VI Hamiltonian formulation

Equivalent to Lagrange formulation

Used for quantum mechanics
Statistical mechanics more intuitive in most cases.

1) Hamiltonian case of motion

Assume (for what follows):

- Holonomic
- MonofORMIC (\( V = V(q^i) \)) or
- Systems depend on velocities in previously discussed special cases only.

a) Legendre transformation

Lagrangian case of motion:

\[
\frac{d}{dt} \frac{\partial L}{\partial \dot{q}_i} - \frac{\partial L}{\partial q_i} = 0
\]
for \( n \) independent variables \( q_i \), in eqs of motion of second order:

Hamiltonian formulation:
in eqs of motion of first order:
variables: in generalized \( q_i \),
in canonical momenta \( \dot{p}_i \):

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

\((q, p) \) "canonical variables"

How to switch from \( L(q, \dot{q}; t) \) to \( H(q, p; t) \)?

Legendre transform

Imagine \( f(x, y) \) such that

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

\[
(u = \frac{\partial f}{\partial x}; \ v = \frac{\partial f}{\partial y})
\]

Define \( g = f - ux \)

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

with \( u = \frac{\partial g}{\partial y} \), \( x = \frac{\partial g}{\partial u} \)
Thermodynamics

\[ \text{d}U = \text{d}Q - \text{d}W = \text{ideal gas} \]

\[ = T\text{d}S - P\text{d}V \]

\[ \Rightarrow U = U(S,V), \quad T = \frac{\partial U}{\partial S}, \quad P = -\frac{\partial U}{\partial V} \]

**Enthalpy:** \( H = U + PV = H(S,P) \)

**Free energy (free energy):** \( F = U - TS = F(T,V) \)

**Free energy (free energy):** \( G = U - TS + PV = G(T,P) \)

**Lagrange's equations:**

\[ \text{d}L = \frac{\partial L}{\partial q_i} \text{d}q_i + \frac{\partial L}{\partial \dot{q}_i} \text{d}\dot{q}_i + \frac{\partial L}{\partial t} \text{dt} \]

with \( p_i = \frac{\partial L}{\partial \dot{q}_i} \Rightarrow p_i = \frac{\partial L}{\partial \dot{q}_i} \)
\[ dL = p_i \, dq_i + p_i \, dq_i + \frac{\partial L}{\partial t} \, dt \]

**Hamiltonian:**

\[ H = \dot{q}_i \, p_i - L = \]

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

\[ = \frac{\partial H}{\partial q_i} \, dq_i + \frac{\partial H}{\partial p_i} \, dp_i + \frac{\partial H}{\partial t} \, dt \]

\[ q_i, p_i \text{ independent} \]

\[ \begin{array}{c|c|c}
\hline
\quad & \dot{q}_i & \frac{\partial H}{\partial p_i} \\
\hline
\quad & \frac{\partial H}{\partial q_i} & p_i \\
\hline
\quad & \frac{\partial L}{\partial q_i} & -\frac{\partial L}{\partial t} \\
\hline
\end{array} \]

"canonical equations"

(compare: \( H = \hbar \), but defined in different variables!)

**Construction of Hamiltonian**

(1) Choose \( \{q_i\} = 0 \quad L = T - V \)

(2) Find conjugate momenta \( p_i = \frac{\partial L}{\partial \dot{q}_i} \)
3.) Legendre transform \( H = g_i \cdot p_i - L \)

1.) Find \( g_i \) as function of \( q, p, t \)

5.) replace \( g_i \) in \( H \).

For some cases, where

\[ h = T + V = \text{energy} \]

\[ H = T + V \]

**Examples:**

1.) \( T = \frac{m \cdot v^2}{2} = \frac{m}{2} \left( v^2 + r_1^2 \dot{r}_1^2 + r_2^2 \dot{r}_2^2 \right) \)

\[ V = V(\mathbf{r}, \mathbf{\dot{r}}, \mathbf{\ddot{r}}) \]

\[ p_r = \frac{\partial V}{\partial \dot{r}_1} = m \dot{r}_1 \]

\[ p_\theta = \frac{\partial V}{\partial \dot{r}_2} = m r_1^2 \dot{r}_2 \]

\[ p_\phi = \frac{\partial V}{\partial \dot{r}_\phi} = m r_1 r_2 \dot{r}_\phi \]

\[ T = \frac{p_r^2}{2m} + \frac{p_\theta^2}{2m r_1^2} + \frac{p_\phi^2}{2m r_2^2} \]

2.) \( T = \frac{m \cdot v^2}{2} - \frac{p_i \cdot r_i}{2m^2} \)

3.) particle with mass \( m \), charge \( q \), \( \mathbf{v} \) in electromagnetic field:

\[ L = T - V = \frac{m}{2} \mathbf{v}^2 - q \cdot \mathbf{v} \cdot \mathbf{A}(\mathbf{r}) - q \cdot \mathbf{A}(\mathbf{r}) \cdot \mathbf{v} \]
or \[ L = \frac{m}{\alpha} x_i \dot{x}_i - g y + g A_i \phi \]  \[ \rho_i = \frac{\partial L}{\partial \dot{x}_i} = m \ddot{x}_i + g A_i \]  \[ \Rightarrow \ddot{x}_i = \frac{\rho_i - g A_i}{m} \]  \[ = 0 \]  \[ H = \left( \frac{r - g A}{2m} \right)^2 + g \phi \]  

b) Cyclic coordinates \( q_i \): \[ \frac{\partial L}{\partial q_i} = 0 \]  \[ \Rightarrow \dot{p}_i = 0 = -\frac{\partial H}{\partial q_i} \]  \[ = 0 \] cyclic also in \( H \)!

true:
\[ \frac{dH}{dt} = \frac{\partial H}{\partial q_i} \dot{q}_i + \frac{\partial H}{\partial p_i} \dot{p}_i + \frac{\partial H}{\partial \dot{q}_i} \ddot{q}_i + \frac{\partial H}{\partial \dot{p}_i} \ddot{p}_i = \frac{\partial H}{\partial \dot{q}_i} \]  \[ = -\frac{\partial L}{\partial \dot{q}_i} \]

\( L \) independent of \( t \) => \( H \) indip. of \( t \)  
\[ \Rightarrow H = \text{const} \]  
(most of the time: \( H = E = \text{const} \), but counterexample in book!)