Kanoniske transformationer (i)

Værdien af transformationer: Polære koordinater: $(x, y, z) = (r\cos\phi\sin\theta, r\sin\phi\sin\theta, r\cos\theta)$
$\Rightarrow \quad T = \frac{1}{2}m\big(\dot{x}^2 + \dot{y}^2 + \dot{z}^2\big) = \frac{1}{2}m\big(\dot{r}^2 + r^2\dot{\theta}^2 + r^2\sin^2\theta\dot{\phi}^2\big).$
Hvis $V = V(r, \theta) \Rightarrow \phi$ er en cyklisk koordinat og $p_\phi = mr^2\sin^2\theta\,\dot{\phi}$ er bevaret.
Den ideelle transformation må være én, hvor alle koordinater bliver cykliske.

Opgave 1.10: Punkttransformation: $q_i = q_i(Q_1, Q_2, \ldots, Q_n, t) \qquad (i = 1, \ldots, n)$

$\Rightarrow \dot{q}_i = \dfrac{\partial q_i}{\partial Q_j}\dot{Q}_j + \dfrac{\partial q_i}{\partial t}$ og $\dfrac{\partial \dot{q}_i}{\partial \dot{Q}_j} = \dfrac{\partial q_i}{\partial Q_j}$. For Lagrangefunktionen $L = L(\mathbf{q}, \dot{\mathbf{q}}, t)$ fås

$$\frac{d}{dt}\Big(\frac{\partial L}{\partial \dot{Q}_j}\Big) - \frac{\partial L}{\partial Q_j} = \frac{d}{dt}\Big(\frac{\partial L}{\partial q_i}\frac{\partial q_i}{\partial \dot{Q}_j} + \frac{\partial L}{\partial \dot{q}_i}\frac{\partial \dot{q}_i}{\partial \dot{Q}_j}\Big) - \Big(\frac{\partial L}{\partial q_i}\frac{\partial q_i}{\partial Q_j} + \frac{\partial L}{\partial \dot{q}_i}\frac{\partial \dot{q}_i}{\partial Q_j}\Big)$$

$$= \frac{d}{dt}\Big(\frac{\partial L}{\partial \dot{q}_i}\frac{\partial q_i}{\partial Q_j}\Big) - \Big(\frac{\partial L}{\partial q_i}\frac{\partial q_i}{\partial Q_j} + \frac{\partial L}{\partial \dot{q}_i}\frac{\partial \dot{q}_i}{\partial Q_j}\Big) = \frac{\partial q_i}{\partial Q_j}\frac{d}{dt}\Big(\frac{\partial L}{\partial \dot{q}_i}\Big) + \frac{\partial L}{\partial \dot{q}_i}\frac{\partial \dot{q}_i}{\partial Q_j} - \Big(\frac{\partial L}{\partial q_i}\frac{\partial q_i}{\partial Q_j} + \frac{\partial L}{\partial \dot{q}_i}\frac{\partial \dot{q}_i}{\partial Q_j}\Big)$$

$$= \Big[\frac{d}{dt}\Big(\frac{\partial L}{\partial \dot{q}_i}\Big) - \frac{\partial L}{\partial q_i}\Big]\frac{\partial q_i}{\partial Q_j} = 0.$$

Lagrangeligningerne er *forminvariante* mht. en transformation i **konfigurationsrummet**.

I Hamiltonformuleringen er der $2n$ uafhængige koordinater $\mathbf{q}$ og $\mathbf{p}$, og den tilsvarende generelle transformation i **faserummet** er:

$Q_i = Q_i(\mathbf{q}, \mathbf{p}, t), \quad P_i = P_i(\mathbf{q}, \mathbf{p}, t),$ og omvendt $\quad q_i = q_i(\mathbf{Q}, \mathbf{P}, t), \quad p_i = p_i(\mathbf{Q}, \mathbf{P}, t)$

$H \mapsto K = K(\mathbf{Q}, \mathbf{P}, t), \quad \dot{Q}_i = \dfrac{\partial K}{\partial P_i},\ \dot{P}_i = -\dfrac{\partial K}{\partial Q_i}.$ Krav: Q_i og P_i er kanoniske variable,

men ikke nødvendigvis at $K(\mathbf{Q}, \mathbf{P}, t) = H\big(\mathbf{q}(\mathbf{Q}, \mathbf{P}, t), \mathbf{p}(\mathbf{Q}, \mathbf{P}, t), t\big)$.

Øvelse: Vis at bevægelsesligningerne for de transformerede variable, i tilfældet $n = 1$,

$q = q(Q, P), \quad p = p(Q, P)$ er $\quad \dfrac{\partial H}{\partial Q} = -J_D\dot{P}, \quad \dfrac{\partial H}{\partial P} = J_D\dot{Q},$

hvor J_D er Jacobi-determinanten $J_D = \left|\dfrac{\partial(q, p)}{\partial(Q, P)}\right|$.

Kanoniske transformationer (ii)

$$\dot{Q}_i = \frac{\partial K}{\partial P_i},\ \dot{P}_i = -\frac{\partial K}{\partial Q_i},\ \delta\int_{t_1}^{t_2} \left[p_i\dot{q}_i - H(\mathbf{q},\mathbf{p},t)\right]dt = 0 \Rightarrow \delta\int_{t_1}^{t_2} \left[P_i\dot{Q}_i - K(\mathbf{Q},\mathbf{P},t)\right]dt = 0$$

eller

$$\lambda\big(p_i\dot{q}_i - H\big) = P_i\dot{Q}_i - K + \frac{dF}{dt}, \qquad \text{bemærk} \quad \delta\int_{t_1}^{t_2} \frac{dF}{dt}dt = \delta\Big[F(\mathbf{q},\mathbf{p},\mathbf{Q},\mathbf{P},t)\Big]_{t_1}^{t_2} = 0$$

Udvidet kanonisk transformation: $(\lambda \neq 1)$

$$Q_i = \mu q_i, \quad P_i = \nu p_i \Rightarrow K = K(\mathbf{Q},\mathbf{P},t) = \mu\nu H\Big(\frac{\mathbf{Q}}{\mu},\frac{\mathbf{P}}{\nu},t\Big) = \mu\nu H(q,p,t)$$

idet $\lambda = \mu\nu \quad \Rightarrow \quad \mu\nu\big(p_i\dot{q}_i - H\big) = P_i\dot{Q}_i - K$

