IV The Hamilton Formalism

4.1 Legendre Transformations

* Let \( f(x) \) be a function with \( \frac{df}{dx} = u \). We seek a function \( g(u) \) for which \( \frac{dg}{du} = -x \) or \( dg = -x \, du \).

The Legendre transform \( \mathcal{L}: C^1(I) \to C^1(Y) \), \( f \mapsto g \) where \( Y \subseteq \mathbb{R} \) is the domain of all values taken by \( \frac{df}{dx} \) over \( I \).

The Legendre transform has this property:

Why? \( df = u \, dx = d(ux) - x \, du \) \( \Rightarrow \) \( d(ux) = -x \, du \)

* If \( \frac{d^2f}{dx^2} \neq 0 \) then the Legendre transformation \( f \mapsto g \) is an invertible mapping between functions.

\[
\begin{align*}
  f(x) & \mapsto g(u) = f(x) - ux \\
  g(u) - \frac{dg}{du}u &= f(x) \\
  = -x
\end{align*}
\]

* For two variables \( f(x,y) \), \( df = u(x,y) \, dx + v(x,y) \, dy \)

\[
\frac{\partial f}{\partial x}g_y - \frac{\partial f}{\partial y}g_x
\]

The Legendre transform of \( f(x,y) \) w.r.t. \( y \) is defined by the property:

\( g(x,v) \) with \( dg = u \, dx - v \, dv \) i.e. \( u = \left( \frac{\partial g}{\partial x} \right)_v \), \( v = \frac{\partial g}{\partial v} \)
It is given by \( g(x, y) = f(x, y) - xy = f(x, y) - y \left( \frac{df}{dy} \right)_x \)

Again this is reversible.

Generalizations to more coordinates: easy.

* The Hamilton function of (2.4.3.1) is the negative Lagrangian transform of the Lagrange function w.r.t. the velocity coordinates.

\[
L(q_1, \ldots, q_5, \dot{q}_1, \ldots, \dot{q}_5; t) \rightarrow \sum_{i=1}^{5} p_i \dot{q}_i - L(q_1, \ldots, q_5, \dot{q}_1, \ldots, \dot{q}_5; t)
\]

\[
\equiv H(q_1, \ldots, q_5, p_1, \ldots, p_5; t)
\]

since \( p_i = \frac{\partial L}{\partial \dot{q}_i} \)

I.e. the Hamilton function is equivalent (contains the same information) as the Lagrange function. It describes a mechanical system completely.
4.2 The Hamilton Equations

* Differential of the Hamilton function:

directly: \[ dH = \sum_{i=1}^{s} \left( \frac{\partial H}{\partial q_i} dq_i + \frac{\partial H}{\partial p_i} dp_i \right) - \frac{\partial H}{\partial t} dt \]

from Legendre transform: \[ dH = \sum_{i=1}^{s} \left( p_i dq_i + q_i dp_i \right) - \sum_{i=1}^{s} \left( \frac{\partial L}{\partial q_i} dq_i + \frac{\partial L}{\partial q_i^*} dq_i^* \right) \frac{dq_i}{dt} \frac{dt}{dt} \]

\[ = \sum_{i=1}^{s} \left( p_i dq_i + q_i dp_i \right) - \frac{\partial L}{\partial t} dt \]

\[ \dot{q}_i = \frac{\partial H}{\partial p_i} \quad i = 1, \ldots, s \]

Hamilton's Equations

\[ \dot{p}_i = -\frac{\partial H}{\partial q_i} \quad i = 1, \ldots, s \]

Canonical Equations

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

* Hamilton Equations = 2s equations of motion of 1st order in time. (Compared to 2s equations of motion of 2nd order in the Lagrangian formalism)

They directly describe the motion of the system in phase space \((q(t), p(t))\)

* In symplectic form: let \(X = (q_1, q_2, p_1, \ldots, p_s)\) then in matrix form

\[ \dot{X} = S \cdot \nabla_X H \]  
where \(\nabla_X\) is the gradient vector \((\frac{\partial H}{\partial q_1}, \ldots, \frac{\partial H}{\partial q_s})\)

and  \(S = \begin{pmatrix} 0 & I_s \\ -I_s & 0 \end{pmatrix}\) is the symplectic matrix
* The total time derivative is

