IV The Hamilton Formalism

4.1 Legendre Transformations

$I \to \mathbb{R}$ ($I \subseteq \mathbb{R}$ interval)

* Let $f(x)$ be C^1 function with $df = \frac{df}{dx} dx \equiv u\, dx$

We seek a function $g(u)$ for which $\frac{dg}{du} = -x$ or $dg = -x\, du$

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

$$\boxed{g(u) = f(x) - ux = f(x) - x\frac{df}{dx}}$$

has this property.

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

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

$$f(x) \xmapsto{\mathcal{L}} g(u) = f(x) - ux \xmapsto{\mathcal{L}} g(u) - \underbrace{\frac{dg}{du}}_{=-x} u = f(x)$$

* For two variables $f(x,y)$, $df = \underbrace{u(x,y)}_{\left(\frac{\partial f}{\partial x}\right)_y} dx + \underbrace{v(x,y)}_{\left(\frac{\partial f}{\partial y}\right)_x} dy$

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

$g(x,v)$ with $dg = u\,dx - y\,dv$ i.e. $u = \left(\frac{\partial g}{\partial x}\right)_v$, $y = -\left(\frac{\partial g}{\partial v}\right)_x$

It is given by $g(x,v) = f(x,y) - vy = f(x,y) - y\left(\frac{\partial f}{\partial y}\right)_x$

Again this is reversible.

Generalizations to more coordinates: easy.

* The Hamilton Function of (2.4.3.1) is the negative Legendre transform of the Lagrange fct. w.r.t. the velocity coordinates

$$\boxed{\begin{aligned} L(q_1,\dots,q_s,\dot{q}_1,\dots,\dot{q}_s,t) &\xrightarrow{\mathcal{L}} \sum_{i=1}^{s} p_i\dot{q}_i - L(q_1,\dots,q_s,\dot{q}_1,\dots,\dot{q}_s,t) \\ &\equiv H(q_1,\dots,q_s,p_1,\dots,p_s,t) \end{aligned}}$$

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

I.e. the Hamilton fct. is equivalent (carries the same information) as the Lagrange fct. It describes a mechanical system completely.

4.2 The Hamilton Equations

* Differential of the Hamilton fct.:

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 transf.: $$dH = \sum_{i=1}^{s} \left(p_i d\dot{q}_i + \dot{q}_i dp_i \right) - \sum_{i=1}^{s} \left(\underbrace{\frac{\partial L}{\partial q_i}}_{=\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_i} = \dot{p}_i} dq_i + \frac{\partial L}{\partial \dot{q}_i} d\dot{q}_i \right) - \frac{\partial L}{\partial t} dt$$

$$= \sum_{i=1}^{s} \left(-\dot{p}_i dq_i + \dot{q}_i dp_i \right) - \frac{\partial L}{\partial t} dt$$

$$\Rightarrow \boxed{\begin{aligned} \dot{q}_i &= \frac{\partial H}{\partial p_i} \qquad i = 1, .., s \\ \dot{p}_i &= -\frac{\partial H}{\partial q_i} \qquad i = 1, .., s \\ -\frac{\partial L}{\partial t} &= \frac{\partial H}{\partial t} \end{aligned}}$$

Hamilton's Equations
or
Canonical Equations

* Hamilton Equations = $2s$ equations of motion of 1^{st} order in time (compared to s e.o.m. of 2^{nd} order in the Lagrange formalism)
They directly describe the motion of the system in phase space $(q(t), p(t))$

* In symplectic form: Let $X = (q_1, .., q_s, p_1, .., p_s)$ then in matrix form

$$\dot{X} = S \cdot \nabla_X H$$ where ∇_X is the gradient vector $\left(\frac{\partial}{\partial q_1}, \ldots, \frac{\partial}{\partial p_s}\right)$

and $$S = \begin{array}{c} \left(\begin{array}{cc} 0 & \mathbb{1} \\ -\mathbb{1} & 0 \end{array} \right) \begin{array}{l} \} \ s \text{ rows} \\ \} \ s \text{ rows} \end{array} \\ \begin{array}{cc} \underbrace{}_{s} & \underbrace{}_{s} \end{array} \end{array}$$ is the symplectic matrix

* The total time derivative is

$$\boxed{\frac{dH}{dt} = \frac{\partial H}{\partial t}}$$

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

Why? $$\frac{dH}{dt} = \sum_{i=1}^{s} \frac{\partial H}{\partial q_i} \underbrace{\dot{q}_i}_{\frac{\partial H}{\partial p_i}} + \sum_{i=1}^{s} \frac{\partial H}{\partial p_i} \underbrace{\dot{p}_i}_{-\frac{\partial H}{\partial q_i}} + \frac{\partial H}{\partial t} = \frac{\partial H}{\partial t}$$

