14.4. Liouvillesche Satz

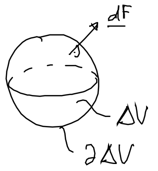
$$\boxed{\begin{array}{l} \text{Phasenraumdichte: } \rho(\underline{X},t) \\ \quad \text{Wahrscheinlichkeit: } \rho(\underline{X},t)\,d^{6N}X \\ \text{Normierung: } \int_V \rho(\underline{X},t)\,d^{6N}X = 1 \end{array}} \qquad (14.31)$$

$$\boxed{\underline{X}(t) = \{q_i(t), p_i(t)\}} \qquad (14.32)$$

Erwartungswert = Mittelwert einer Observable

$$\langle A \rangle = \int d^{6N}X\,\rho(\underline{X},t)\,A(\underline{X},t) \qquad (14.32)$$

- Kontinuitätsgl.: Herleitung



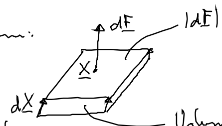
$$\frac{d}{dt}\int_{\Delta V} \rho(\underline{X},t)\,d^{6N}X \underset{\substack{\Delta V\\ \text{fest}}}{=} \int_{\Delta V} \frac{\partial}{\partial t}\rho(\underline{X},t)\,d^{6N}X$$

$$= -\int_{\partial\Delta V} \underline{j}(\underline{X},t)\cdot d\underline{F} \qquad (14.33)$$

mit Wahrscheinlichkeitsstromdichte:

$$\boxed{\underline{j}(\underline{X},t) = \rho(\underline{X},t)\,\dot{\underline{X}}(t)} \qquad (14.34)$$

Warum:



Verschiebung des Phasenraumpunktes bei $\underline{X}$ in Zeit dt

Volumen: Fläche × Höhe $= d\underline{X}\cdot d\underline{F}$

$\longrightarrow \rho\, d\underline{X}\cdot d\underline{F}$ ... Wahrscheinlichkeit, daß System in Zeit dt Fläche $|d\underline{F}|$ durchquert

$\xrightarrow{\text{pro } dt} \rho\frac{d\underline{X}}{dt}\cdot d\underline{F} = \underline{j}\cdot d\underline{F}$

Satz von Gauß (in 6N Dimensionen)

$$\boxed{\begin{array}{l} \int_{\partial\Delta V} \underline{j}\cdot d\underline{F} = \int_{\Delta V} \operatorname{div}\underline{j}\; d^{6N}X \\ \text{mit } \operatorname{div} = \underline{\nabla}_{\underline{X}}\cdot = \begin{pmatrix} \frac{\partial}{\partial X_1} \\ \vdots \\ \frac{\partial}{\partial X_{6N}} \end{pmatrix}\cdot \end{array}} \qquad (14.35)$$

$$(14.33) \xrightarrow[(14.35)]{(14.34)} \int_{\Delta V} \Big[\frac{\partial}{\partial t}\varrho + \underbrace{\mathrm{div}(\varrho \dot{\underline{X}})}_{\uparrow}\Big] d^{6N}X = 0$$

$$\xrightarrow[\text{beliebig}]{\Delta V} \quad \boxed{\frac{\partial \varrho}{\partial t} + \mathrm{div}(\varrho \dot{\underline{X}}) = 0}$$

... Kontinuitätsgleichg. für ϱ

- Liouvillesche Satz:

Herleitg.: $\mathrm{div}(\varrho \dot{\underline{X}}) = \sum_j \Big[\frac{\partial}{\partial q_j}(\varrho \dot q_j) + \frac{\partial}{\partial p_j}(\varrho \dot p_j)\Big]$

$$\underline{X} = \begin{pmatrix} q_1 \\ \vdots \\ q_{3N} \\ p_1 \\ \vdots \\ p_{3N} \end{pmatrix} \qquad = \sum_j \Big[\frac{\partial \varrho}{\partial q_j} \underbrace{\dot q_j}_{=\frac{\partial H}{\partial p_j}} + \frac{\partial \varrho}{\partial p_j} \underbrace{\dot p_j}_{-\frac{\partial H}{\partial q_j}} + \underbrace{\varrho\Big(\frac{\partial}{\partial q_j} \underbrace{\dot q_j}_{\frac{\partial H}{\partial p_j}} + \frac{\partial}{\partial p_j} \underbrace{\dot p_j}_{-\frac{\partial H}{\partial q_j}}\Big)}_{=0}\Big]$$

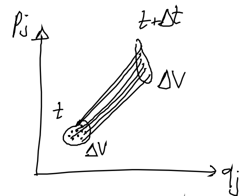
$$\mathrm{div}(\varrho \dot{\underline{X}}) \overset{(14.14)}{=} \{\varrho, H\} \qquad (14.37)$$

$$(14.37) \text{ in } (14.36) \longrightarrow \boxed{0 = \frac{\partial \varrho}{\partial t} + \{\varrho, H\}} \quad (14.38)$$