Kanonisk transformation: $(\lambda = 1)$ $\qquad p_i\dot{q}_i - H = P_i\dot{Q}_i - K + \dfrac{dF}{dt}$

$$\Leftrightarrow \qquad p_i dq_i - P_i dQ_i + (K - H)dt = dF$$

Udtrykket viser at q_i, Q_i og t er de uafhængige variable i F, og $F = F(\mathbf{q},\mathbf{Q},t)$ kaldes for *frembringerfunktionen* eller *generatoren* for den kanoniske transformation.

$$F = F_1 = F_1(\mathbf{q},\mathbf{Q},t) \Rightarrow dF = dF_1 = \frac{\partial F_1}{\partial q_i}dq_i + \frac{\partial F_1}{\partial Q_i}dQ_i + \frac{\partial F_1}{\partial t}dt, \qquad \text{som indsat giver}$$

$$\Big(p_i - \frac{\partial F_1}{\partial q_i}\Big)dq_i + \Big(-P_i - \frac{\partial F_1}{\partial Q_i}\Big)dQ_i + \Big(K - H - \frac{\partial F_1}{\partial t}\Big)dt = 0, \qquad \text{eller}$$

$$p_i = \frac{\partial F_1}{\partial q_i} \quad (1), \qquad P_i = -\frac{\partial F_1}{\partial Q_i} \quad (2), \qquad K = H + \frac{\partial F_1}{\partial t} \quad (3)$$

De tre ligninger fastlægger transformationen: (2) er en relation mellem P_i og $(\mathbf{q},\ \mathbf{Q},t)$ som bestemmer $q_i = q_i(\mathbf{Q},\mathbf{P},t)$. Indsættes dette i (1) fås $p_i = p_i\big(\mathbf{q}(\mathbf{Q},\mathbf{P},t),\mathbf{Q},t\big)$. Ligning (3) giver sluttelig $K = K(\mathbf{Q},\mathbf{P},t)$, når de to resultater indsættes i denne ligning.

Kanoniske transformationer (iii)

Kanonisk transformation: $p_i dq_i - P_i dQ_i + (K - H)dt - dF = 0$

Genererende funktion $F_2(\mathbf{q}, \mathbf{P}, t)$ kombineret med Legendre transformation:

$$F = F_2(\mathbf{q}, \mathbf{P}, t) - Q_i P_i\,, \qquad dF_2 = \frac{\partial F_2}{\partial q_i} dq_i + \frac{\partial F_2}{\partial P_i} dP_i + \frac{\partial F_2}{\partial t} dt \quad \Rightarrow$$

$$p_i dq_i - P_i dQ_i + (K - H)dt - dF_2 + Q_i dP_i + P_i dQ_i = 0 \qquad \text{eller}$$

$$\Big(p_i - \frac{\partial F_2}{\partial q_i}\Big) dq_i + \Big(Q_i - \frac{\partial F_2}{\partial P_i}\Big) dP_i + \Big(K - H - \frac{\partial F_2}{\partial t}\Big) dt = 0 \qquad \text{og dermed}$$

$$p_i = \frac{\partial F_2}{\partial q_i}\,, \qquad Q_i = \frac{\partial F_2}{\partial P_i}\,, \qquad K = H + \frac{\partial F_2}{\partial t}$$

(i) $F = F_1(\mathbf{q}, \mathbf{Q}, t) \quad \Rightarrow \quad p_i = \dfrac{\partial F_1}{\partial q_i}, \qquad P_i = -\dfrac{\partial F_1}{\partial Q_i}, \qquad K = H + \dfrac{\partial F_1}{\partial t}$

(ii) $F = F_2(\mathbf{q}, \mathbf{P}, t) - Q_i P_i \quad \Rightarrow \quad p_i = \dfrac{\partial F_2}{\partial q_i}, \qquad Q_i = \dfrac{\partial F_2}{\partial P_i}, \qquad K = H + \dfrac{\partial F_2}{\partial t}$

(iii) $F = F_3(\mathbf{p}, \mathbf{Q}, t) + q_i p_i \quad \Rightarrow \quad q_i = -\dfrac{\partial F_3}{\partial p_i}, \qquad P_i = -\dfrac{\partial F_3}{\partial Q_i}, \qquad K = H + \dfrac{\partial F_3}{\partial t}$

(iv) $F = F_4(\mathbf{p}, \mathbf{P}, t) + q_i p_i - Q_i P_i \quad \Rightarrow \quad q_i = -\dfrac{\partial F_4}{\partial p_i}, \qquad Q_i = \dfrac{\partial F_4}{\partial P_i}, \qquad K = H + \dfrac{\partial F_4}{\partial t}$

+ forskellige kombinationer af (i)–(iv) for forskellige frihedsgrader:

F. eks. (ii) og (iv) $\qquad F = F_5(q_1, p_2, P_1, P_2, t) - Q_1 P_1 + q_2 p_2 - Q_2 P_2 \;\Rightarrow$

$$p_1 = \frac{\partial F_5}{\partial q_1}\,, \qquad Q_1 = \frac{\partial F_5}{\partial P_2}\,, \qquad q_2 = -\frac{\partial F_5}{\partial p_2}\,, \qquad Q_2 = \frac{\partial F_5}{\partial P_2}\,, \quad K = H + \frac{\partial F_5}{\partial t}$$

