به‌عنوان یک مثال، اکنون یک معادله ریاضی بر روی صفحه نوشته شده است. معادله درونیت که با نماد $\dot{q}_i$ نشان داده شده است، به صورت $\frac{d}{dt} \left( \frac{\partial H}{\partial \dot{q}_i} \right) = \frac{\partial H}{\partial q_i}$ نمایش داده شده است. در این مثال، $H$ نماد ارتفاع معادله و $q_i$ نماد مقیاس معادله است. همچنین در صفحه نوشته شده است که $q_i$ نماد مختصات مولکولی است و $p_i$ نماد آنتی‌سیمپاتیک مولکولی است. در هر صورت، این معادله به‌عنوان یک مثال از معادله مولکولی نشان داده شده است.
دل سیستم سکویی، دانسته‌ای از افزایش‌های نداشته و داشته باشد، (ت، ن، پ) را می‌گذاریم.


c_{1}^2 + c_{2}^2 + c_{3}^2 = 1


Legendre Transform: \( (t, p, s) \) لقب گرفته‌اند.

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\[ df = u \, dx + v \, dy \]

\[ u = \frac{\partial f}{\partial x} \quad v = \frac{\partial f}{\partial y} \]

\[ g = f - uz \]

\[ dg = df - u \, dx - v \, dy = \frac{\partial g}{\partial x} \, dx + \frac{\partial g}{\partial y} \, dy - v \, dy - x \, du \]

\[ g = v \, dy - x \, du \]

\[ x = \frac{\partial g}{\partial u}, \quad v = \frac{\partial g}{\partial e} \]


c_{1}^2 + c_{2}^2 + c_{3}^2 = 1


Legendre Transform: \( (t, p, s) \) لقب گرفته‌اند.

\[ du = dQ - dW \]

\[ du = T \, ds - P \, dV \]

\[ u = u(s, V) \]

\[ v = v(s, V) \]
\[ du = T\,ds - P\,dv \quad u = u(S, V) \]

\[ T = \frac{\partial u}{\partial S}, \quad P = -\frac{\partial u}{\partial V} \]

If the Helmholtz free energy is a function of \( S \) and \( P \), then

\[ H = H(S, P) \]

Enthalpy is defined as

\[ H = U + PV \]

Where the change in enthalpy is given by

\[ dh = du + P\,dv + V\,dP = T\,ds - P\,dv + P\,dv + V\,dP \]

\[ dh = T\,ds + V\,dP \]

Helmholtz free energy \( F(T, V) \)

\[ F = U - TS \]

\[ G = H - TS \]

\[ dl = \frac{\partial l}{\partial q_i} dq_i + \frac{\partial l}{\partial q_i} dq_i + \frac{\partial l}{\partial t} dt \]

\[ p_i = \frac{\partial l}{\partial q_i}, \quad p_i = \frac{\partial l}{\partial q_i} \]
\[ dL = \dot{p}_i \, dq_i + p_i \, dq_i + \frac{\partial L}{\partial t} \, dt \]

\[ H(q, p, t) = \dot{q}_i \, p_i - L(q, q, t) \]

\[ dh = \dot{q}_i \, dp_i + p_i \, dq_i - p_i \, dq_i - \frac{\partial L}{\partial t} \, dt \]

\[ \Rightarrow dh = \dot{q}_i \, dp_i - p_i \, dq_i - \frac{\partial L}{\partial t} \, dt \] (1)

\[ H = H(q, p) \Rightarrow dh = \frac{\partial H}{\partial q_i} \, dq_i + \frac{\partial H}{\partial p_i} \, dp_i + \frac{\partial H}{\partial t} \, dt \] (2)

Canonical equation of Hamiltonian system \( 2n + 1 \).

\[ \dot{q}_i = \frac{\partial H}{\partial p_i} \]

\[ -p_i = \frac{\partial H}{\partial q_i} \]

\[ \frac{\partial L}{\partial t} = \frac{\partial H}{\partial t} \]

C. G. J. Jacobi (1837) Comptes rendus de l'Académie des Sciences de Paris, s. p. 61 (1837)
The term symplectic comes from the Greek for "intertwined" and is particularly appropriate for Hamilton's equations where $\dot{q}$ is matched with a derivative with respect to $p$ and $p$ similarly with negative of a $q$ derivative. H. Weyl first introduced the term in 1939 in his book "The Classical Groups".

