Hamiltonian Dynamics:

wish to replace $\dot{q}$ in Lagrange formulation by a "better" variable

(1) $\dot{q}$ is ill-defined in quantum mechanics

$q \to \psi(q)$ which is spread out in q-space

$P(q)$ = prob of being at q $= |\psi(q)|^2$

$P(\dot{q}) = ?$

(2) Lagrange's Eqs are $2^{\underline{nd}}$ order in time, awkward mathematics

common analysis for $y''(x) = f(x)$

$z = y'(x)$ and $z'(x) = f(x)$ - coupled 1^{st} order eqs

Nicely visualized in the "phase plane"

(3) p is better than $\dot{q}$ because

p = constant $\leftrightarrow$ L independent of q

$\leftrightarrow$ symmetry of problem

(4) L does not have any direct significance but

(it turns out) H = result of $\dot{q} \to p$ in L does

(5) Simple "change of variables" awkward:

if $L(q, \dot{q}) \to \hat{L}(q, p(q, \dot{q}))$

$$\frac{\partial L}{\partial q} = \frac{\partial \hat{L}}{\partial q} + \frac{\partial \hat{L}}{\partial p}\frac{\partial p}{\partial q}$$

$$\frac{\partial L}{\partial \dot{q}} = \frac{\partial \hat{L}}{\partial p}\frac{\partial p}{\partial \dot{q}}, \quad \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}}\right) = \cdots$$

mess in general

Simple idea: $L = \frac{1}{2}m\dot{x}^2 - V(x)$

$\rightarrow m\ddot{x} = -V'(x)$ $\quad H \equiv p\dot{q} - L = \text{constant}$ $\quad p \equiv \frac{\partial L}{\partial \dot{q}} = m\dot{x}$

and $H = p^2/2m + V(x)$

Notice $\frac{\partial H}{\partial x} = V'(x)$ + $\frac{\partial H}{\partial p} = p/m$

so $\dot{p} = -\frac{\partial H}{\partial x}$ $\quad \dot{x} = \frac{\partial H}{\partial p}$ with $H = H(x,p)$

Here change of variable $(x,\dot{x}) \rightarrow (x,p)$ is simple

General case: "Legendre transform"

start with $f(x)$ + wish to trade in x for $w = f'(x)$

(" $L(q,\dot{q})$ " $\dot{q}$ $\quad p = \frac{\partial L}{\partial \dot{q}}$)

assume $w = f'(x) \longleftrightarrow x = x(w)$

define $g(w) = xw - f(x)\Big|_{x=x(w)}$

notice $dg = x\,dw + \cancel{w\,dx} - \cancel{f'(x)\,dx}$

so $g = g(w)$ and x can be recovered from $\frac{dg}{dw} = x$

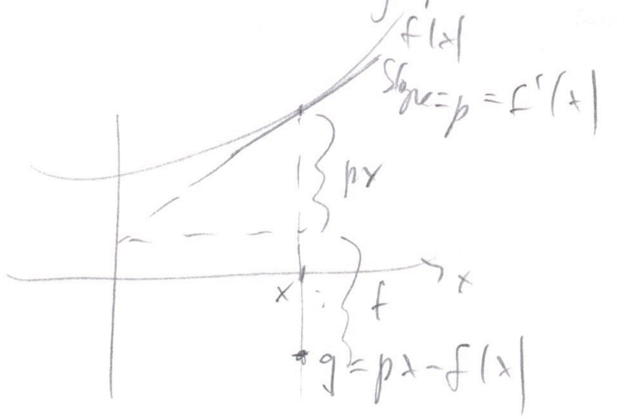
To go back, repeat the procedure:

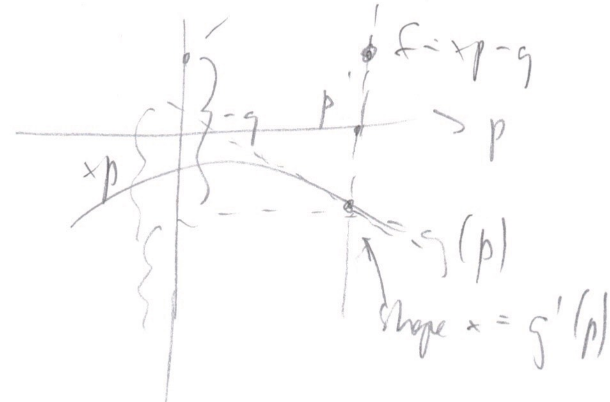
let $F \equiv xw - g\Big|_{w=w(x)}$

$dF = \cancel{x\,dw} + w\,dx - \cancel{g'(w)\,dw}$

or $\frac{dF}{dx} = w = \frac{df}{dx} \rightarrow F = f$

NB: $f(x)$ and $g(p)$ have the same information





More: google legendre xform.

— x —

Back to mechanics:

Instead of $L(q, \dot q, t)$ with $\frac{d}{dt}\frac{\partial L}{\partial \dot q_i} = \frac{\partial L}{\partial q_i}$

replace $\dot q_i$ by $p_i = \frac{\partial L}{\partial \dot q_i}$ so $p_i = p_i(q, \dot q)$

so $\dot q_i = \dot q_i(p, q)$

let $H(q, p, t) = \sum_i \dot q_i p_i - L \Big|_{\dot q_i = \dot q_i(q,p)}$

then $dH = \sum_i \cancel{d\dot q_i\, p_i} + \dot q_i\, dp_i - \sum_i \underbrace{\frac{\partial L}{\partial q_i}}_{\dot p_i} dq_i - \cancel{\underbrace{\frac{\partial L}{\partial \dot q_i}}_{p_i} d\dot q_i} - \frac{\partial L}{\partial t}$

$= \sum \dot q_i\, dp_i - \dot p_i\, dq_i - \frac{\partial L}{\partial t} dt$

So indeed q, p are the arguments of H. This means

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

compare: get "Hamilton's Eqs"

$$\dot{p}_i = -\frac{\partial H}{\partial q_i}, \quad \dot{q}_i = +\frac{\partial H}{\partial p_i}, \quad \frac{\partial H}{\partial t} = -\frac{\partial L}{\partial t}.$$

Notice also

$$\frac{dH}{dt} = \sum_i \frac{\partial H}{\partial p_i} \underbrace{\dot{p}_i}_{= -\frac{\partial H}{\partial q_i}} + \frac{\partial H}{\partial q_i} \underbrace{\dot{q}_i}_{= +\frac{\partial H}{\partial p_i}} + \frac{\partial H}{\partial t} = \frac{\partial H}{\partial t} = -\frac{\partial L}{\partial t}$$

so H is a constant unless L depends <u>explicitly</u> on t.

Also: if H is independent of some q_I (cyclic or ignorable coord.)

then $\dot{p}_I = -\frac{\partial H}{\partial q_I} = 0$ and p_I = constant.

Example $L = \sum_{i=1}^{n} \frac{1}{2} m_i \dot{\underline{r}}_i^2 - V(\underline{r}_1 \dots \underline{r}_n)$

classical n-particle system w fixed mass.

$$\underline{p}_i = \frac{\partial L}{\partial \dot{\underline{r}}_i} = m_i \dot{\underline{r}}_i \rightarrow \dot{\underline{r}}_i = \underline{p}_i / m$$

$$H = \sum_i \underline{p}_i \cdot \underbrace{(\underline{p}_i/m)}_{\dot{\underline{r}}_i} - \Big[\sum \tfrac{1}{2} m_i \underbrace{(\underline{p}_i/m)}_{\dot{\underline{r}}_i}^2 - V \Big]$$

$$= \sum_i \underline{p}_i^2/2m_i + V(\{\underline{r}_i\}) = E = \text{constant here}$$