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

i.e. \( H = \text{const} \), with no explicit time-dependence

Way 2: \( \frac{\partial H}{\partial t} = \sum_{i=1}^{5} \frac{\partial H}{\partial q_i} \dot{q}_i + \sum_{i=1}^{5} \frac{\partial H}{\partial \dot{q}_i} \dot{\dot{q}}_i + \frac{\partial H}{\partial t} = \frac{\partial H}{\partial t} \)

\[
\frac{\partial H}{\partial \dot{q}_i} \dot{\dot{q}}_i - \frac{\partial H}{\partial q_i}
\]

* Let \( q_i \) be cyclical coord. \( \iff \frac{\partial L}{\partial \dot{q}_i} = 0 \) \( \iff \dot{q}_i = \text{const.} \)

Hence \( \dot{q}_i = -\frac{\partial H}{\partial \dot{q}_i} = 0 \) i.e. \( H \) does not depend on \( q_i \)

\( \dot{q}_i \equiv c_i \) is fixed by initial conditions \( \Rightarrow \) effective degrees of freedom reduced by one

* Partial Lagrange transformation (e.g. if we only transform cyclical coordinate)

Transform coordinates \( q_1 \ldots q_n \), leave \( q_{n+1} \ldots q_s \)

The Hamiltonian is

The Hamiltonian is

\[
R(\dot{q}_1, \ldots, \dot{q}_s; q_1, \ldots, q_n) = \sum_{i=1}^{n} p_i \dot{q}_i - L = H - \sum_{i=n+1}^{s} p_i \dot{q}_i
\]

\( R = H \) for \( n=s \) and \( R = -L \) for \( n=0 \)

The equations of motion are

\[
\dot{q}_i = \frac{\partial R}{\partial \dot{q}_i} \quad i = 1, \ldots, n
\]

\[
\dot{p}_i = -\frac{\partial R}{\partial q_i} \quad i = 1, \ldots, n
\]

\[
\frac{\partial R}{\partial \dot{q}_i} = \frac{\partial R}{\partial \dot{q}_i} = 0 \quad i = n+1, \ldots, s
\]

i.e. \( R \) is like Hamiltonian for \( q_1, \ldots, q_n \) and like Lagrange fit. for \( q_{n+1}, \ldots, q_s \)

Way 2: Compare coefficients of \( dR \) as done above for \( dH \).

\[ (LL 841) \]
* Hamiltonian for single particle in potential energy \( U(x, y, z) \):

- in cartesian coord., \( H = \frac{1}{2m} (p_x^2 + p_y^2 + p_z^2) + U(x, y, z) \)

Why? \( L = \frac{1}{2m} (x^2 + y^2 + z^2) = U \); \( p_i = \frac{\partial L}{\partial \dot{q}_i} = m \dot{q}_i \)

\[ H = \frac{1}{2m} (x^2 + y^2 + z^2) - L = \frac{1}{2m} (x^2 + y^2 + z^2) + U = \frac{1}{2m} (p_x^2 + p_y^2 + p_z^2) + U \]

- in cylindrical coord. \( H = \frac{1}{2m} \left( p_r^2 + \frac{p_\theta^2}{r^2} + p_z^2 \right) + U(r, \theta, z) \)

- in spherical coord. \( H = \frac{1}{2m} \left( p_r^2 + \frac{p_\theta^2}{r^2} + \frac{p_\phi^2}{r^2 \sin^2 \theta} \right) + U(r, \theta, \phi) \)

* Particle with charge \( q \) in electromagnetic fields \( \vec{E}, \vec{B} \) with potentials \( \phi, \vec{A} \).

Recall \( L = \frac{1}{2m} \dot{r}^2 - q (\vec{A} \cdot \dot{\vec{r}}) \)

The Hamiltonian is \( H = \frac{1}{2m} (p - q \vec{A})^2 + q \phi \)

Why? \( \text{HW 10} \)

* Harmonic oscillator

\[ L = \frac{1}{2} m q'^2 - \frac{1}{2} k q^2 \quad \Rightarrow \quad p = \frac{\partial L}{\partial q'} = m q' \]

\[ \Rightarrow H(q, p) = \frac{p^2}{2m} + \frac{1}{2} k q^2 \]

Canonical equations:

\[ \dot{q} = \frac{\partial H}{\partial p} = \frac{p}{m} \quad \Rightarrow \quad \dot{p} = m \ddot{q} \]

\[ \dot{p} = -\frac{\partial H}{\partial q} = -k q \]

\( \frac{d}{dt} \left[ q^2 + \frac{k}{m} q \right] = 0 \quad \text{as it should} \)

Since \( \frac{\partial H}{\partial t} = 0 \quad \Rightarrow \quad E = H = \text{const.} \)

\[ \Rightarrow \quad \frac{p^2}{2mE} + \frac{q^2}{\frac{k}{m} E} = 1 \]

Lince phase space curves are ellipses around the origin with semi axes \( \sqrt{2mE} \) and \( \sqrt{\frac{2k}{m} E} \)
4.3 Poisson Brackets

* Let $f$ and $g$ be functions of $q = (q_1, q_2, \ldots, q_6)$, $p = (p_1, p_2, \ldots, p_6)$ and $t$.