Eksempler på kanoniske transformationer

$$\text{(i):}\quad F_2 = q_i P_i \quad\Rightarrow\quad p_i = \frac{\partial F_2}{\partial q_i} = P_i\,,\quad Q_i = \frac{\partial F_2}{\partial P_i} = q_i \quad \text{(identitet)}$$

$$\text{(ii):}\quad F_1 = q_i Q_i \quad\Rightarrow\quad p_i = \frac{\partial F_1}{\partial q_i} = Q_i\,,\quad P_i = -\frac{\partial F_1}{\partial Q_i} = -q_i \quad \text{(ombytning)}$$

$$(q_i, p_i) \mapsto (-P_i, Q_i) \Rightarrow \dot{p}_i = -\frac{\partial H}{\partial q_i} \mapsto \dot{Q}_i = -\frac{\partial H}{\partial(-P_i)}\,,\quad \dot{q}_i = \frac{\partial H}{\partial p_i} \mapsto -\dot{P}_i = \frac{\partial H}{\partial Q_i}$$

$$\text{(iii):}\quad F_2 = f_j(\mathbf{q}, t) P_j \quad\Rightarrow\quad Q_i = \frac{\partial F_2}{\partial P_i} = f_i(\mathbf{q}, t)\,,\quad p_i = \frac{\partial F_2}{\partial q_i} = \frac{\partial f_j}{\partial q_i} P_j$$

Den første ligning bestemmer $q_i = q_i(\mathbf{Q}, t)$. Den anden ligning kan vendes om ved udregningen: $\dfrac{\partial q_i}{\partial Q_k} p_i = \dfrac{\partial q_i}{\partial Q_k}\dfrac{\partial f_j}{\partial q_i} P_j = \dfrac{\partial Q_j}{\partial q_i}\dfrac{\partial q_i}{\partial Q_k} P_j = \dfrac{\partial Q_j}{\partial Q_k} P_j = P_k. \qquad (f_j \equiv Q_j).$

Denne kanoniske transformation er identisk med punkttransformationen af Lagrangefunktionen: $L = L(\mathbf{q}, \dot{\mathbf{q}}, t)$, hvor $q_i = q_i(\mathbf{Q}, t)$ og $\dot{q}_i = \dfrac{\partial q_i}{\partial Q_j}\dot{Q}_j + \dfrac{\partial q_i}{\partial t}$. Det sidste udtryk betyder:

$$P_k = \frac{\partial L}{\partial \dot{Q}_k} = \frac{\partial L}{\partial q_i}\frac{\partial q_i}{\partial \dot{Q}_k} + \frac{\partial L}{\partial \dot{q}_i}\frac{\partial \dot{q}_i}{\partial \dot{Q}_k} = p_i \frac{\partial \dot{q}_i}{\partial \dot{Q}_k} = p_i \frac{\partial q_i}{\partial Q_k}, \qquad \text{som ovenfor.}$$

Benyttes i stedet $F_2 = f_j(\mathbf{q}, t) P_j + g(\mathbf{q}, t)$ er $Q_i = f_i(\mathbf{q}, t)$ som før, men den kanoniske bevægelsesmængde P_k ændres og bestemmes nu af ligningen: $p_i = \dfrac{\partial f_j}{\partial q_i} P_j + \dfrac{\partial g}{\partial q_i}$

Denne transformation svarer til punkttransformationen af L, hvor $q_i = q_i(\mathbf{Q}, t)$ kombineres med at Lagrangefunktionen L erstattes af $L' = L - \dfrac{dg}{dt}$. [Øvelse].

Den harmoniske oscillator (i)

Hamilton for den éndimensionale harmoniske oscillator:

$$H = T + V = \frac{p^2}{2m} + \tfrac{1}{2} k\, q^2 \quad \text{eller} \quad H = \frac{1}{2m}\left(p^2 + m^2\omega^2 q^2\right), \quad \omega^2 = \frac{k}{m}$$

Find en kanonisk transformation, $(q,p) \mapsto (Q,P)$, hvor Q er en cyklisk koordinat:

$$p = f(P)\cos Q, \quad q = \frac{f(P)}{m\omega}\sin Q \quad \Rightarrow \quad K = H = \frac{f^2(P)}{2m}\left(\cos^2 Q + \sin^2 Q\right) = \frac{f^2(P)}{2m}$$

Benyt $F_1 = \tfrac{1}{2} m\omega q^2 \cot Q \Rightarrow p = \dfrac{\partial F_1}{\partial q} = m\omega q \cot Q \quad (1), \quad P = -\dfrac{\partial F_1}{\partial Q} = \dfrac{m\omega q^2}{2\sin^2 Q} \quad (2).$

$(2) \;\Rightarrow\; q = \sqrt{\dfrac{2P}{m\omega}}\sin Q$, hvorefter $(1) \;\Rightarrow\; p = \sqrt{2Pm\omega}\cos Q \quad$ eller $\quad f(P) = \sqrt{2Pm\omega}$ [trykfejl i ligning (9.39b)].

Resultat: Transformationen $q = \sqrt{\dfrac{2P}{m\omega}}\sin Q, \quad p = \sqrt{2Pm\omega}\cos Q \quad$ er kanonisk og $\Rightarrow$

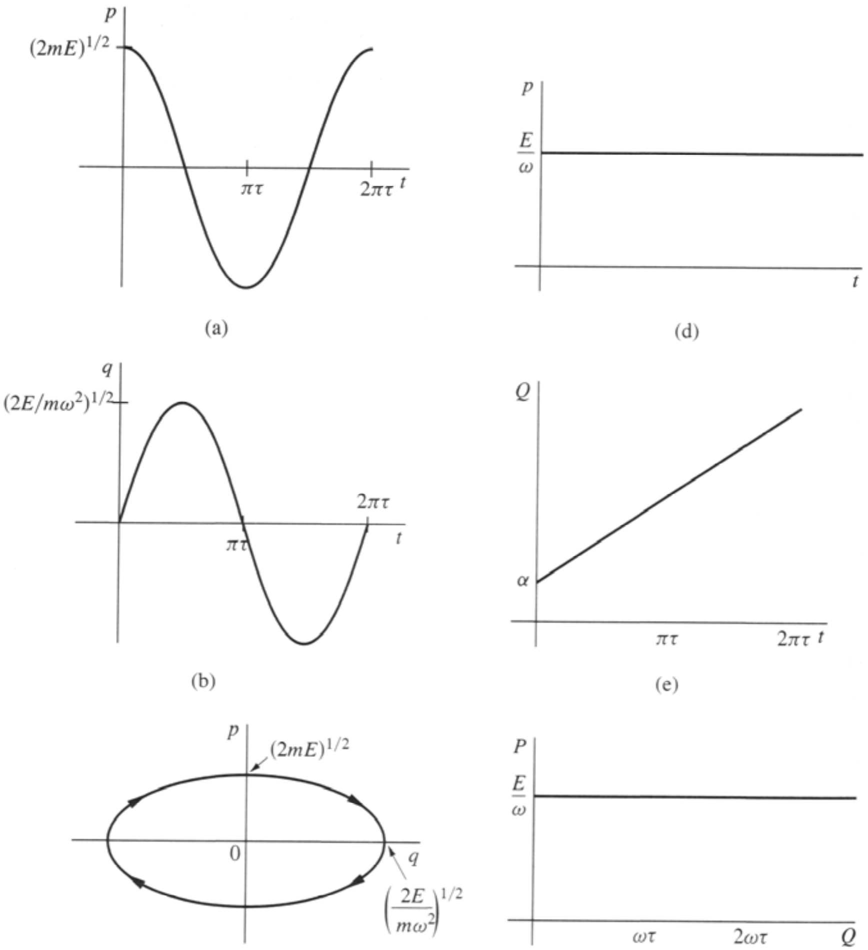
$K = H = \dfrac{f^2(P)}{2m} = \omega P, \quad$ som er cyklisk i $Q \quad \Rightarrow \quad P$ er bevægelseskonstant.