* Let q_j be cyclical coord. $\Leftrightarrow \frac{\partial L}{\partial q_j} = 0 \Leftrightarrow p_j = \text{const.}$

Hence $\dot{p}_j = -\frac{\partial H}{\partial q_j} = 0$ i.e. H does not depend on q_j

$p_j \equiv c_j$ is fixed by initial conditions $\Rightarrow$ effective degrees of freedom reduced by one

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

Transform coordinates $q_1, \dots, q_n$, leave $q_{n+1}, \dots, q_s$

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The Routhian is

$$R(q_1, \dots, q_n; p_1, \dots, p_n; q_{n+1}, \dots, q_s; \dot{q}_{n+1}, \dots, \dot{q}_s) = \sum_{i=1}^{n} p_i \dot{q}_i - L = H - \sum_{i=n+1}^{s} p_i \dot{q}_i$$

$R = H$ for $n = s$ and $R = -L$ for $n = 0$

The equations of motion are

$$\dot{q}_i = \frac{\partial R}{\partial p_i} \qquad i = 1, \dots, n \qquad\qquad \frac{d}{dt}\frac{\partial R}{\partial \dot{q}_i} - \frac{\partial R}{\partial q_i} = 0 \qquad i = n+1, \dots, s$$

$$\dot{p}_i = -\frac{\partial R}{\partial q_i} \qquad i = 1, \dots, n \qquad\qquad \frac{\partial R}{\partial t} = -\frac{\partial L}{\partial t}$$

i.e. R is like Hamiltonian for $q_1, \dots, q_n$ and like Lagrange fct. for $q_{n+1}, \dots, q_s$

Why? Compare coefficients of dR as done above for dH. (LL §41)

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

    $$H = m(\dot{x}^2+\dot{y}^2+\dot{z}^2) - L = \frac{1}{2}m(\dot{x}^2+\dot{y}^2+\dot{z}^2) + U = \frac{1}{2m}(p_x^2+p_y^2+p_z^2) + U$$
  - in cylindrical coord: $H = \frac{1}{2m}\left(p_r^2 + \frac{p_\phi^2}{r^2} + p_z^2\right) + U(r,\phi,z)$
  - 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 $L = \frac{1}{2}m\dot{\vec{r}}^2 - q(\phi - \dot{\vec{r}}\cdot\vec{A})$

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

  Why? HW 10

* Harmonic oscillator

  $L = \frac{1}{2}m\dot{q}^2 - \frac{1}{2}kq^2$; $\quad p = \frac{\partial L}{\partial \dot{q}} = m\dot{q}$

  $\Rightarrow H(p,q) = \frac{p^2}{2m} + \frac{1}{2}kq^2$

  Canonical equations: $\left.\begin{aligned} \dot{q} &= \frac{\partial H}{\partial p} = \frac{p}{m} \Rightarrow \dot{p} = m\ddot{q} \\ \dot{p} &= -\frac{\partial H}{\partial q} = -kq \end{aligned}\right\} \Rightarrow \ddot{q} + \frac{k}{m}q = 0$

  as it should

  Since $\frac{\partial H}{\partial t} = 0 \Rightarrow E \equiv H = \text{const.}$

  $\Rightarrow \frac{p^2}{2mE} + \frac{q^2}{\frac{2E}{k}} = 1$ hence phase space curves are ellipses around the origin with semi axes $\sqrt{2mE}$ and $\sqrt{\frac{2E}{k}}$

4.3 Poisson Brackets

* Let f and g be functions of $q = (q_1, \ldots, q_s)$, $p = (p_1, \ldots, p_s)$ and t.

  We define the Poisson bracket of f and g as

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

In symplectic form $[f, g] = (\nabla_x f)^T S (\nabla_x g)$

* Obviously for functions f_1, f_2, g and a const c we have

$$[f, g] = -[g, f] \qquad \text{(anti-symmetry)}$$

$$[f, c] = 0 = [c, g] \qquad \text{(zero element)}$$

$$\left.\begin{aligned} [f_1 + f_2, g] &= [f_1, g] + [f_2, g] \\ [c f_1, g] &= c[f_1, g] = [f_1, c g] \end{aligned}\right\} \text{((bi) linearity)}$$

$$[f_1 f_2, g] = f_1 [f_2, g] + f_2 [f_1, g] \qquad \text{product rule}$$

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

* For the Hamiltonian H

$$[f, H] = \sum_{k=1}^{s} \left(\underbrace{\frac{\partial H}{\partial p_k}}_{\dot{q}_k} \frac{\partial f}{\partial q_k} - \underbrace{\frac{\partial H}{\partial q_k}}_{-\dot{p}_k} \frac{\partial f}{\partial p_k} \right) = \sum_{k=1}^{s} \left(\frac{\partial f}{\partial q_k} \dot{q}_k + \frac{\partial f}{\partial p_k} \dot{p}_k \right)$$

