14.4. Liouvillesche Satz

- $\underline{X}(t) = \begin{pmatrix} q_1 \\ \vdots \\ q_{3N} \\ p_1 \\ \vdots \\ p_{3N} \end{pmatrix}$ ... Punkt im Phasenraum

- Dichte $\rho(\underline{X}, t)$ im Phasenraum

  $\rho(\underline{X}, t)\, d^{6N}X$ ... Wahrscheinlichkeit, System im Zustand/Gebiet $[\underline{X}, \underline{X}+d\underline{X}]$ anzutreffen (14.31)

  $\int_V \rho\, d^{6N}X = 1$ ... Normierung

- Kontinuitätsgl.:

$$\boxed{\frac{\partial \rho}{\partial t} + \operatorname{div}(\rho \dot{\underline{X}}) = 0} \quad (14.36)$$

$$\text{mit } \operatorname{div} = \underline{\nabla}_{\underline{X}} \cdot = \begin{pmatrix} \frac{\partial}{\partial x_1} \\ \vdots \\ \frac{\partial}{\partial x_{6N}} \end{pmatrix} \cdot = \begin{pmatrix} \frac{\partial}{\partial q_1} \\ \vdots \\ \frac{\partial}{\partial p_{3N}} \end{pmatrix} \cdot$$

- Liouvillescher Satz:

Herleitung: $\operatorname{div}(\rho \dot{\underline{X}}) = \sum_j \left[\frac{\partial}{\partial q_j}(\rho \dot{q}_j) + \frac{\partial}{\partial p_j}(\rho \dot{p}_j) \right]$

$$\underline{X} = \begin{pmatrix} q_1 \\ \vdots \\ q_{3N} \\ p_1 \\ \vdots \\ p_{3N} \end{pmatrix} \quad = \sum_j \left[\frac{\partial}{\partial q_j}\rho \underbrace{\dot{q}_j}_{= \frac{\partial H}{\partial p_j}} + \frac{\partial}{\partial p_j}\rho \underbrace{\dot{p}_j}_{= -\frac{\partial H}{\partial q_j}} + \underbrace{\rho\left(\frac{\partial}{\partial q_j} \underbrace{\dot{q}_j}_{\frac{\partial H}{\partial p_j}} + \frac{\partial}{\partial p_j} \underbrace{\dot{p}_j}_{-\frac{\partial H}{\partial q_j}} \right)}_{= 0} \right]$$

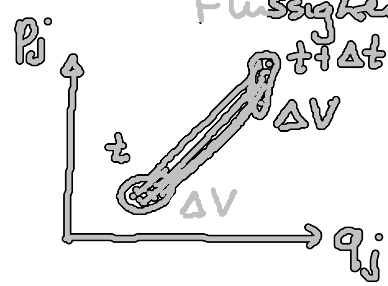
$$\longrightarrow \operatorname{div}(\rho \dot{\underline{X}}) \overset{(14.14)}{=} \{\rho, H\} \quad (14.37)$$

(14.37) in (14.36) $\longrightarrow$

$$\boxed{0 = \frac{\partial \rho}{\partial t} + \{\rho, H\}} \quad (14.38)$$

... Liouvillesche Satz

(i) (14.38) $\overset{\uparrow}{=}$ $\frac{d\varrho}{dt} = 0$ ... Dichte entlang Systembahn ist
(14.13) konstant = „inkompressible"
Flüssigkeit



(ii) thermodynam. Gleichgewicht:

$$\boxed{\frac{\partial\varrho}{\partial t} = 0 \longrightarrow \{\varrho, H\} = 0} \quad (14.39)$$

mögliche Lsg: $\varrho = \varrho(H) = \varrho\left(H(\{q_j\}, \{p_j\})\right) = \sum_n \varrho_n H^n$

$$\{H^n, H\} = 0$$

Bsp: kanonische Ensemble:
$$\boxed{\begin{array}{l} \varrho = \frac{1}{Z} e^{-H/k_B T} \\ \text{"}Z = \int d^{6N}X \, e^{-H/k_B T}\text{"} \end{array}}$$

14.5 Kanonische Transformationen

[lat: best angepaßt]

• Idee: alle q_j zyklisch & $\frac{\partial H}{\partial t} = 0$

$\longrightarrow \dot{p}_j = -\frac{\partial H}{\partial q_j} = 0 \longrightarrow p_j = \alpha_j = \text{konst.}$

$\longrightarrow H = H(\alpha_1, \dots, \alpha_s) \longrightarrow \dot{q}_j = \frac{\partial H}{\partial \alpha_j} = \omega_j(\alpha_1, \dots, \alpha_s) = \text{konst.}$

$$\longrightarrow \boxed{q_j = \omega_j t + \beta_j} \quad (14.41)$$

Bem: (i) (14.41) definiert <u>integrable</u> Systeme (... „die Ausnahme")
(ii) die Regel: <u>nicht</u> integrable Systeme (Bsp: 3-Körper-Problem)

Ziel: Trafos $\{q_i, p_j\} \longrightarrow \{Q_k, P_k\}$, so daß alle Q_k zyklisch!