$H = T + V = E \quad \Rightarrow \quad P = \dfrac{E}{\omega}.$

Hamiltons bevægelsesligning for Q er $\dot{Q} = \dfrac{\partial H}{\partial P} = \omega \quad \Rightarrow \quad Q = Q(t) = \omega t + \alpha$

Slutresultat: $\quad q = \sqrt{\dfrac{2E}{m\omega^2}}\sin(\omega t + \alpha), \qquad p = \sqrt{2mE}\cos(\omega t + \alpha)$

Den harmoniske oscillator (ii)



$$Q = \omega t + \alpha\,, \qquad P = \frac{E}{\omega}$$

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

$$p = \sqrt{2mE}\cos(\omega t + \alpha)$$

Faserumsvolumen:

$$A(E_0) = \iint_{E<E_0} dp dq = \int p dq = \pi ab = \frac{2\pi E_0}{\omega}$$

Indsættes det kvantemekaniske resultat $\Delta E = \hbar\omega$ fås det kvasi-klassiske resultat, at “faserumsvolumnet” pr. kvantetilstand er $\Delta A = 2\pi\hbar = h$ (pr. frihedsgrad).

Indføres normaliserede variable (“kaos”):

$$q' = \sqrt{\frac{m\omega^2}{2}}\,q, \qquad p' = \frac{p}{\sqrt{2m}}$$

bliver det tilsvarende bane i (q', p')-faserummet en cirkel med arealet:
$A' = \pi E$

Den symplektiske metode (i)

Begrænset kanonisk transformation (ingen eksplicit t-afhængighed):

$$Q_i = Q_i(\mathbf{q},\mathbf{p}), \quad P_i = P_i(\mathbf{q},\mathbf{p}); \quad q_i = q_i(\mathbf{Q},\mathbf{P}), \quad p_i = p_i(\mathbf{Q},\mathbf{P}); \qquad K = H + \frac{\partial F}{\partial t} = H$$

$$\left.\begin{aligned} \dot{Q}_i &= \frac{\partial Q_i}{\partial q_j}\dot{q}_j + \frac{\partial Q_i}{\partial p_j}\dot{p}_j = \frac{\partial Q_i}{\partial q_j}\frac{\partial H}{\partial p_j} - \frac{\partial Q_i}{\partial p_j}\frac{\partial H}{\partial q_j} \\ \dot{Q}_i &= \frac{\partial H}{\partial P_i} = \frac{\partial H}{\partial p_j}\frac{\partial p_j}{\partial P_i} + \frac{\partial H}{\partial q_j}\frac{\partial q_j}{\partial P_i} \end{aligned}\right\} \quad \frac{\partial Q_i}{\partial q_j} = \frac{\partial p_j}{\partial P_i}\,, \qquad \frac{\partial Q_i}{\partial p_j} = -\frac{\partial q_j}{\partial P_i}$$

Betragtes istedet $\dot{P}_i$ fås analogt $\qquad \dfrac{\partial P_i}{\partial q_j} = -\dfrac{\partial p_j}{\partial Q_i}\,, \qquad \dfrac{\partial P_i}{\partial p_j} = \dfrac{\partial q_j}{\partial Q_i}$

Symplektisk notation, $\quad \overline{\overline{J}} \equiv \begin{pmatrix} \mathbf{0} & \mathbf{1} \\ -\mathbf{1} & \mathbf{0} \end{pmatrix}, \quad \eta_i = q_i, \quad \eta_{i+n} = p_i \quad (i = 1, 2, \ldots, n)$

Hamiltons bevægelsesligninger $\dot{q}_i = \dfrac{\partial H}{\partial p_i}, \quad \dot{p}_i = -\dfrac{\partial H}{\partial q_i}$ omformes til $\quad \dot{\boldsymbol{\eta}} = \overline{\overline{J}}\,\dfrac{\partial H}{\partial \boldsymbol{\eta}}$

Nye kanoniske koordinater: $\boldsymbol{\zeta} = \boldsymbol{\zeta}(\boldsymbol{\eta}) \quad \Rightarrow \quad \dot{\boldsymbol{\zeta}} = \overline{\overline{M}}\dot{\boldsymbol{\eta}}\,, \quad M_{ij} = \dfrac{\partial \zeta_i}{\partial \eta_j}$

$$\dot{\boldsymbol{\zeta}} = \overline{\overline{M}}\,\overline{\overline{J}}\frac{\partial H}{\partial \boldsymbol{\eta}} = \overline{\overline{M}}\,\overline{\overline{J}}\widetilde{\overline{\overline{M}}}\frac{\partial H}{\partial \boldsymbol{\zeta}}\,, \qquad \frac{\partial H}{\partial \eta_i} = \frac{\partial H}{\partial \zeta_j}\frac{\partial \zeta_j}{\partial \eta_i} = M_{ji}\frac{\partial H}{\partial \zeta_j} = \left(\widetilde{\overline{\overline{M}}}\right)_{ij}\frac{\partial H}{\partial \zeta_j}$$