Hence

$$\boxed{\frac{df}{dt} = \frac{\partial f}{\partial t} + [f, H]}$$

In particular: f integral of motion $\Leftrightarrow$ $\frac{\partial f}{\partial t} = -[f, H]$

if $\frac{\partial f}{\partial t} = 0$ $\quad$ f int. of motion and $\cancel{\frac{\partial f}{\partial t}}$ $\Leftrightarrow$ $[f, H] = 0$

* Poisson brackets of coordinates:

$$[f, q_k] = -\frac{\partial f}{\partial p_k} \qquad [f, p_k] = +\frac{\partial f}{\partial q_k}$$

In particular:
$$\boxed{[q_i, q_k] = 0 \qquad [p_i, p_k] = 0 \qquad [p_i, q_k] = -\delta_{ik}}$$

* Jacobi Identity: $\boxed{[f, [g,h]] + [g, [h,f]] + [h, [f,g]] = 0}$

for fcts. f, g, h

Why? LL §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? $\frac{d}{dt}[f,g] = \left[\frac{\partial f}{\partial t}, g\right] + \left[f, \frac{\partial g}{\partial t}\right] + \underbrace{[H, [f,g]]}_{= -[f, [g,H]] - [g, [H,f]] \quad \text{(Jacobi)}}$

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

$$= \left[\frac{df}{dt}, g\right] + \left[f, \frac{dg}{dt}\right] = 0$$

* Connection with quantum mechanics (QM)

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

classical mechanics	QM
function f	operator $\hat{f}$
Hamiltonian H	Hamilton operator $\hat{H}$
$[p_i, q_k] = -\delta_{ik}$	$\frac{i}{\hbar}[\hat{p}_i, \hat{q}_k] = -\delta_{ik}$
$\frac{df}{dt} = \frac{\partial f}{\partial t} + [f, H]$	$\frac{d}{dt}\hat{f} = \frac{\partial}{\partial t}\hat{f} + \frac{i}{\hbar}[\hat{H}, \hat{f}]$

4.4 Modified Action

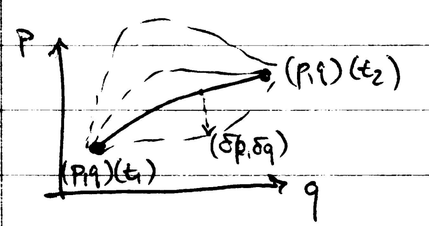
4.4.1 Modified Hamilton Principle for Phase Space

* We define the modified action in phase space

$$\boxed{S = \int_{t_1}^{t_2} \left(\sum_{i=1}^{s} p_i \dot{q}_i - H(p,q,t) \right) dt}$$

We interpret $S \equiv S[p,q]$ 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 <u>equal-time</u> variations $\delta p_i(t)$, $\delta q_i(t)$, $i = 1, .., s$ with all $2s$ variations <u>independent</u> of each other and $\delta p(t_1) = 0 = \delta p(t_2)$; $\delta q(t_1) = 0 = \delta q(t_2)$



* Modified Hamilton Principle:

$\delta S = 0$ for a $(p(t), q(t))$ $\iff$ $$\dot{q}_j = \frac{\partial H}{\partial p_j}, \quad \dot{p}_j = -\frac{\partial H}{\partial q_j}, \quad j = 1, .., s$$

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

Why? Parameterize variations through parameters, e.g. $(\delta p, \delta q) = (\delta p_\alpha, \delta q_\alpha)$ with $(\delta p_\alpha, \delta q_\alpha)_{\alpha=0} = (0,0)$. $p_\alpha = p + \delta p_\alpha$, $q_\alpha = q + \delta q_\alpha$

Then $\delta S = \frac{\partial}{\partial\alpha} \int_{t_1}^{t_2} dt \left(\sum_{i=1}^{s} p_\alpha \dot{q}_\alpha - H(p_\alpha, q_\alpha, t) \right) d\alpha$

$$\Rightarrow \delta S = 0 \iff 0 = d\alpha \int_{t_1}^{t_2} dt \left(\sum_{i=1}^{s} \left(\frac{\partial p_{\alpha j}}{\partial \alpha} \dot{q}_{\alpha j} + p_{\alpha j} \underbrace{\frac{\partial \dot{q}_{\alpha j}}{\partial \alpha}}_{\frac{d}{dt}\frac{\partial q_{\alpha j}}{\partial \alpha}} - \frac{\partial H}{\partial q_{\alpha j}} \frac{\partial q_{\alpha j}}{\partial \alpha} - \frac{\partial H}{\partial p_{\alpha j}} \frac{\partial p_{\alpha j}}{\partial \alpha} \right) \right)_{\alpha=0}$$

equal-time variations!