Example – central force motion

$$L = \tfrac{1}{2} m (\dot{r}^2 + r^2\dot{\theta}^2) - V(r)$$

$$p_r = \frac{\partial L}{\partial \dot{r}} = m\dot{r} \quad , \quad p_\theta = \frac{\partial L}{\partial \dot{\theta}} = mr^2\dot{\theta} \quad (= L_z)$$

$$H = p_r \dot{r} - p_\theta \dot{\theta} - L$$

$$= p_r^2/2m + p_\theta^2/2mr^2 + V(r)$$

$$\dot{r} = \frac{\partial H}{\partial p_r} = p_r/m \qquad \dot{p}_r = -\frac{\partial H}{\partial r} = -\frac{p_\theta^2}{mr^3} - V'(r)$$

$$\dot{\theta} = \frac{\partial H}{\partial p_\theta} = p_\theta/mr^2 \qquad \dot{p}_\theta = -\frac{\partial H}{\partial \theta} = 0$$

θ = ignorable coordinate

p_θ = constant = l angular momentum

$$\rightarrow \quad m\ddot{r} = -\frac{l^2}{mr^3} - V'(r) \qquad \text{: usual eq.}$$

Example – bead on a wire in 2d $\quad y = f(x)$

Lagrangian $\quad L = \frac{1}{2}m\left(\dot{x}^2 + \dot{y}^2\right) - mgy$

$$\to \frac{m}{2}\left(1 + f'(x)^2\right)\dot{x}^2 - mg\,f(x)$$

$$\frac{d}{dt}\left[m\left(1 + f'(x)\right)^2 \dot{x}\right] = -mg f' + m f' f'' \dot{x}^2$$

Hamiltonian $\quad p = \frac{\partial L}{\partial \dot{x}} = m\dot{x}\left(1 + f(x)^2\right)$

$$H = p\dot{x} - L = p \cdot \frac{p}{m(1+f'^2)} - \left(\frac{m}{2}\left(1+f'^2\right)\left(\frac{p}{m(1+f'^2)}\right)^2 - mgf\right)$$

$$= \frac{p^2}{2m(1+f'^2)} + mgf$$

$$\dot{x} = \frac{\partial H}{\partial p} = \frac{p}{m(1+f'^2)} \qquad \dot{p} = -\frac{\partial H}{\partial x}$$

$$= \frac{p^2 f' f''}{m(1+f'^2)^2} - mgf'$$

$\to$ same equation for $\ddot{x}$

Other example of Legendre xfm is thermodynamics:

1st law $\quad dU = dQ - dW$

$\qquad$ work done by system

$\qquad$ heat added to system

and for inf. reversible processes $dQ = TdS$

where S = entropy $= k_B \log W = -k\sum_i p_i \log p_i$ = int. factor

$= \ldots$

So $\quad dU = TdS - pdV - $ (other forms of work)

dV is directly controllable but dS may not be.

Instead of S, a better independent variable might be

$$T = \frac{\partial U}{\partial S} \qquad \left(U = U(S,V) \to dU = \frac{\partial U}{\partial S} dS + \cdots \right)$$

Legendre xfm: $\quad$ Let $F = U - TS$ $\quad$ (opp sign for historical reasons)

$$dF = TdS - pdV - (TdS + SdT)$$

$$= -SdT - pdV$$

$\hookrightarrow$ $F = F(T,V)$ = Helmholtz free energy

$$S = -\frac{\partial F}{\partial T} \quad \text{if its needed.}$$

Hamiltonians + time evolution:

look at any $f(q, p, t)$

$$\frac{df}{dt} = \sum_i \left(\frac{\partial f}{\partial q_i} \dot{q}_i + \frac{\partial f}{\partial p_i} \dot{p}_i \right) + \frac{\partial f}{\partial t}$$

$$= \sum_i \left(\frac{\partial f}{\partial q_i} \frac{\partial H}{\partial p_i} - \frac{\partial f}{\partial p_i} \frac{\partial H}{\partial q_i} \right) + \frac{\partial f}{\partial t}$$

$$\equiv \{ f, H \} + \frac{\partial f}{\partial t}$$

"Poisson bracket" of f with H

Generally $\{A, B\} = \sum_i \left(\frac{\partial A}{\partial q_i} \frac{\partial B}{\partial p_i} - \frac{\partial B}{\partial q_i} \frac{\partial A}{\partial p_i} \right)$

e.g. $\{q_j, p_k\} = \sum_i \left(\delta_{ij} \delta_{ik} - 0 \right) = \delta_{jk}$