Kanonisk transformation $\quad \dot{\boldsymbol{\zeta}} = \overline{\overline{J}}\dfrac{\partial H}{\partial \boldsymbol{\zeta}} \quad \Rightarrow \quad \overline{\overline{M}}\,\overline{\overline{J}}\widetilde{\overline{\overline{M}}} = \overline{\overline{J}} \quad (1)$

Matricer der opfylder (1) kaldes symplektiske. Denne direkte metode forudsætter at de nye koordinater eksplicit defineres ud fra de gamle $\boldsymbol{\zeta} = \boldsymbol{\zeta}(\boldsymbol{\eta})$.

$$\overline{\overline{M}}\,\overline{\overline{J}} = \overline{\overline{J}}\widetilde{\overline{\overline{M}}}^{-1} \quad \Rightarrow \quad \overline{\overline{J}}\,\overline{\overline{M}}\,\overline{\overline{J}}^2 = \overline{\overline{J}}^2\widetilde{\overline{\overline{M}}}^{-1}\overline{\overline{J}} \quad \Rightarrow \quad \overline{\overline{J}}\,\overline{\overline{M}} = \widetilde{\overline{\overline{M}}}^{-1}\overline{\overline{J}} \quad \Rightarrow \quad \widetilde{\overline{\overline{M}}}\,\overline{\overline{J}}\,\overline{\overline{M}} = \overline{\overline{J}}$$

Den symplektiske metode (ii)

Tidsafhængig kanoniske transformation: $\boldsymbol{\zeta} = \boldsymbol{\zeta}(\boldsymbol{\eta}, t)\,, \quad \overline{\overline{M}} = \dfrac{\partial \boldsymbol{\zeta}}{\partial \boldsymbol{\eta}} \quad \Rightarrow \quad \overline{\overline{M}}\,\overline{\overline{J}}\,\widetilde{\overline{\overline{M}}} = \overline{\overline{J}}$

Vi vil vise at den symplektiske ligning er gyldig for en *infinitesimal* (tidsafhængig) kanonisk transformation, $Q_i = q_i + \delta q_i\,, \quad P_i = p_i + \delta p_i \quad$ eller $\quad \boldsymbol{\zeta} = \boldsymbol{\eta} + \delta\boldsymbol{\eta}$

En infinitesimal kanonisk transformation kan genereres ved at benytte

$$F_2 = F_2(\mathbf{q}, \mathbf{P}, t) = q_j P_j + \epsilon\, G(\mathbf{q}, \mathbf{P}, t) \quad \Rightarrow \quad p_i = \frac{\partial F_2}{\partial q_i} = P_i + \epsilon\, \frac{\partial G}{\partial q_i} \quad \Rightarrow \quad \delta p_i = -\epsilon\, \frac{\partial G}{\partial q_i}$$

$$Q_i = \frac{\partial F_2}{\partial P_i} = q_i + \epsilon\, \frac{\partial G}{\partial P_i} = q_i + \epsilon\, \frac{\partial G}{\partial p_i} + \mathcal{O}(\epsilon^2) \quad \Rightarrow \quad \delta q_i = \epsilon\, \frac{\partial G}{\partial p_i} \quad \text{eller} \quad \delta\boldsymbol{\eta} = \epsilon\, \overline{\overline{J}}\, \frac{\partial G}{\partial \boldsymbol{\eta}}$$

$$\overline{\overline{M}} = \frac{\partial \boldsymbol{\zeta}}{\partial \boldsymbol{\eta}} = \overline{\overline{1}} + \frac{\partial \delta\boldsymbol{\eta}}{\partial \boldsymbol{\eta}} = \overline{\overline{1}} + \epsilon\, \overline{\overline{J}}\, \frac{\partial^2 G}{\partial \boldsymbol{\eta} \partial \boldsymbol{\eta}}\,, \qquad \left(\frac{\partial^2 G}{\partial \boldsymbol{\eta} \partial \boldsymbol{\eta}}\right)_{ij} = \frac{\partial^2 G}{\partial \eta_i \partial \eta_j} = \left(\frac{\partial^2 G}{\partial \boldsymbol{\eta} \partial \boldsymbol{\eta}}\right)_{ji}$$

Benyttes $\quad \widetilde{\overline{\overline{A}}\,\overline{\overline{B}}} = \widetilde{\overline{\overline{B}}}\,\widetilde{\overline{\overline{A}}}, \qquad \widetilde{\overline{\overline{J}}} = -\overline{\overline{J}} \qquad$ fås

$$\widetilde{\overline{\overline{M}}} = \overline{\overline{1}} - \epsilon\, \frac{\partial^2 G}{\partial \boldsymbol{\eta} \partial \boldsymbol{\eta}}\, \overline{\overline{J}} \quad \Rightarrow \quad \overline{\overline{M}}\,\overline{\overline{J}}\,\widetilde{\overline{\overline{M}}} = \left(\overline{\overline{1}} + \epsilon\, \overline{\overline{J}}\, \frac{\partial^2 G}{\partial \boldsymbol{\eta} \partial \boldsymbol{\eta}}\right) \overline{\overline{J}} \left(\overline{\overline{1}} - \epsilon\, \frac{\partial^2 G}{\partial \boldsymbol{\eta} \partial \boldsymbol{\eta}}\, \overline{\overline{J}}\right) = \overline{\overline{J}} + \mathcal{O}(\epsilon^2)$$

Den symplektiske ligning gælder for en vilkårlig infinitesimal kanonisk transformation, også hvis transformationen (G) afhænger eksplicit af t. Den symplektiske ligning gælder derfor ved hvert skridt af følgende sekvens af kanoniske transformationer:

$$\boldsymbol{\eta} \mapsto \boldsymbol{\zeta}(t_0) \mapsto \boldsymbol{\zeta}(t_0 + \delta t) \mapsto \boldsymbol{\zeta}(t_0 + 2\delta t) \mapsto \cdots \mapsto \boldsymbol{\zeta}(t_0 + t).$$

Antager vi at serien er konvergent har vi dermed at den symplektiske ligning er gyldig også når den kanoniske transformation afhænger eksplicit af t.