partial integration for the second term:

$$\int_{t_1}^{t_2} dt\, p_{\alpha j} \frac{d}{dt} \frac{\partial q_{\alpha j}}{\partial \alpha} = \underbrace{\left(p_{\alpha j} \frac{\partial q_{\alpha j}}{\partial \alpha} \right)\Big|_{t_1}^{t_2}}_{=0 \text{ for } p_{\alpha=0}(t_1) = p_{\alpha=0}(t_2) = 0 \text{ etc.}} - \int_{t_1}^{t_2} dt\, \dot{p}_{\alpha j} \frac{\partial q_{\alpha j}}{\partial \alpha}$$

Using $\delta q_j = \frac{\partial q_j}{\partial \alpha} d\alpha$, $\delta p_j = \frac{\partial p_j}{\partial \alpha} d\alpha$ we have

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

$\square$ since all variations $\delta q_i, \delta p_j$ independent

4.4.2 The Action with Free Endpoint

* We considered action with fixed initial and end times t_1 and t_2 and fixed initial and final points $\underbrace{q(t_1)}_{\equiv q_1}$, $\underbrace{q(t_2)}_{\equiv q_2}$ in Sec. II.

Now allow variations of the endpoint q_2!

* We have $$\delta S = \underbrace{\left[\sum_{i=1}^{s} \frac{\partial L}{\partial \dot{q}_i}\delta q_i\right]_{t_1}^{t_2}}_{\text{this term used to vanish for } \delta q_i(t_2)=0} + \int_{t_1}^{t_2} \sum_{i=1}^{s} \underbrace{\left(\frac{\partial L}{\partial q_i} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}_i}\right)}_{\text{vanishes for physical trajectory}} \delta q_i \, dt$$ (see derivation in 2.1)

$$\Rightarrow \delta S = \sum_{i=1}^{s} p_i \, \delta q_i \qquad \text{where } \delta q_i \equiv \delta q_i(t_2)$$

and in particular for action depending on end point: $\boxed{\frac{\partial S}{\partial q_i} = p_i}$

* Now also allow $t_2 \equiv t$ to be a parameter that can be varied:

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

From the definition: $\boxed{\frac{dS}{dt} = L}$

on the other hand $$\frac{dS}{dt} = \frac{\partial S}{\partial t} + \sum_{i=1}^{s} \frac{\partial S}{\partial q_i}\dot{q}_i = \frac{\partial S}{\partial t} + \sum_{i=1}^{s} p_i \dot{q}_i$$

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

$$\Rightarrow \boxed{dS = \sum_{i=1}^{s} p_i \, dq_i - H \, dt}$$ total differential of the action as a function of time and final point

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

4.4.3 The Variational Principles of Maupertuis, Fermat and Jacobi

* Assume a mechanical system with $\frac{\partial L}{\partial t} = 0 = -\frac{\partial H}{\partial t}$

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 $S = \int \sum_{i=1}^{s} p_i\,dq_i - E(t - t_1)$

$$\underset{\text{Combine}}{\Rightarrow} \quad \delta\left(\int \sum_{i=1}^{s} p_i\,dq_i\right) = 0$$

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

$$\boxed{\bar{S} = \int \sum_{i=1}^{s} p_i\,dq_i = \int\left(\sum_{i=1}^{s} p_i \dot{q}_i\right) dt}$$

Principle of Maupertuis: The motion of a system minimizes the abbreviated action for variations of the path at 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.

$$\delta\left(\int_{t_1}^{t} dt\right) = \delta(t - t_1) = 0$$

Why? $U = \text{const.} \Rightarrow \sum_{i=1}^{s} p_i \dot{q}_i = 2T = \text{const.}$

$$\Rightarrow \delta \int \left(\sum_{i=1}^{s} p_i \dot{q}_i\right) dt = 2T \int dt \neq 0$$

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

Energy $E = \frac{1}{2} \sum_{i,j} a_{ij} \dot{q}_i \dot{q}_j + U \Rightarrow dt = \sqrt{\dfrac{\sum_{i,j} a_{ij} dq_i \, dq_j}{2(E-U)}}$

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

* The condition $\delta \bar{S} = 0$ in the form $(*)$ is called Jacobi Principle.