We define the Poisson bracket of $f$ and $g$ as

$$
\{f, g\} = \sum_{i=1}^{6} \left( \frac{\partial f}{\partial q_i} \frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i} \frac{\partial g}{\partial q_i} \right)
$$

in symplectic form $\{f, g\} = \sum_{i=1}^{6} \left( \frac{\partial f}{\partial q_i} \frac{d}{dt} \frac{\partial g}{\partial q_i} - \frac{\partial f}{\partial p_i} \frac{d}{dt} \frac{\partial g}{\partial p_i} \right)$.

* Obviously for functions $f, f_1, g$ and a constant $c$ we have

$$
\{f, g\} = -\{g, f\} \quad \text{(anti-symmetry)}
$$

$$
\{f, c\} = 0 = \{c, g\} \quad \text{(zero element)}
$$

$$
\{f_1 + f_2, g\} = \{f_1, g\} + \{f_2, g\} \quad \text{(bi-linearity)}
$$

$$
\{c f_1, g\} = c \{f_1, g\} = \{f_1, c g\}
$$

$$
\{f_1 f_2, g\} = f_1 \{f_2, g\} + f_2 \{f_1, g\} \quad \text{(product rule)}
$$

$$
\frac{\partial}{\partial t} \{f, g\} = \left\{ \frac{\partial f}{\partial t}, g \right\} + \left\{ f, \frac{\partial g}{\partial t} \right\}
$$

* For the Hamiltonian $H$

$$
\{H, H\} = \sum_{k=1}^{6} \left( \frac{\partial H}{\partial q_k} \frac{\partial q_k}{\partial t} - \frac{\partial H}{\partial p_k} \frac{\partial p_k}{\partial t} \right) = \sum_{k=1}^{6} \left( \frac{\partial H}{\partial q_k} \frac{\partial q_k}{\partial t} + \frac{\partial H}{\partial p_k} \frac{\partial p_k}{\partial t} \right)
$$

Hence,

$$
\frac{df}{dt} = \frac{\partial f}{\partial t} + \{f, H\}
$$
In particular: if integral of motion \( \Rightarrow \frac{df}{dt} = -[f, H] \)
\[ \frac{df}{dt} = 0 \] if int. of motion and \( \frac{df}{dt} \) \( \Rightarrow \) \( [f, H] = 0 \)

* Poisson brackets of coordinates:

\[
[f_i, q_k] = \frac{\partial f_i}{\partial q_k}, \quad [p_k, q_i] = +\frac{\partial f_i}{\partial q_k}
\]

In particular:

\[
[f_i, q_k] = 0, \quad [p_i, q_k] = 0, \quad [p_i, q_k] = \delta_{ik}
\]

* Jacobi Identity:

\[
[f, [g, h]] + [g, [h, f]] + [h, [f, g]] = 0
\]

for fields \( f, g, h \)

Why: L \& S.42

* Poisson Theorem: Let \( f, g \) be integrals of motion, i.e. \( \frac{df}{dt} = 0 = \frac{dg}{dt} \)

Then \( [f, g] \) is also integral of motion.

Why: \[
\frac{d}{dt} [f, g] = [\frac{df}{dt}, g] + [f, \frac{dg}{dt}] + [h_i, [f, g]]
\]

\[
= -[f, [g, h]] - [g, [h, f]] \quad \text{(Jacobi)}
\]

\[
= [\frac{df}{dt}, g] + [f, \frac{dg}{dt} + [h_i, g]]
\]

\[
= [\frac{df}{dt}, g] + [f, \frac{dg}{dt}] = 0
\]
* Connection with quantum mechanics (QM)

The Poisson bracket has the same algebraic structure (Lie product) as the commutator in QM.