Poissonparentes

Poissonparentesen for to funktioner $u(\mathbf{q}, \mathbf{p}, t)$ og $v(\mathbf{q}, \mathbf{p}, t)$ defineres:

$$[u, v]_{\mathbf{q},\mathbf{p}} = \sum_i \left(\frac{\partial u}{\partial q_i} \frac{\partial v}{\partial p_i} - \frac{\partial u}{\partial p_i} \frac{\partial v}{\partial q_i} \right) \qquad \text{eller} \qquad [u, v]_{\boldsymbol{\eta}} = \widetilde{\frac{\partial u}{\partial \boldsymbol{\eta}}}\, \overline{\overline{J}}\, \frac{\partial v}{\partial \boldsymbol{\eta}}$$

Simple resultater (trykfejl i lærebogen: ligningen før (9.71) og (9.71)):

$$[q_j, q_k]_{\mathbf{q},\mathbf{p}} = 0, \quad [p_j, p_k]_{\mathbf{q},\mathbf{p}} = 0, \quad [q_j, p_k]_{\mathbf{q},\mathbf{p}} = -[p_j, q_k]_{\mathbf{q},\mathbf{p}} = \delta_{jk} \qquad \text{eller} \qquad [\boldsymbol{\eta}, \boldsymbol{\eta}]_{\boldsymbol{\eta}} = \overline{\overline{J}}$$

Transformation af variable $(\mathbf{q}, \mathbf{p}) \mapsto (\mathbf{Q}, \mathbf{P})$ eller $\boldsymbol{\zeta} = \boldsymbol{\zeta}(\boldsymbol{\eta}, t)$, hvor $\overline{\overline{M}} = \dfrac{\partial \boldsymbol{\zeta}}{\partial \boldsymbol{\eta}}$:

$$[\boldsymbol{\zeta}, \boldsymbol{\zeta}]_{\boldsymbol{\eta}} = \frac{\partial \boldsymbol{\zeta}}{\partial \boldsymbol{\eta}}\, \overline{\overline{J}}\, \widetilde{\frac{\partial \boldsymbol{\zeta}}{\partial \boldsymbol{\eta}}} = \overline{\overline{M}}\, \overline{\overline{J}}\, \widetilde{\overline{\overline{M}}} = \overline{\overline{J}} \quad \Leftrightarrow \quad \text{kanonisk transformation } (\overline{\overline{M}} \text{ er symplektisk}).$$

$[\boldsymbol{\zeta}, \boldsymbol{\zeta}]_{\boldsymbol{\eta}} = [\boldsymbol{\zeta}, \boldsymbol{\zeta}]_{\boldsymbol{\zeta}} = \overline{\overline{J}}$ er uafhængig af en kanonisk transformation.

$$\frac{\partial v}{\partial \eta_i} = \frac{\partial v}{\partial \zeta_j} \frac{\partial \zeta_j}{\partial \eta_i} = \frac{\partial v}{\partial \zeta_j} M_{ji} = \left(\widetilde{\overline{\overline{M}}}\right)_{ij} \frac{\partial v}{\partial \zeta_j} \Rightarrow \frac{\partial v}{\partial \boldsymbol{\eta}} = \widetilde{\overline{\overline{M}}} \frac{\partial v}{\partial \boldsymbol{\zeta}}, \quad \widetilde{\frac{\partial u}{\partial \boldsymbol{\eta}}} = \widetilde{\widetilde{\overline{\overline{M}}} \frac{\partial u}{\partial \boldsymbol{\zeta}}} = \widetilde{\frac{\partial u}{\partial \boldsymbol{\zeta}}}\, \overline{\overline{M}}$$

$$[u, v]_{\boldsymbol{\eta}} = \widetilde{\frac{\partial u}{\partial \boldsymbol{\eta}}}\, \overline{\overline{J}}\, \frac{\partial v}{\partial \boldsymbol{\eta}} = \widetilde{\frac{\partial u}{\partial \boldsymbol{\zeta}}}\, \overline{\overline{M}}\, \overline{\overline{J}}\, \widetilde{\overline{\overline{M}}}\, \frac{\partial v}{\partial \boldsymbol{\zeta}} = \widetilde{\frac{\partial u}{\partial \boldsymbol{\zeta}}}\, \overline{\overline{J}}\, \frac{\partial v}{\partial \boldsymbol{\zeta}} \equiv [u, v]_{\boldsymbol{\zeta}}$$

Alle poissonparenteser er kanonisk invariante (invariante overfor kanoniske transformationer), hvilket også gælder (pr. definition) for Hamiltons bevægelsesligninger. Bemærk, at vi ikke fremover behøver at specificere, hvilke koordinater der benyttes ved udregningen af Poissonparenteserne: $[u, v]_{\boldsymbol{\eta}} = [u, v]_{\boldsymbol{\zeta}} = [u, v]$.

Klassisk mekanik $\mapsto$ Kvantemekanik: Poissonparentes $\mapsto$ Kommutator mellem to operatorer (Dirac), $\quad [u, v]_{\text{Klassisk}} \mapsto \dfrac{1}{i\hbar} [\hat{u}, \hat{v}]_{\text{Kvantemekanisk}} \qquad ([\hat{x}, \hat{p}_x] = i\hbar)$

Poissonparentes algebra:

$[u, u] = 0$
$[u, v] = -[v, u]$ (antisymmetri)
$[au + bv, w] = a[u, w] + b[v, w],$ a og b er konstanter (linearitet).
$[uv, w] = u[v, w] + [u, w]v$ (produktregel)
$[u, [v, w]] + [v, [w, u]] + [w, [u, v]] = 0$ (Jacobis identitet)

Den sidste sætning bevises i lærebogen. Dette bevis samt de næste 2 sider er kursorisk læsning [side 391-393(nederst)].