- **Bisher**: $\boxed{\text{Punkttransformation: } Q_k = Q_k(\{q_j\}, t)}$ (14.42)

Beh: $\boxed{\text{Punkttrafos lassen Lagrange Glg. invariant}}$

Bew: Umkehrung: $q_j = q_j(\{Q_k\}, t) \longrightarrow \dot{q}_j = \sum_k \frac{\partial q_j}{\partial Q_k}\dot{Q}_k + \frac{\partial q_j}{\partial t}$ (*)

Zeige: $\frac{d}{dt}\frac{\partial L}{\partial \dot{Q}_k} - \frac{\partial L}{\partial Q_k} = 0$!

$+\frac{\partial L}{\partial q_j}\frac{\partial q_j}{\partial \dot{Q}_k} = 0$

$$= \sum_j \overbrace{\frac{d}{dt}\Big(\frac{\partial L}{\partial \dot{q}_j}\underbrace{\frac{\partial \dot{q}_j}{\partial \dot{Q}_k}}_{\overset{(*)}{=}\frac{\partial q_j}{\partial Q_k}}\Big)}^{\left(\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_j}\right)\frac{\partial q_j}{\partial Q_k} + \cancel{\frac{\partial L}{\partial \dot{q}_j}\underbrace{\frac{d}{dt}\frac{\partial q_j}{\partial Q_k}}_{\frac{\partial \dot{q}_j}{\partial Q_k}}}} - \sum_j\Big(\frac{\partial L}{\partial q_j}\frac{\partial q_j}{\partial Q_k} + \cancel{\frac{\partial L}{\partial \dot{q}_j}\frac{\partial \dot{q}_j}{\partial Q_k}}\Big)$$

$$= \sum_j \underbrace{\Big(\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_j} - \frac{\partial L}{\partial q_j}\Big)}_{=0}\frac{\partial q_j}{\partial Q_k} = 0 \checkmark$$

- $\boxed{\textbf{kanonische Trafos}: \quad Q_k = Q_k(\{q_j\}, \{p_j\}, t)}$

$$P_k = P_k(\{q_j\},\{p_j\},t) \qquad (14.43)$$

wenn Hamiltonsche Bewgl. forminvariant bleiben, mit neuer Hamiltonfunktion $\bar{H} = \bar{H}(\{Q_k\},\{P_k\},t)$

also: $$L(\{q_j\},\{\dot{q}_j\},t) \overset{\text{kanon}}{\underset{\text{Trafo}}{=}} L(\{Q_k\},\{\dot{Q}_k\},t) + \frac{d}{dt}F \qquad (14.44)$$

vgl. Kap. 13.5 c)

$$\overset{\text{Legendre}}{\underset{\text{Trafo}}{\longleftrightarrow}} \quad \boxed{\sum_j p_j \dot{q}_j - H = \sum_j P_j \dot{Q}_j - \bar{H} + \frac{d}{dt}F} \qquad (14.45)$$

- erzeugende Funktion F

(i) bestimmt kanonische Trafo!

(ii) soll also von $\underbrace{\{q_j\}, \{p_j\}, \{Q_j\}, \{P_j\}}_{\substack{2f \text{ unabh.} \\ 2f \text{ abhängige Variable [vgl. (14.43)]}}}$ abhängen

$\longrightarrow$ 4 Möglichkeiten

$$F_1(\{q_j\},\{Q_j\},t) \qquad F_2(\{q_j\},\{P_j\},t)$$
$$F_3(\{p_j\},\{Q_j\},t) \qquad F_4(\{p_j\},\{P_j\},t) \qquad (14.46)$$

(i) $F_1(\{q_j\},\{Q_j\},t)$:

Bilde $$\frac{d}{dt}F_1 = \sum_j \left(\frac{\partial F_1}{\partial q_j}\dot{q}_j + \frac{\partial F_1}{\partial Q_j}\dot{Q}_j \right) + \frac{\partial F_1}{\partial t}$$

in (14.45) & Koeff.vgl. bei $\dot{q}_j, \dot{Q}_j$, da $\{q_j\}, \{Q_j\}$ unabh. Variable

$$\text{für } \dot{q}_j \longrightarrow \boxed{p_j = \frac{\partial F_1}{\partial q_j}} \cdots\cdots \xrightarrow{\text{Umkehrg.}} Q_k = Q_k(\{q_j\}, \{p_j\}, t)\,!$$

$$\text{für } \dot{Q}_j \longrightarrow \boxed{P_j = -\frac{\partial F_1}{\partial Q_j}} \cdots\cdots \longrightarrow P_k = P_k(\{q_j\}, \{Q_j\}, t)$$
$$= P_k(\{q_j\}, \{p_j\}, t)\,!$$

$$\text{Rest} \longrightarrow \boxed{\bar{H} = H + \frac{\partial F_1}{\partial t}}$$