$$\eta_i = q_i, \quad \eta_{i+n} = p_i, \quad \eta = \begin{pmatrix} q_1 \\ q_2 \\ \vdots \\ q_n \\ p_1 \\ \vdots \\ p_n \end{pmatrix}$$

$$\frac{\partial H}{\partial \eta_i} = \frac{\partial H}{\partial \eta_{i+n}}$$

$$\mathbf{J} = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$$

$$\mathbf{J}^T = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} = -\mathbf{J} = \mathbf{J}^{-1}$$

$$\mathbf{J}^{T} = \mathbf{JJ}^{T} = \mathbf{I} \quad \mathbf{J}^{2} = -\mathbf{I} \quad \det \mathbf{J} = +1$$
\[ \eta = \int \frac{\partial H}{\partial \dot{\eta}} \]

\[
\begin{bmatrix}
q_1 \\
q_2 \\
\dot{q}_1 \\
\dot{q}_2
\end{bmatrix} =
\begin{bmatrix}
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1 \\
-1 & 0 & 0 & 0 \\
0 & -1 & 0 & 0
\end{bmatrix}
\begin{bmatrix}
\dot{p}_1 \\
\dot{p}_2 \\
p_1 \\
p_2
\end{bmatrix}
\]

Symplectic

Canonical Transform

...
\[ Q_i = Q_i(q, p, t) \]
\[ P_i = P_i(q, p, t) \]

A point transformation of phase space is defined by:

\[ \dot{Q} = \frac{\partial k}{\partial P_i} \]
\[ \dot{P}_i = -\frac{\partial k}{\partial Q_i} \]

The Hamiltonian is given by:

\[ H(q, p, t) = \sum_i (P_i Q_i - K(Q_i, P_i, t)) \]

With:

\[ \lambda (P_i Q_i - H) = P_i Q_i - K + \frac{dF}{dt} \]

Where \( F \) is a scaled function of the coordinates.
\[ Q_i' = \mu q_i, \quad P_i' = \nu P_i, \]

\[ Q' = \mu q, \quad P' = \nu P \]

\[ K'(Q', P') = \mu \nu H(q, p) \]

\[ \mu \nu (P_i q_i - H) = P_i' Q_i' - K' \]

\[ P_i q_i - H = P_i Q_i - K + \frac{dF}{dt} \]

1 ≠ 1 Extended canonical transformation.

1 = 1 Canonical transformation.

\[ Q_i = Q_i(q, p) \]

Restricted Canonical transformation.

\[ P_i = P_i(q, p) \]

Does not depend on time, explicitly.

\[ F \text{ is called "generating function" of transformation } \]

\[ F = F_q(q, Q, t) \]

\[ P_i q_i - H = P_i Q_i - K + \frac{dF}{dt} \]

\[ K = H + \frac{\partial F}{\partial t} \]
\[ Q_i = Q_i (q, p) \]
\[ P_i = P_i (q, p) \]

\[ \dot{Q}_i = \frac{\partial Q_i}{\partial q_j} \dot{q}_j + \frac{\partial Q_i}{\partial p_j} \dot{p}_j = \frac{\partial Q_i}{\partial q_j} \dot{q}_j + \frac{\partial Q_i}{\partial p_j} \dot{p}_j = \frac{\partial Q_i}{\partial q_j} \frac{\partial H}{\partial q_j} - \frac{\partial Q_i}{\partial p_j} \frac{\partial H}{\partial p_j} \]

\[ \dot{p}_j = \frac{\partial H}{\partial q_j} \]

\[ \dot{q}_j = \frac{\partial H}{\partial p_j} \]

\[ Q_i = \frac{\partial H}{\partial p_i} \]

That is, the transformation is canonical if

\[ \begin{pmatrix} \frac{\partial Q_i}{\partial q_j} \\ \frac{\partial Q_i}{\partial p_j} \end{pmatrix} = \begin{pmatrix} \frac{\partial P_j}{\partial q_i} \\ \frac{\partial P_j}{\partial p_i} \end{pmatrix} \]

\[ \begin{pmatrix} \frac{\partial P_i}{\partial q_j} \\ \frac{\partial P_i}{\partial p_j} \end{pmatrix} = - \begin{pmatrix} \frac{\partial Q_j}{\partial q_i} \\ \frac{\partial Q_j}{\partial p_i} \end{pmatrix} \]