Det differentielle volumenelement i faserummet er kanonisk invariant:

$$d\eta = dq_1 dq_2 \ldots dq_n dp_1 dp_2 \ldots dp_n, \qquad d\zeta = dQ_1 dQ_2 \ldots dQ_n dP_1 dP_2 \ldots dP_n$$

Sammenhænget mellem de to volumenelementer er givet ved absolutværdien af Jacobi-determinanten:

$$d\zeta = |J_D| d\eta = \left| \left| \frac{\partial(Q_1, \ldots, Q_n, P_1, \ldots, P_n)}{\partial(q_1, \ldots, q_n, p_1, \ldots, p_n)} \right| \right| d\eta = \left| \left| \frac{\partial \boldsymbol{\zeta}}{\partial \boldsymbol{\eta}} \right| \right| d\eta = ||\overline{\overline{M}}|| d\eta = d\eta,$$

idet $\widetilde{\overline{\overline{M}}}\,\overline{\overline{J}}\,\overline{\overline{M}} = \overline{\overline{J}} \quad \Rightarrow \quad |\overline{\overline{M}}|^2 |\overline{\overline{J}}| = |\overline{\overline{J}}|$

Den symplektiske betingelse medfører eksistensen af en genererende funktion F for transformationen:

De to metoder er ækvivalente [beviset på side 395-396(nederst) er kursorisk læsning].

Poissonparenteser i Hamiltonteorien (i)

Vilkårlig funktion $u = u(\mathbf{q}, \mathbf{p}, t)$

$$\frac{du}{dt} = \frac{\partial u}{\partial q_i}\dot{q}_i + \frac{\partial u}{\partial p_i}\dot{p}_i + \frac{\partial u}{\partial t} = \frac{\partial u}{\partial q_i}\frac{\partial H}{\partial p_i} - \frac{\partial u}{\partial p_i}\frac{\partial H}{\partial q_i} + \frac{\partial u}{\partial t} = [u, H] + \frac{\partial u}{\partial t}$$

Hamiltonligningerne kan omskrives enten ved at benytte

(1) $u = u(q_i) = q_i$ eller $u = u(p_i) = p_i$ i ligningen ovenfor, i hvilke tilfælde $\dfrac{\partial u}{\partial t} = 0$

(2) definitionen, ligning (9.67), af en Poissonparentes:

$$[q_i, H] = \frac{\partial q_i}{\partial q_j}\frac{\partial H}{\partial p_j} - \frac{\partial q_i}{\partial p_j}\frac{\partial H}{\partial q_j} = \delta_{ij}\dot{q}_j - 0(-\dot{p}_j) = \dot{q}_i$$

$$[p_i, H] = \frac{\partial p_i}{\partial q_j}\frac{\partial H}{\partial p_j} - \frac{\partial p_i}{\partial p_j}\frac{\partial H}{\partial q_j} = 0\,\dot{q}_j - \delta_{ij}(-\dot{p}_j) = \dot{p}_i$$

I symplektisk notation, $\dot{\boldsymbol{\eta}} = [\boldsymbol{\eta}, H]$ og dermed også $\dot{\boldsymbol{\eta}} = \overline{\overline{J}}\dfrac{\partial H}{\partial \boldsymbol{\eta}} = [\boldsymbol{\eta}, H]$

Benyttes $u = H$ fås umiddelbart det kendte resultat: $\dfrac{dH}{dt} = [H, H] + \dfrac{\partial H}{\partial t} = \dfrac{\partial H}{\partial t}$

Er u en bevægelseskonstant, $\dot{u} = 0$, fås $[H, u] = \dfrac{\partial u}{\partial t}$ og dermed $[H, u] = 0$, hvis u ikke afhænger eksplicit af t (kvantemekanik: Operatoren, svarende til en bevægelseskonstant, kommuterer med Hamiltonen).

Jacobis identitet, $[u, [v, w]] + [v, [w, u]] + [w, [u, v]] = 0$, kan i nogle tilfælde benyttes til at identificere nye bevægelseskonstanter: Indsættes $w = H$ og er u og v bevægelseskonstanter $\Rightarrow$ $[H, [u, v]] = 0$, eller at $[u, v]$ er en ny bevægelseskonstant.

Poissonparenteser i Hamiltonteorien (ii)

Infinitesimal kanonisk transformation: $F_2 = q_i P_i + \epsilon G(\mathbf{q}, \mathbf{P}, t) \quad \Rightarrow \quad \boldsymbol{\eta} \mapsto \boldsymbol{\zeta} = \boldsymbol{\eta} + \delta\boldsymbol{\eta}$

(9.63) $\delta\boldsymbol{\eta} = \epsilon \overline{\overline{J}} \dfrac{\partial G}{\partial \boldsymbol{\eta}} \quad \Rightarrow \quad \delta u = u(\boldsymbol{\eta} + \delta\boldsymbol{\eta}) - u(\boldsymbol{\eta}) = \widetilde{\dfrac{\partial u}{\partial \boldsymbol{\eta}}} \delta\boldsymbol{\eta} = \epsilon \widetilde{\dfrac{\partial u}{\partial \boldsymbol{\eta}}} \overline{\overline{J}} \dfrac{\partial G}{\partial \boldsymbol{\eta}} \equiv \epsilon[u, G]$

Benyttes $G = P_i = p_i + \mathcal{O}(\epsilon) \Rightarrow \delta\eta_j = \epsilon[\eta_j, G] = \epsilon[\eta_j, p_i] = \epsilon\, \delta_{ij}$ dvs. $\delta q_i = \epsilon$ og $\delta\eta_{j \neq i} = 0$

eller $\quad \delta u = \epsilon[u, p_i] = \delta q_i [u, p_i] \quad \Rightarrow \quad \dfrac{\delta u}{\delta q_i} = \dfrac{\partial u}{\partial q_i} = [u, p_i]$