Classical mechanics \( \mathcal{CM} \)

function \( f \)
operator \( \hat{f} \)

Hamiltonian \( H \)
Hamilton operator \( \hat{H} \)

\[ [p_i, q_k] = -\delta_{ik} \]
\[ \frac{i}{\hbar} [\hat{p}_i, \hat{q}_k] = -\delta_{ik} \]

\[ \frac{df}{dt} = \frac{\partial f}{\partial t} + \{f, H\} \]
\[ \frac{d}{dt} \hat{f} = \frac{\partial \hat{f}}{\partial t} + \frac{i}{\hbar} [\hat{H}, \hat{f}] \]
4.4 Modified Action

4.4.1 Modified Hamilton Principle for Phase Space

We define the modified action in phase space

\[
S = \int_{t_1}^{t_2} \left( \sum_{i=1}^{s} p_i \dot{q}_i - \sum_{i,j} \frac{\partial H}{\partial q_{ij}} \right) dt
\]

We interpret \( S = S[p, q] \) as a functional on phase space curves (instead of only trajectories \( q \)).

* Let \( (p(t), q(t)) \) be the phase space curve of a system. We allow equal-time variations \( \delta p_i(t), \delta q_i(t), i = 1, \ldots, s \) with all 2s variations independent of each other and \( \delta p(t_1) = 0 = \delta p(t_2), \delta q(t_1) = 0 = \delta q(t_2) \)

\[
\begin{align*}
\delta S & = 0 \quad \text{for } (p(t), q(t)) \\
\delta p_i & = \frac{\partial H}{\partial \dot{p}_i}, \quad j = 1, \ldots, s \\
\delta q_i & = -\frac{\partial H}{\partial \dot{q}_i}
\end{align*}
\]

(i.e. \((p(t), q(t))\) is phase space curve of the system)

Why? Parameterize variations through parameters, e.g. \((\delta p, \delta q) = (\delta p_x, \delta q_x)\) with \((\delta p_x, \delta q_x)_{x=0} = (0, 0), \ p_x = p + \delta p_x, \ q_x = q + \delta q_x\)
Then \[ \delta S = \frac{\partial}{\partial \alpha} \int_{t_1}^{t_2} \left( \sum_{i=1}^{S} \left( \frac{\partial p_i}{\partial q_i} \dot{q}_i + \dot{p}_i \frac{\partial q_i}{\partial q_i} - \frac{\partial H}{\partial q_i} \frac{\partial q_i}{\partial p_i} - \frac{\partial H}{\partial p_i} \frac{\partial p_i}{\partial q_i} \right) \right) \, dt \]

\[ \Rightarrow \delta S = 0 \iff 0 = \frac{\partial}{\partial \alpha} \int_{t_1}^{t_2} \left( \sum_{i=1}^{S} \left( \frac{\partial p_i}{\partial q_i} \dot{q}_i + \dot{p}_i \frac{\partial q_i}{\partial q_i} - \frac{\partial H}{\partial q_i} \frac{\partial q_i}{\partial p_i} - \frac{\partial H}{\partial p_i} \frac{\partial p_i}{\partial q_i} \right) \right) \, dt \]

\[ \text{equal-time variations!} \quad \frac{d}{dt} \frac{\partial H}{\partial q_i} \]

Partial integration for the second term:

\[ \int_{t_1}^{t_2} \frac{d}{dt} \left( \frac{\partial q_i}{\partial \alpha} \right) \, dt = \left. \frac{\partial q_i}{\partial \alpha} \frac{\partial q_i}{\partial p_i} \right|_{t_1}^{t_2} \int_{t_1}^{t_2} \frac{d}{dt} \left( \frac{\partial q_i}{\partial p_i} \right) \, dt \]

\[ = 0 \quad \text{for} \quad p_{i,0} = p_{i}(t) = 0 \text{ etc.} \]

Using \( \delta q_i = \frac{\partial q_i}{\partial \alpha} \, \delta \alpha \), \( \delta p_i = \frac{\partial p_i}{\partial \alpha} \, \delta \alpha \) we have

\[ \delta S = 0 \iff 0 = \int_{t_1}^{t_2} \sum_{i=1}^{S} \left[ \delta p_i \left( \frac{\dot{q}_i - \frac{\partial H}{\partial q_i}}{\dot{p}_i} \right) - \delta q_i \left( \dot{p}_i + \frac{\partial H}{\partial q_i} \right) \right] \, dt \]

\[ \square \text{ since all variations } \delta q_i, \delta p_i \text{ independent} \]
4.4.2 The Action with Free Endpoint

* We considered action with fixed initial and end times $t_i$ and $t_e$ and fixed
initial and final points $q_1(t_i) = q_1$, $q_2(t_e) = q_2$ in Sec. II.