$\{q_j, q_k\} = \{p_j, p_k\} = 0$

→ Just like commutators in Quantum Mechanics

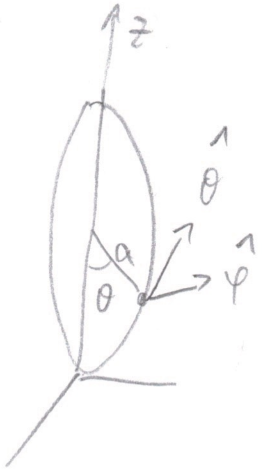
$$\underbrace{[q, p]}_{\text{operators}} \equiv qp - pq \rightarrow \underbrace{q\left(-i\hbar \frac{\partial}{\partial q}\right) - \left(-i\hbar \frac{\partial}{\partial q}\right) q}_{= i\hbar}$$

+ if $A(t)$ is a time-dependent operator

$$\frac{dA}{dt} = [A, H] + \frac{\partial A}{\partial t}$$

QM Hamiltonian

Example Bead on a vertical circular loop rotating at $\omega(t)$



$$\dot{\underline{r}} = a\dot{\theta}\,\hat{\theta} + a\sin\theta\,\omega(t)\,\hat{\varphi}$$

$$T = \frac{m}{2}\left(a^2\dot{\theta}^2 + \omega^2(t)\,a^2\sin^2\theta\right)$$

$$y = a(1-\cos\theta) \rightarrow V = mga(1-\cos\theta)$$

so $$L = \frac{ma^2}{2}\left(\dot{\theta}^2 + \omega^2(t)\sin^2\theta\right) + mga\cos\theta$$

$$p_\theta = \frac{\partial L}{\partial\dot{\theta}} = ma^2\dot{\theta}$$

$$H = p_\theta^2/2m - \frac{1}{2}ma^2\omega^2(t)\sin^2\theta - mga\cos\theta$$

H = const iff ω = constant ($\partial L/\partial t = 0$ then)

$E \neq$ constant because driving the loop does work

Hamilton Eqs: $$\dot{\theta} = \frac{\partial H}{\partial p_\theta} = p_\theta/ma^2$$

$$\dot{p}_\theta = -\frac{\partial H}{\partial\theta} = \frac{1}{2}ma^2\omega^2\sin 2\theta - mga\sin\theta$$

or $$\ddot{\theta} = -\frac{g}{a}\sin\theta + \frac{1}{2}\omega^2(t)\sin 2\theta$$

Possible equilibria at $\theta = 0$ & π

$\theta = 0$ case $$\ddot{\theta} \rightarrow -\frac{g}{a}\theta + \frac{1}{2}\omega^2(t)\cdot 2\theta + \dots$$
$$= -\left(g/a - \omega^2\right)\theta + \dots$$

$\therefore$ stable for $\omega^2(t) < g/a$

$\theta = \pi$ case let $\varphi = \pi - \theta$ so $\begin{cases} \ddot{\theta} = -\ddot{\varphi} \\ \sin\theta = +\sin\varphi \\ \sin 2\theta = 2\sin\theta\cos\theta = -2\sin\varphi\cos\varphi \end{cases}$

$$-\ddot{\varphi} \rightarrow -\frac{g}{a}\varphi - \frac{1}{2}\omega^2(t)\cdot 2\varphi$$

$$\text{or } \ddot{\varphi} = +\left(g/a + \omega^2(t)\right)\varphi \quad \text{: always unstable}$$

3rd possibility: $\omega =$ constant and $\frac{g}{a}\sin\theta = \frac{1}{2}\omega^2\sin 2\theta$

$$\text{or } \cos\theta_0 = \frac{g}{a\omega^2}$$

expand again: $\theta = \theta_0 + \varphi$

$$\ddot{\varphi} = -\frac{g}{a}\sin(\theta_0 + \varphi) + \frac{1}{2}\omega^2\sin 2(\theta_0 + \varphi)$$