... Liouvillescher Satz

(i) $(14.38) \underset{(14.13)}{=} \frac{d\varrho}{dt} = 0$ ... Dichte entlang Systembahn $X(t)$ ist konstant

$\Rightarrow$ Ensemble von Systemen = „inkompressible Flüssigkeit"



(ii) thermodynam. Gleichgewicht:

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

mögliche Lsg: $\varrho = \varrho(H) = \varrho(H(\{q_j\}, \{p_j\}))$ $\Big[= \sum_n \varrho_n H^n\Big]$

weil $\{H, H\} = 0$

<u>Bsp:</u> kanonische Ensemble: $\boxed{\begin{aligned} \varrho &= \frac{1}{Z} e^{-\frac{H}{k_B T}} \\ Z &= \int d^{6N}X \, e^{-H/k_B T} \end{aligned}}$ (14.40)

14.5 Kanonische Transformationen
[lat. bestangepaßt]

- Motivierende Idee:

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

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

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

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

Bem.: (i) (14.41) definiert integrable Systeme (..., „die Ausnahme" ...)

(ii) die Regel: nicht-integrable Systeme: Bsp: 3-Körper-Problem

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

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

Beh.: $\boxed{\text{Punkttrafos lassen Lagrange Gln. forminvariant}}$

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

$$= \sum_j \frac{d}{dt}\Big(\frac{\partial L}{\partial \dot{q}_j} \underbrace{\frac{\partial \dot{q}_j}{\partial \dot{Q}_k}}_{(*)\ \frac{\partial q_j}{\partial Q_k}} + \underbrace{\frac{\partial L}{\partial q_j} \frac{\partial q_j}{\partial \dot{Q}_k}}_{=0}\Big) - \sum_j \Big(\frac{\partial L}{\partial q_j} \frac{\partial q_j}{\partial Q_k} + \cancel{\frac{\partial L}{\partial \dot{q}_j} \frac{\partial \dot{q}_j}{\partial Q_k}}\Big)$$

$$\overbrace{\Big(\frac{d}{dt} \frac{\partial L}{\partial \dot{q}_j}\Big) \frac{\partial q_j}{\partial Q_k}} + \cancel{\frac{\partial L}{\partial \dot{q}_j} \frac{d}{dt} \frac{\partial q_j}{\partial Q_k}}$$

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

- jetzt:

$$\boxed{\begin{array}{l} \text{Kanonische Trafos:} \quad Q_k = Q_k(\{q_j\}, \{p_j\}, t) \\ \qquad\qquad\qquad\qquad\quad P_k = P_k(\{q_j\}, \{p_j\}, t) \\ \text{wenn Hamiltonsche Bew. gl. forminvariant bleiben} \\ \text{bzgl. neuer Hamiltonfunktion } \bar{H} = \bar{H}(\{Q_k\}, \{P_k\}, t) \end{array}}$$

äquivalent: $L(\{q_j\}, \{\dot{q}_j\}, t) \xlongequal[\text{Trafo}]{\text{kanon.}} L(\{Q_k\}, \{\dot{Q}_k\}, t) + \underbrace{\frac{d}{dt} F}_{\text{Eichtrafo vgl. Kap. 13.5 c)}}$ (14.44)

$\longrightarrow$ Legendre Trafo:

$$\boxed{\sum_j p_j \dot{q}_j - H = \sum_j P_j \dot{Q}_j - \bar{H} + \frac{d}{dt} F} \quad (14.45)$$

• erzeugende Funktion F:

(i) bestimmt Trafo!

(ii) soll also von $\underbrace{\{q_j\}, \{p_j\}, \{Q_j\}, \{P_j\}}_{\substack{2f \text{ unabhängig} \\ 2f \text{ abhängige Variable}}}$ 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

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

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

$\xrightarrow{\text{Rest}}$ $\boxed{\bar{H} = H + \frac{\partial F_1}{\partial t}}$ $\qquad = P_k(\{q_j\}, \{p_j\}, t)$

... F_1 erzeugt kanon. Trafo

(ii) $F_2(\{q_j\}, \{P_j\}, t) \underset{\text{Trafo}}{\overset{\text{Legendre}}{=}} F_1 + \sum_j P_j Q_j \qquad P_j = -\frac{\partial F_1}{\partial Q_j}, \quad Q_j \longrightarrow -P_j \qquad (14.48)$ [vgl. Legendre Trafo]

$\xrightarrow{\text{Theorie der Legendre Trafo}}$
$$\boxed{\begin{aligned} p_j &= \frac{\partial F_2}{\partial q_j} \\ Q_j &= +\frac{\partial F_2}{\partial P_j} \\ \bar{H} &= H + \frac{\partial F_2}{\partial t} \end{aligned}} \qquad (14.49)$$

... F_2 erzeugt kanon. Trafo