... F_1 erzeugt kanonische Trafo

(ii) $F_2(\{q_j\}, \{P_j\}, t) \underset{\text{trafo}}{\overset{\text{Leg.}}{=}} F_1 + \sum_j P_j Q_j$ (14.48)

$\left[\, y(x)\,,\ p = \frac{\partial y}{\partial x}\right.$

$\rightarrow \psi(p) = y(x) - px$

$\left. x = -\frac{\partial \psi}{\partial p} \,\right]$

$$\longrightarrow \boxed{\begin{aligned} p_j &= \frac{\partial F_2}{\partial q_j} \\ Q_j &= +\frac{\partial F}{\partial P_j} \\ \bar{H} &= H + \frac{\partial F_2}{\partial t} \end{aligned}} \quad (14.49)$$

... F_2 erzeugt kanon. Trafo

(iii) $F_3(\{p_j\}, \{Q_j\}, t) \underset{\text{trafo}}{\overset{\text{Leg.}}{=}} F_1 - \sum_j p_j q_j$ (14.50) $\longrightarrow$

$$\boxed{\begin{aligned} q_j &= -\frac{\partial F_3}{\partial p_j} \\ P_j &= -\frac{\partial F_3}{\partial Q_j} \\ \bar{H} &= H + \frac{\partial F_3}{\partial t} \end{aligned}} \quad (14.51)$$

(iv) $F_4(\{p_i\},\{P_j\},t) \underset{\text{trafo}}{\overset{\text{Leg.}}{=}} F_1 + \sum_j P_j Q_j - \sum_j p_j q_j$ ... F_3 erzeugt kanon. Trafo

$$\longrightarrow \boxed{\begin{aligned} q_j &= -\frac{\partial F_4}{\partial p_j} \\ Q_j &= \frac{\partial F_4}{\partial P_j} \\ \bar{H} &= H + \frac{\partial F_4}{\partial t} \end{aligned}} \quad (14.53)$$

... F_4 erzeugt kanon Trafo

Beispiele:

(i) identische Trafo: $F_2 = \sum_j q_j P_j \longrightarrow$

$$p_j = \frac{\partial F_2}{\partial q_j} = P_j$$
$$Q_j = \frac{\partial F_2}{\partial P_j} = q_j \quad !$$
$$\bar{H} = H$$

(ii) $\boxed{\text{Punkttrafo} = \text{kanon. Trafo}}$

$$F_2 = \sum_j f_j(\{q_k\},t)\, P_j \xrightarrow[Q_j = \frac{\partial F_2}{\partial P_j}]{} Q_j = f_j(\{q_k\},t), \quad \bar{H} = H + \frac{\partial F_2}{\partial t}$$

(iii) $F_1 = \sum_j q_j Q_j \longrightarrow$

$$\left.\begin{aligned} p_j &= \frac{\partial F_1}{\partial q_j} = Q_j \\ P_j &= -\frac{\partial F_1}{\partial Q_j} = -q_j \end{aligned}\right\} \text{Vertauschung von Koord. \& Impulse}$$

(iv) harmonischer Oszillator: $(x,p) = (q,p)$

$$\boxed{H = \frac{p^2}{2m} + \frac{m\omega^2}{2} q^2} \quad (14.54)$$

, mit Federkonst.: $f = m\omega^2$

$$F_1 = \frac{m}{2}\omega q^2 \cot Q \longrightarrow \begin{aligned} p &= \frac{\partial F_1}{\partial q} = m\omega q \cot Q \quad (1) \\ P &= -\frac{\partial F_1}{\partial Q} = \frac{m\omega q^2}{2} \frac{1}{\sin^2 Q} \quad (2) \end{aligned}$$

$$\left.\begin{aligned} &(2) \longrightarrow \quad q = \sqrt{\frac{2P}{m\omega}} \sin Q \quad (3) \\ &(3) \text{ in } (1) \longrightarrow \quad p = \sqrt{2m\omega P} \cos Q \quad (4) \end{aligned}\right\} \text{kanon. Umkehrtrafo !!}$$

(3), (4) in H: $H = \bar{H} - \omega P \cos^2 Q + \omega P \sin^2 Q$

$\longrightarrow$ $\boxed{H = \omega P \longleftrightarrow \text{Impuls: } P = \frac{\text{Energie } E = H}{\omega}}$

Q ... zykl. Koord. $\longrightarrow$ Bewgl. $\dot{Q} = \frac{\partial H}{\partial P} = \omega$

$\downarrow$

$P = \text{const.}$

$\longrightarrow$ $Q = \omega t + \alpha$

$\longrightarrow$ $q \overset{(2)}{=} \sqrt{\frac{2E}{m\omega^2}} \sin(\omega t + \alpha)$ ✓