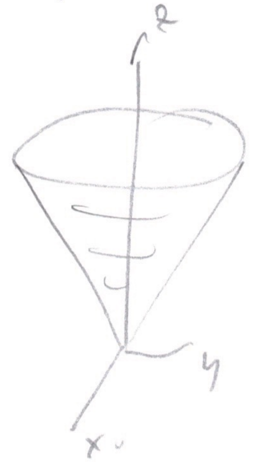
$$\sin\theta_0 + \varphi\cos\theta_0 \qquad \sin 2\theta_0 + 2\varphi\cos 2\theta_0$$

$$= \left(-\frac{g}{a}\cos\theta_0 + \omega^2\underbrace{\cos 2\theta_0}_{2\cos^2\theta_0 - 1}\right)\varphi$$

$$= -\omega^2\sin^2\theta_0\cdot\varphi$$

stable

Example 13.4 particle moving on an inverted cone



$$L = \frac{m}{2}\left(\dot r^2 + r^2\dot\varphi^2 + \dot z^2\right) - mgz$$

$$\xrightarrow{\text{cone: } r = cz} \frac{m}{2}\left[(c^2+1)\dot z^2 + c^2 z^2 \dot\varphi^2\right] - mgz$$

$$p_z \; \frac{\partial L}{\partial \dot z} = m(c^2+1)\dot z$$

$$p_\varphi = \frac{\partial L}{\partial \dot\varphi} = mc^2z^2\dot\varphi \qquad (= L_z)$$

$$H = p_z \cdot \frac{p_z}{m(c^2+1)} + p_\varphi \cdot \frac{p_\varphi}{mc^2z^2} - \frac{m}{2}\left[(c^2+1)\left(\frac{p_z}{m(c^2+1)}\right)^2 + c^2z^2\left(\frac{p_\varphi}{mc^2z^2}\right)^2\right] + mgz$$

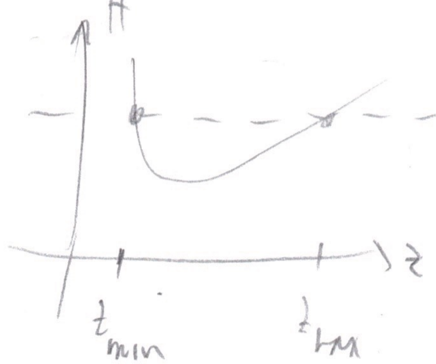
$$\equiv \frac{p_z^2}{2m(c^2+1)} + \frac{p_\varphi^2}{2mc^2z^2} + mgz \qquad (= E = \text{constant})$$

^ potential barrier at $z=0$

$$\dot z = \frac{\partial H}{\partial p_z} = \frac{p_z}{m(c^2+1)} \qquad \dot\varphi = \frac{\partial H}{\partial p_\varphi} = \frac{p_\varphi}{mc^2z^2}$$

$$\dot p_z = -\frac{\partial H}{\partial z} = \frac{p_\varphi^2}{mc^2z^3} - mg \qquad \dot p_\varphi = -\frac{\partial H}{\partial \varphi} = 0 \quad \text{: cons. of } L_z$$

Notice $V_{eff} \to \infty$ for $z \to 0$ and $z \to \infty$ so $z_{min} < z < z_{max}$



$$(c^2+1)\ddot{z} = -g + \frac{p_\varphi^2}{m^2c^2z^3}$$

Motion: $\dot{\varphi} = \frac{p_\varphi}{mcz} > 0$

So m rotates around the cone bouncing back & forth between z_{min} & z_{max}.

Special case $z = z_0$ = constant so $\ddot{z} = 0$, $z_0 = \left(\frac{p_\varphi^2}{m^2c^2g}\right)^{1/3}$

stability? let $z = z_0 + x$

$$(c^2+1)\ddot{x} = -g + \left(\frac{p_\varphi}{mc}\right)^2 \frac{1}{(z_0+x)^3} \sim \frac{1}{z_0^3}\left(1 - \frac{3x}{z_0} + \cdots\right)$$

$$= -\frac{3}{z_0^4}\left(\frac{p_\varphi}{mc}\right)^2 x =$$

$$= -\frac{3g}{z_0}x \qquad \text{stable again}$$