Ved (uendelig mange) succesive anvendelser af generatoren svarende til G genereres en (aktiv) forskydning af systemet i faserummet, fra (0) til (1), hvor $q_i(0) \mapsto q_i(1)$ mens alle andre koordinater er uændret. En Taylor-rækkeudvikling giver, $\Delta q_i = q_i(1) - q_i(0)$,

$$
\begin{aligned}
u(1) &= u(0) + \frac{du(0)}{dq_i}\Delta q_i + \tfrac{1}{2}\frac{d^2u(0)}{dq_i^2}(\Delta q_i)^2 + \cdots \\
&= u(0) + [u, p_i]_0 \Delta q_i + \tfrac{1}{2}[[u, p_i], p_i]_0 (\Delta q_i)^2 + \tfrac{1}{3!}[[[u, p_i], p_i], p_i]_0 (\Delta q_i)^3 + \cdots
\end{aligned}
$$

Eksempelvis: (i) $(q_i, p_i) = (x, p_x) \Rightarrow p_x = m\dot{x}$ genererer en forskydning af m stykket $x(1) - x(0)$ i x aksens retning. (ii) $(q_i, p_i) = (\phi, p_\phi) = (\phi, L_z) \Rightarrow L_z = \sum_i (\mathbf{r}_i \times \mathbf{p}_i) \cdot \hat{\mathbf{z}}$ genererer en rotation af et mange-partikel system vinklen $\phi(1) - \phi(0)$ omkring z-aksen.

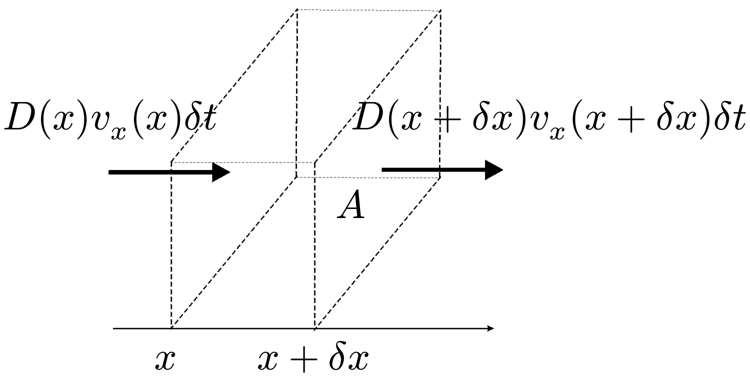
Benyttes $u = H$ og er p_i en bevægelseskonstant, $[H, p_i] = 0, \quad \Leftrightarrow \quad H(1) = H(0)$:
Hvis Hamiltonfunktionen er invariant overfor en infinitesimal kanonisk transformation, så er dens generator en bevægelseskonstant.

Tidsudvikling: For $u = u(\mathbf{q}, \mathbf{p})$ og dermed $\dfrac{du}{dt} = [u, H]$ fås analogt:
$u(t) = u(0) + [u, H]_0 t + \tfrac{1}{2}[[u, H], H]_0 t^2 + \tfrac{1}{3!}[[[u, H], H], H]_0 t^3 + \cdots$

H er generatoren for en infinitesmal tidsforskydning af systemet. (t, H) kan opfattes som kanoniske variable. F.eks. hvis t er en cyklisk koordinat så er $\dot{H} = 0$.

Liouvilles teorem

Ensemble: En udgave af et makroskopisk ($n = 10^{23}$ partikler) system med et bestemt valg af $2n$ begyndelsesbetingelser (der er i overensstemmelse med givne begrænsninger).
$D = D(\mathbf{q}, \mathbf{p}, t)$: sandsynlighedstætheden af ensembler i faserummet. Statistisk midling: $\langle B(t)\rangle = \int BD d\Omega$, hvor $d\Omega$ er det differentielle volumen i faserummet og $\int D d\Omega = 1$.
Det enkelte ensemble kan afbildes som et punkt i faserummet, $E_i(t)$. Antallet af ensembler, $E_1, E_2, \ldots$, i faserummet er konstant $\Rightarrow$ *kontinuitetsligning*:



$$\delta D A \delta x = D(x) A v_x(x)\delta t - D(x+\delta x) A v_x(x+\delta x)\delta t$$

$$\left.\frac{\delta D}{\delta t}\right|_x = -\frac{D(x+\delta x)v_x(x+\delta x) - D(x)v_x(x)}{\delta x}$$

eller i flere dimensioner

$$\frac{\partial D(\mathbf{x},t)}{\partial t} + \sum_i \frac{\partial}{\partial x_i}\big[D(\mathbf{x},t)\dot{x}_i(\mathbf{x},t)\big] = 0$$

δD er den tidslige ændring af D på stedet $\mathbf{x}$.

I det $2n$-dimensionale faserum:

$$\frac{\partial D}{\partial t} + \sum_{i=1}^{n}\left[\frac{\partial(D\dot{q}_i)}{\partial q_i} + \frac{\partial(D\dot{p}_i)}{\partial p_i}\right] = \frac{\partial D}{\partial t} + \sum\left[\dot{q}_i\frac{\partial D}{\partial q_i} + \dot{p}_i\frac{\partial D}{\partial p_i} + D\left(\frac{\partial \dot{q}_i}{\partial q_i} + \frac{\partial \dot{p}_i}{\partial p_i}\right)\right] = 0$$

$$\frac{\partial \dot{q}_i}{\partial q_i} = \frac{\partial}{\partial q_i}\frac{\partial H}{\partial p_i}, \qquad \frac{\partial \dot{p}_i}{\partial p_i} = -\frac{\partial}{\partial p_i}\frac{\partial H}{\partial q_i} \qquad \Rightarrow \qquad \frac{\partial \dot{q}_i}{\partial q_i} + \frac{\partial \dot{p}_i}{\partial p_i} = 0, \qquad \text{dvs.}$$

$$\frac{dD}{dt} = \frac{\partial D}{\partial t} + \sum\left(\frac{\partial D}{\partial q_i}\dot{q}_i + \frac{\partial D}{\partial p_i}\dot{p}_i\right) = \frac{\partial D}{\partial t} + [D, H] = 0 \qquad \text{(Liouvilles teorem)}$$

I **ligevægt** er $\langle B(t)\rangle$ = konstant og derfor $\dfrac{\partial D}{\partial t} = 0 \quad \Rightarrow$

$[D, H] = 0 \quad \Rightarrow \quad D$ kan kun afhænge af bevægelseskonstanter ($T + V$, $\mathbf{P}$, og $\mathbf{L}$).