{\partial L}{\partial q_i} - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right)\right] \delta q_i$$

$$= \int_{t_1}^{t_2} dt \left[\frac{\partial L}{\partial \vec{q}} - \frac{d}{dt}\frac{\partial L}{\partial \dot{\vec{q}}}\right] \cdot \left[\delta \vec{q}_{\parallel} + \underbrace{\delta \vec{q}_{\perp}}_{=0} \right]$$

$$\boxed{\int_{t_1}^{t_2} dt \left[\frac{\partial L}{\partial \vec{q}} - \frac{d}{dt}\frac{\partial L}{\partial \dot{\vec{q}}}\right] \cdot \delta \vec{q}_{\parallel} = 0}$$

$$\Rightarrow \frac{\partial L}{\partial \vec{q}} - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{\vec{q}}}\right) \perp \text{ surface}$$

$$\Rightarrow \frac{\partial L}{\partial \vec{q}} - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{\vec{q}}}\right) = \lambda \vec{\nabla} G$$

several constraints: $\frac{\partial L}{\partial \vec{q}} - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{\vec{q}}}\right) = \sum_i \lambda_i \vec{\nabla} G_i$

$$L \longrightarrow L' = L - \sum_i \lambda_i G_i$$

$$L' = L'(\{q_i\}, \{\dot{q}_i\}, \lambda_i)$$

$$\frac{\partial L'}{\partial q_i} = \frac{d}{dt}\left(\frac{\partial L'}{\partial \dot q_i}\right) = \frac{d}{dt}\frac{\partial}{\partial \dot q_i}\left(L - \sum_j \lambda_j G_j\right)$$

$$= \frac{d}{dt}\left(\frac{\partial L}{\partial \dot q_i}\right) - \sum_j \lambda_j \frac{d}{dt}\frac{\partial}{\partial \dot q_i} G_j$$

$$\frac{\partial L'}{\partial \lambda_i} = \frac{d}{dt}\underbrace{\frac{\partial L'}{\partial \dot\lambda_i}}_{=0} = 0 \qquad = -G_i \Rightarrow \boxed{G_i = 0}$$

Noether Theorem

relation symmetries $\leftrightarrow$ conservation laws

continuous symmetry $\underbrace{S}_{\text{transformation}}(\underbrace{\alpha}_{\text{parameter}})$

$$q_i(t) \xrightarrow{S(\alpha)} q_i'(t) = q_i(t,\alpha)$$

$$q_i(t,0) = q_i(t)$$

$$\alpha = 0 \Leftrightarrow S(\alpha) = \mathbb{1}$$

Requirement: L is invariant under S

$$q_i \longrightarrow q_i' = q_i(t,\alpha)$$

$$L \longrightarrow L$$

$$L(\{q_i(t,0)\},\{\dot{q}_i(t,0)\}) = L(\{q_i(t,\alpha)\},\{\dot{q}_i(t,\alpha)\})$$

$$\frac{d}{d\alpha} L = 0 \quad \text{or} \quad 0 = \sum_i \left[\frac{\partial L}{\partial q_i} \frac{\partial q_i}{\partial \alpha} + \frac{\partial L}{\partial \dot{q}_i} \frac{\partial \dot{q}_i}{\partial \alpha} \right] \underset{\text{mot.}}{\overset{\text{eq.}}{=}}$$

$$= \sum_i \left[\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right) \frac{\partial q_i}{\partial \alpha} + \frac{\partial L}{\partial \dot{q}_i} \frac{d}{dt} \frac{\partial q_i}{\partial \alpha} \right] =$$

$$= \frac{d}{dt} \sum_i \left[\frac{\partial L}{\partial \dot{q}_i} \frac{\partial q_i}{\partial \alpha} \right] = 0$$

$$\Rightarrow \sum_i \left[\frac{\partial L}{\partial \dot{q}_i} \frac{\partial q_i}{\partial \alpha} \right] = \text{const.}$$

conservation law related to $S(\alpha)$

Translation in Space

$$\vec{r}_i = \begin{pmatrix} x_i \\ y_i \\ z_i \end{pmatrix} \longrightarrow \begin{pmatrix} x_i + \alpha \\ y_i \\ z_i \end{pmatrix} = \vec{r}_i\,'$$

$$\dot{\vec r}_i \longrightarrow \dot{\vec r}_i \qquad L \longrightarrow L$$

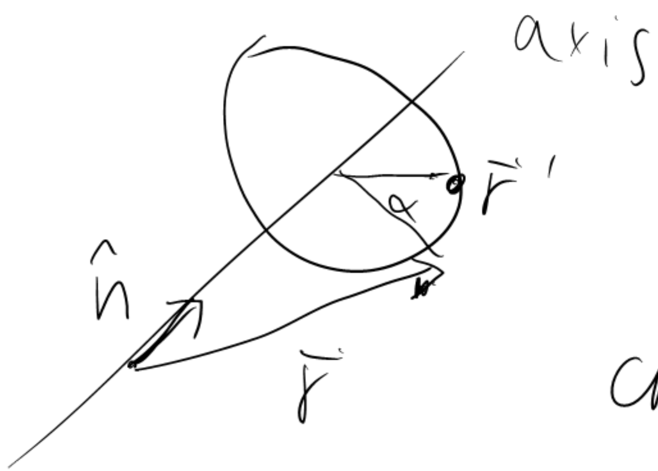
corresponds to conservation of momentum:

$$\text{const.} \equiv P_x = \sum_i \left[\frac{\partial L}{\partial \dot x_i} \underbrace{\frac{\partial x_i}{\partial \alpha}}_{1} + \frac{\partial L}{\partial \dot y_i} \underbrace{\frac{\partial y_i}{\partial \alpha}}_{=0} + \frac{\partial L}{\partial \dot z_i} \underbrace{\frac{\partial z_i}{\partial \alpha}}_{=0} \right]$$

$$= \sum_i \frac{\partial L}{\partial \dot x_i} = \sum_i (\text{particle momenta})$$

$$\Rightarrow \vec P = \text{const.}$$

Rotation in space



$\hat{n}$: unit vector along the axis

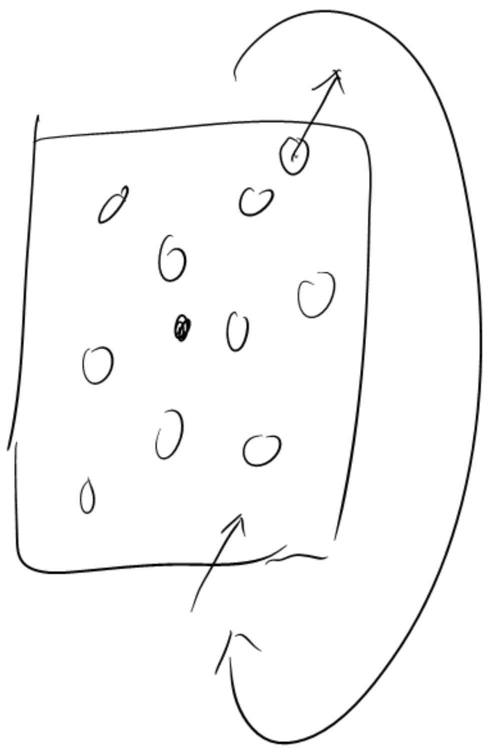
α: angle

$$\text{const.} = \sum_i \underbrace{\frac{\partial L}{\partial \dot{\vec{r}}_i}}_{= \vec{p}_i} \cdot \underbrace{\frac{\partial \vec{r}_i}{\partial \alpha}}_{= \hat{n} \times \vec{r}_i} =$$

$$= \sum_i \vec{p}_i \cdot (\hat{n} \times \vec{r}_i) = \hat{n} \cdot \underbrace{\sum_i (\vec{r}_i \times p_i)}_{= \vec{L} \text{ angular mom.}}$$

$\text{const.} = \hat{n} \cdot \vec{L}$ $\quad \hat{n}$ arbitrary

$\Rightarrow \vec{L} = \text{const.}$



periodic
boundary
conditions

Molecular
Dynamics

Gauge Invariance

$$U \longrightarrow U + \underbrace{\Delta U}_{\text{constant}}$$

$$m_i \ddot{\vec{r}}_i = -\frac{\partial U}{\partial \vec{r}_i} \qquad\qquad L \to L - \Delta U$$

More general: $\quad L \longrightarrow L + \frac{d}{dt}\Psi(\{q_i\}, t)$

$\to$ dynamics is not changed $\qquad$ for any function Ψ

WHY?

$$S = \int_{t_1}^{t_2} dt\, L(\{q_i\}, \{\dot{q}_i\}, t)$$

$$\longrightarrow \int_{t_1}^{t_2} dt \left(L + \frac{d}{dt}\Psi \right) = S + \Psi \Big|_{t_1}^{t_2} =$$

$$= S - \Psi(\{q_i(t_1)\}, t_1) + \Psi(\{q_i(t_2)\}, t_2) =$$

$$= S \underbrace{- \Psi(\{q_{i1}\}, t_1) + \Psi(\{q_{i2}\}, t_2)}_{\text{FIXED}}$$

does not depend on trajectory

THEOREM. We search for an M:

$L \to L + M$: Dynamics is unchanged for ANY Lagrangian L : M MUST HAVE the form $M = \frac{d}{dt}\psi(\{q_i\}, t)$

Proof: $$\frac{d}{dt}\left(\frac{\partial M}{\partial \dot{q}}\right) = \frac{\partial M}{\partial q}$$ For ANY trajectory $q(t)$

(just ONE degree of freedom)