Now allow variations of the endpoint $q_2$.

* We have

$$\delta S = \left[ \int_{t_i}^{t_e} \sum_{i=1}^{s} \frac{\partial L}{\partial \dot{q}_i} \delta q_i \right] dt + \int_{t_i}^{t_e} \left( \partial L/\partial q_i - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}_i} \right) \delta q_i \, dt \quad \text{(see derivation in Sec. II)}$$

This term used to vanish for $\delta q_i(t_i) = 0$

$$\Rightarrow \delta S = \sum_{i=1}^{s} p_i \delta q_i \quad \text{where} \quad \delta q_i = \delta q_i(t_e)$$

And in particular for action depending on endpoint:

$$\frac{\delta S}{\delta q_i} = p_i$$

* Now also allow $t_i$ to be a parameter that can be varied.

Note: mathematically we simply define $S$ on a larger function space.

From the definition:

$$\frac{dS}{dt} = L$$

On the other hand

$$\frac{dS}{dt} = \frac{\delta S}{\delta t} + \sum_{i=1}^{s} \frac{\delta S}{\delta q_i} q_i = \frac{\delta S}{\delta t} + \sum_{i=1}^{s} p_i \dot{q}_i$$

$$\Rightarrow \frac{\delta S}{\delta t} = L - \sum_{i=1}^{s} p_i \dot{q}_i = -H$$

$$\Rightarrow dS = \sum_{i=1}^{s} p_i \, dq_i - H \, dt$$

$$\Rightarrow S = \int \sum_{i=1}^{s} \left( p_i \, dq_i - H \, dt \right)$$

Total differential of the action as a function of time and final point.
4.4.3 The Variational Principles of Maupertuis, Fermat and Jacobi

* Assume a Mechanical system with $\frac{dx}{dt} = 0 = \frac{dt}{dt}$

Consider variations of the trajectory with fixed end points but variable time and constant energy $E$.

Then $\delta S = -H \delta t \Rightarrow \delta S + E \delta t = 0$ since $E = H = \text{const.}$

On the other hand $S = \int_{t_i}^{t_f} \mathbf{p} \cdot d\mathbf{q} = E(t - t_i)$

$\Rightarrow \delta \left( \int_{t_i}^{t_f} \mathbf{p} \cdot d\mathbf{q} \right) = 0$

* We define the abbreviated action $\bar{S}$ of the system as

$$\bar{S} = \int_{t_i}^{t_f} \mathbf{p} \cdot d\mathbf{q} = \int_{t_i}^{t_f} (\mathbf{p} \cdot \dot{\mathbf{q}}) dt$$

Principle of Maupertuis: The motion of a system minimizes the abbreviated action for variations of the path of constant energy but different times, i.e. $\delta \bar{S} = 0$

* The special case of free motion ($U = \text{const.}$) leads to Fermat's Principle:

For free system the motion is the one with the shortest duration between initial and final point, i.e.

$$\delta \left( \int_{t_i}^{t_f} dt \right) = \delta (t - t_i) = 0$$
Why? \[ U = \text{const.} \Rightarrow \sum_{i=1}^{N} p_i \dot{q}_i = 2T = \text{const.} \]

\[ \Rightarrow \sum_{i=1}^{N} \left( \frac{1}{2} \right) p_i \dot{q}_i \, dt = 2T \int dt = 0 \]

Same as in geometrical optics!

- We can eliminate time completely from the variational principle and only base it on the shape of the trajectory.

Consider: \[ L = \frac{1}{2} \sum_{i,j} a_{ij} \dot{q}_i \dot{q}_j - U \Rightarrow p_i = \sum_j \dot{q}_j \]

Energy: \[ E = \frac{1}{2} \sum_{i,j} a_{ij} \dot{q}_i \dot{q}_j + U \Rightarrow dt = \sqrt{2(E-U) \sum_{i,j} a_{ij} \dot{q}_i \dot{q}_j} \]

Hence: \[ S = \int \sum_{i,j} a_{ij} \frac{dq_i}{dt} \, dq_j = \int \sqrt{2(E-U) \sum_{i,j} a_{ij} \, dq_i \, dq_j} \]  \( (*) \)

- The condition \( \delta S = 0 \) in the form \( (*) \) is called Jacobi Principle.