8. Hamilton's equations

"Lagrange vs Hamilton":

- Equivalent equations and the same physics; just different methods.
- Hamilton's procedure suitable within quantum and statistical mechanics.

We assume holonomic systems, and potentials that are conservative, $V = V(q)$, or velocity dependent, $U = U(q, \dot{q})$, such that $Q_i = -\partial U/\partial q_i + \frac{d}{dt}\partial U/\partial \dot{q}_i$, to include E.M. fields in our description.

- Lagrange: $\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_i} - \frac{\partial L}{\partial q_i} = 0 \; ; \; i = 1, 2, \cdots, n$

  I.e., n 2. order differential equations.

  State of system: Point in n-dim. configuration space with axes q_i

- Hamilton: $2n$ 1. order diff. eqns.

  State of system: Point in $2n$-dim. phase space with axes q_i and p_i, with

$$p_i = \frac{\partial L}{\partial \dot{q}_i} \quad ; \quad i = 1, 2, \cdots, n$$

q, p are <u>canonical variables</u>

- Both formulations result in $2n$ integration constants and require $2n$ initial conditions for complete solution.

8.1 Legendre transformations and Hamiltons eqns of motion

Transition from Lagrange to Hamilton involves a change of variables, from $(q, \dot{q}, t)$ to (q, p, t) with $p_i = \partial L / \partial \dot{q}_i$.

Legendre transformation:

Assume function $f(x,y)$ such that

$$df = u \cdot dx + v \cdot dy \quad ; \quad u(x,y) = \frac{\partial f}{\partial x} \;, \quad v(x,y) = \frac{\partial f}{\partial y}$$

Want to change variables ("basis") from (x,y) to (u,y).
Define $g = f - u \cdot x$ (old function minus product of new and old variable). Then:

$$dg = df - u\,dx - x\,du = v\,dy - x\,du$$

with

$$v = v(u,y) = \frac{\partial g}{\partial y} \quad ; \quad x = x(u,y) = -\frac{\partial g}{\partial u}$$

Ex: Thermodynamics

1. + 2. law : $T dS = dU + p dV \Rightarrow dU = T dS - p dV$

$$U = U(S,V), \quad T = \partial U / \partial S, \quad p = -\partial U / \partial V$$

More convenient with enthalpy $H = H(S,p) = U + pV$ for isentropic and isobaric processes:

$$dH = dU + p dV + V dp = T dS + V dp \quad ; \quad T = \partial H / \partial S, \quad V = \partial H / \partial p$$

More convenient with Gibbs' free energy $G(T,p) = H - TS$ for isothermal and isobaric processes:

$$dG = dH - T dS - S dT = V dp - S dT \; ; \quad V = \partial G / \partial p \,, \quad S = -\partial G / \partial T$$

The natural Legendre transf. for changing variables from $(q, \dot{q}, t)$ to (q, p, t) is:

$$H = p\dot{q} - L = H(q, p, t)$$

With summation over repeated index:

$$dH = d(p_i \dot{q}_i - L) = p_i \, d\dot{q}_i + \dot{q}_i \, dp_i - dL$$

In addition, with $H = H(q_i, p_i, t)$:

$$dH = \frac{\partial H}{\partial q_i} dq_i + \frac{\partial H}{\partial p_i} dp_i + \frac{\partial H}{\partial t} dt$$

We have also:

$$dL = \frac{\partial L}{\partial q_i} dq_i + \frac{\partial L}{\partial \dot{q}_i} d\dot{q}_i + \frac{\partial L}{\partial t} dt$$

Canonical momentum: $p_i = \partial L / \partial \dot{q}_i$

Lagrange's equations:

$$\frac{\partial L}{\partial q_i} = \frac{d}{dt} \frac{\partial L}{\partial \dot{q}_i} = \frac{d}{dt} p_i = \dot{p}_i$$

The terms with $d\dot{q}_i$ cancel

$$\Rightarrow dH = -\dot{p}_i \, dq_i + \dot{q}_i \, dp_i - \frac{\partial L}{\partial t} dt$$

Comparison $(dH = dH)$ yields:

$$\boxed{\dot{q}_i = \frac{\partial H}{\partial p_i} \, , \quad \dot{p}_i = -\frac{\partial H}{\partial q_i}}$$

Hamilton's $\overbrace{\text{equations}}^{\text{(canonical)}}$ of motion

and $\frac{\partial H}{\partial t} = -\frac{\partial L}{\partial t}$

[whereas $\frac{dH}{dt} = -\frac{\partial L}{\partial t}$ for the energy function $H(q, \dot{q}, t)$]

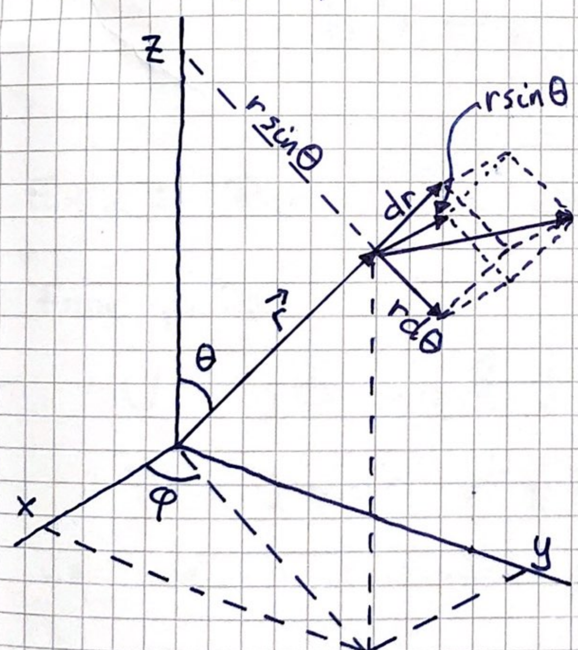
In summary, the typical recipe in the Hamilton(ian) formalism:

1. Construct $L(q, \dot{q}, t)$
2. Define canonical momenta $p_i = \partial L / \partial \dot{q}_i$
3. Construct $H = p_i \dot{q}_i - L = H(q, \dot{q}, p, t)$
4. Use $p_i = \partial L / \partial \dot{q}_i$ to express $\dot{q} = \dot{q}(q, p, t)$
5. Eliminate $\dot{q}_i$ from H to arrive at $H(q, p, t)$
6. Use H to solve the canonical equations of motion

Two important examples:

Ex 1: Particle in central forcefield, $V = V(r)$

Reminder, spherical coordinates: $q_i = (r, \theta, \varphi)$



$$d\vec{r} = \hat{r}\, dr + \hat{\theta}\, r\, d\theta + \hat{\varphi}\, r \sin\theta\, d\varphi$$

$$\Downarrow$$

$$\dot{\vec{r}} = \hat{r}\, \dot{r} + \hat{\theta}\, r \dot{\theta} + \hat{\varphi}\, r \sin\theta \cdot \dot{\varphi}$$

$$\Downarrow$$

$$T = \frac{1}{2} m v^2$$

$$= \frac{1}{2} m \left(\dot{r}^2 + r^2 \dot{\theta}^2 + r^2 \sin^2\theta \cdot \dot{\varphi}^2 \right)$$

Canonical momenta:

$$p_r = \frac{\partial L}{\partial \dot{r}} = m\dot{r}, \quad p_\theta = \frac{\partial L}{\partial \dot{\theta}} = m r^2 \dot{\theta}, \quad p_\varphi = \frac{\partial L}{\partial \dot{\varphi}} = m r^2 \sin^2\theta \cdot \dot{\varphi}$$

Write down Hamiltonian:

$$H = p_i \dot{q}_i - L = p_i \dot{q}_i - T + V$$

$$= m\dot{r}\dot{r} + mr^2\dot{\theta}\dot{\theta} + mr^2\sin^2\theta\,\dot{\varphi}\dot{\varphi}$$

$$-\frac{1}{2}m\dot{r}^2 - \frac{1}{2}mr^2\dot{\theta}^2 - \frac{1}{2}mr^2\sin^2\theta\,\dot{\varphi}^2 + V(r)$$

$$= \frac{1}{2}m\left(\dot{r}^2 + r^2\dot{\theta}^2 + r^2\sin^2\theta\,\dot{\varphi}^2\right) + V(r)$$

$$= T + V$$

Eliminate $\dot{q}_i$:

$$\dot{r} = p_r/m, \quad \dot{\theta} = p_\theta/mr^2, \quad \dot{\varphi} = p_\varphi/mr^2\sin^2\theta$$

$$\Rightarrow H(q,p) = \frac{1}{2m}\left(p_r^2 + \frac{p_\theta^2}{r^2} + \frac{p_\varphi^2}{r^2\sin^2\theta}\right) + V(r)$$

$$= H(r, \theta, p_r, p_\theta, p_\varphi)$$

Ex 2: Particle in electromagnetic field

From p. 25:

$$U = q\phi - q\vec{A}\cdot\vec{v} = q\phi - qA_i\dot{x}_i \quad \text{(sum over } i\text{)}$$

$$T = \frac{1}{2}mv^2 = \frac{1}{2}m\dot{x}_i\dot{x}_i$$

i.e., we use cartesian coordinates, $x_1 = x$ etc.

$$L = T - U = \frac{1}{2}m\dot{x}_i\dot{x}_i + qA_i\dot{x}_i - q\phi$$

$$p_i = \partial L/\partial \dot{x}_i = m\dot{x}_i + qA_i \quad \Rightarrow \dot{x}_i = \frac{1}{m}(p_i - qA_i)$$

$$H = p_i \dot{x}_i - L$$
$$= (m\dot{x}_i + qA_i)\dot{x}_i - \frac{1}{2} m \dot{x}_i \dot{x}_i - qA_i \dot{x}_i + q\phi$$
$$= \frac{1}{2} m \dot{x}_i \dot{x}_i + q\phi$$

= mechanical energy + potential energy

= total energy

But: $H \neq T + U$ due to velocity dependence of U

We eliminate $\dot{x}_i$:

$$H(x_i, p_i, t) = \frac{1}{2m}(p_i - qA_i)(p_i - qA_i) + q\phi$$
$$= \frac{1}{2m}(\vec{p} - q\vec{A})^2 + q\phi$$

$\vec{p}$ = canonical momentum

$\vec{p} - q\vec{A}$ = mechanical momentum

$\phi = \phi(x_i, t)$, $\vec{A} = \vec{A}(x_i, t)$

If $\vec{A}$ and ϕ are time independent:

$$\frac{\partial L}{\partial t} = 0$$

and

$$\frac{dH}{dt} = \frac{\partial H}{\partial t} = -\frac{\partial L}{\partial t} = 0$$