<u>Ansatz</u>: $M = a_0(q,t) + a_1(q,t)\dot{q} + a_2(q,t)\frac{1}{2}\dot{q}^2 + \ldots$

$$\frac{\partial M}{\partial \dot{q}} = a_1(q,t) + a_2(q,t)\dot{q} + \ldots$$

$$\frac{d}{dt}\left(\frac{\partial M}{\partial \dot{q}}\right) = \frac{\partial a_1}{\partial q}\dot{q} + \frac{\partial a_1}{\partial t} + \frac{\partial a_2}{\partial q}\dot{q}^2 + \frac{\partial a_2}{\partial t}\dot{q} + a_2\ddot{q} + \ldots =$$

$$= \ldots + \ddot{q}\underbrace{\left(a_2 + a_3\ldots + a_4\ldots + a_5\ldots\right)}_{\text{Should be ZERO}}$$

otherwise: $\ddot{q} = \ldots \to$ <u>one</u> trajectory and not so many!

$$M = a_0(q,t) + a_1(q,t)\,\dot{q}$$

$$\frac{\partial M}{\partial \dot{q}} = a_1 \qquad \frac{d}{dt}\frac{\partial M}{\partial \dot{q}} = \frac{\partial a_1}{\partial q}\dot{q} + \frac{\partial a_1}{\partial t}$$

$$\frac{\partial M}{\partial q} = \frac{\partial a_0}{\partial q} + \frac{\partial a_1}{\partial q}\dot{q}$$

$$\left.\begin{matrix} \\ \\ \end{matrix}\right\} \quad \frac{\partial a_1}{\partial t} = \frac{\partial a_0}{\partial q}$$

Def. $\phi(q,t) = \int dq\, a_1(q,t) \Rightarrow a_1 = \dfrac{\partial \phi}{\partial q}$

$$\frac{\partial a_1}{\partial t} = \frac{\partial^2 \phi}{\partial q\, \partial t} = \frac{\partial^2 \phi}{\partial t\, \partial q} = \frac{\partial a_0}{\partial q} \Rightarrow a_0 = \frac{\partial \phi}{\partial t} + C(t)$$

Def.: $\Psi = \phi + \int dt \; c(t)$

$$\frac{\partial \Psi}{\partial t} = \frac{\partial \phi}{\partial t} + c(t) \Rightarrow a_0 = \frac{\partial \Psi}{\partial t}$$

$$\frac{\partial \Psi}{\partial q} = \frac{\partial \phi}{\partial q} = a_1$$

$$\Rightarrow M = a_0 + a_1 \dot{q} = \frac{\partial \Psi}{\partial t} + \frac{\partial \Psi}{\partial q} \dot{q} = \frac{d}{dt} \Psi$$

Generalized Noether - Theorem

$$q_i(t) \xrightarrow{S(\alpha)} q_i(t, \alpha) \qquad S(\alpha = 0) = \mathbb{1}$$

L is NOT invariant, but rather

$$L \xrightarrow{S(\alpha)} L + \alpha \frac{d}{dt} \psi(\{q_i\}, t) + O(\alpha^2)$$

$$\frac{dL}{d\alpha} = \frac{d}{dt}\psi \qquad \left[\text{compared to } \frac{dL}{d\alpha} = 0\right]$$

$\longrightarrow$ does not change the dynamics

$$\frac{dL}{d\alpha} = \frac{d}{dt}\left(\sum_i \frac{\partial L}{\partial \dot{q}_i} \frac{\partial q_i}{\partial \alpha}\right) = \frac{d}{dt}\psi$$

$$\sum_i \frac{\partial L}{\partial \dot{q}_i} \frac{\partial q_i}{\partial \alpha} - \psi = \text{const.}$$

<u>Galilei Transforms</u>

constant velocity

$$\begin{pmatrix} x_i \\ y_i \\ z_i \end{pmatrix} \longrightarrow \begin{pmatrix} x_i - vt \\ y_i \\ z_i \end{pmatrix}$$

$$\dot{x}_i^2 + \dot{y}_i^2 + \dot{z}_i^2 \longrightarrow \dot{x}_i'^2 + \dot{y}_i^2 + \dot{z}_i^2$$

$$\dot{x}_i'^2 = \dot{x}_i^2 + v^2 - 2v\dot{x}_i = \dot{x}_i^2 + \frac{d}{dt}\left[v^2 t - 2v x_i\right]$$

$$L \longrightarrow L + \frac{d}{dt}\sum_i m_i \frac{1}{2}\left(v^2 t - 2v x_i\right)$$

$v \longrightarrow 0$:

$$L \longrightarrow L - v\frac{d}{dt}\underbrace{\sum_i m_i x_i}_{-4}$$

$$\frac{\partial L}{\partial \dot{x}_i} = p_{ix} \qquad \frac{\partial x_i}{\partial v} = -t$$

$$\text{const.} = \sum_i p_{ix}(-t) + \sum_i m_i x_i \quad \Big| : \underbrace{\sum_i m_i}_{= M \text{ total mass}}$$

$$\vec{R} = \frac{\sum_i m_i \vec{r}_i}{\sum_i m_i} \quad \text{center of mass}$$

$$\text{const.} = -t \frac{P_x}{M} + R_x$$

$$R_x = \text{const.} + t \frac{P_x}{M}$$