Hamiltonian Dynamics:

alternative to Lagrangian or $F = ma$

advantages: (1) better to work with p & q than q & $\dot{q}$

- forces related to symmetry laws

$\dot{q}$ is not special

- connect to QM

(2) H has dynamical significance itself –

- often $= E$

- generator of time translations (later)

(3) Systematic procedure for changing variables to "clever" ones.

Toy example $\quad L = \frac{1}{2} m\dot{x}^2 - U(x)$

$$p = \frac{\partial L}{\partial \dot{x}} = m\dot{x} \quad \rightarrow \quad \dot{x} = p/m$$

$$H \equiv p\dot{x} - L = \frac{m}{2}\dot{x}^2 + U(x) = p^2/2m + U(x)$$

$= $ conserved fn of x & p.

notice that "automatically" $H = H(q, p)$:

$$dH = d(p\dot{x} - L) = dp\,\dot{x} + p\,d\dot{x} - \underbrace{\frac{\partial L}{\partial x}}_{= \dot{p}} dx - \underbrace{\frac{\partial L}{\partial \dot{x}}}_{= p} d\dot{x}$$

$$= \dot{x}\,dp - \dot{p}\,dx$$

with no $d\dot{x}$ term.

Latter is example of Legendre transformation, familiar (?) from thermodynamics / stat mech.

In latter, compute $S(E, V) = k_B \log(\#\text{states})$

$$\to \quad E = E(S, V)$$

$$dE = \left(\frac{\partial E}{\partial S}\right)_V dS + \left(\frac{\partial E}{\partial V}\right)_S dV = T\,dS - p\,dV$$

However, S is often an inconvenient variable – hard to control or measure directly – so prefer to have fns of T + V.

So let A = Helmholtz free energy

$$= E - TS \qquad \text{where } T = \left(\frac{\partial E}{\partial S}\right)$$

+ then

$$dA = dE - d(TS)$$

$$= (T\,dS - p\,dV) - (T\,dS + S\,dT)$$

$$= -S\,dT - p\,dV \quad \to \quad A = A(T, V)$$

$$\left(\frac{\partial A}{\partial T}\right)_V \qquad \left(\frac{\partial A}{\partial V}\right)_T$$

Both cases: replace dependent variable $(S, \dot{q})$ by deriv of fn wrt it $(\partial E/\partial S, \partial L/\partial \dot{q})$, define new fn as shift $(A = E - TS,\ H = p\dot{q} - L)$ + then new fn depends on new variables due ($A(T,V)$, $H(p,q)$).

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General case for dynamics:

Lagrangian $L(q_i, \dot q_i, t)$

momenta $p_i = \frac{\partial L}{\partial \dot q_i}$ satisfy $\dot p_i = \frac{\partial L}{\partial q_i}$

Hamiltonian $H(q_i\, p_i\, t) \equiv \sum_i \dot q_i\, p_i - L$

(, where $\dot q_i = \dot q_i(p, q, t)$)

NB: to actually eliminate the $\dot q_i$ have to be able to invert the fns $p_i = p_i(\dot q_i, q_i)$ for $\dot q_i$, which requires $\frac{\partial p_i}{\partial \dot q_j} = \frac{\partial^2 L}{\partial \dot q_i \partial \dot q_j}$ be non-singular

(implicit for thm of calculus).

If so, $dH = \sum_i (\cancel{d\dot q_i\, p_i} + \dot q_i\, dp_i) - \sum_i \left(\underbrace{\frac{\partial L}{\partial q_i}}_{\dot p_i} dq_i + \cancel{\underbrace{\frac{\partial L}{\partial \dot q_i}}_{p_i} d\dot q_i} \right) - \frac{\partial L}{\partial t} dt$

so $H = H(q_i\, p_i\, t)$

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

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

: Hamilton's (canonical) eqs.

Also note $\quad \frac{dH}{dt} = \underbrace{\sum_i \frac{\partial H}{\partial q_i}\dot{q}_i + \frac{\partial H}{\partial p_i}\dot{p}_i}_{=0} + \frac{\partial H}{\partial t} = -\frac{\partial L}{\partial t}$

More generally, if λ is any parameter in L,

$$H(p, q, t, \lambda) = \sum p_i \dot{q}_i - L(q, \dot{q}, t, \lambda)$$

$$dL = \sum(\dot{p}_i\, dq + p_i\, d\dot{q}_i) + \frac{\partial L}{\partial t} dt + \frac{\partial L}{\partial \lambda} d\lambda$$

$$\rightarrow \quad dH = \sum(-\dot{p}_i\, dq + \dot{q}_i\, dp) - \frac{\partial L}{\partial t} dt - \frac{\partial L}{\partial \lambda} d\lambda$$

$$\text{so} \quad \left(\frac{\partial H}{\partial \lambda}\right)_{p,q,t} = -\left(\frac{\partial L}{\partial \lambda}\right)_{q,\dot{q},t}.$$

Cyclic coordinates:

Lagrangian version: if $\frac{\partial L}{\partial q_i} = 0$ then $p_i = \frac{\partial L}{\partial \dot{q}_i} = $ constant

which is a constraint in integrating the eqs.

($\dot{q}_i$ need not be constant.)

Hamiltonian version – if $\frac{\partial H}{\partial q_i} = 0$ then $p_i =$ constant

and no further work is needed on p_i & $q_i = \int \frac{\partial H}{\partial p_i} dt$

(common case: $H = \underbrace{\frac{p_i^2}{2m_i}}_{\text{ignore}} + \underbrace{\left[\sum_{j \neq i} \frac{p_j^2}{2m_j} + U(q_j \neq q_i)\right]}_{\text{indep of } q_i \text{ \& } p_i}$.)

When does $H = T + U =$ total energy?

Always, if $T = \sum_\alpha \frac{1}{2} m_\alpha \dot{\underline{r}}_\alpha^2$, $U = U(\{\underline{r}_\alpha\})$, and

$\underline{r}_\alpha = r_\alpha(q_1 \cdots q_n)$ indep of t

because then $T = \sum_{ij} \frac{1}{2} m_{ij} \dot{q}_i \dot{q}_j$ $\quad m_{ij} = \sum_\alpha \frac{\partial r_\alpha}{\partial q_i} \cdot \frac{\partial r_\alpha}{\partial q_j}$

& $\sum p_i \dot{q}_i = \sum_i \left(\sum_j m_{ij} \dot{q}_j\right) \dot{q}_i = 2T$

& $H = \sum p_i \dot{q}_i - L = 2T - (T - U) = T + U$.

More generally: $\underline{r}_\alpha = \underline{r}_\alpha(q_1 \cdots q_n, t)$ or E&M

$T = \frac{1}{2} \dot{\underline{q}}^T \cdot \underset{\text{symm. matrix}}{\underline{\underline{M}}} \cdot \dot{\underline{q}} + \dot{\underline{q}}^T \cdot \underset{\text{terms in } \frac{\partial r_\alpha}{\partial t}}{\underline{N}(\underline{q})} + \underset{\text{put in } U}{R(\underline{q})}$

then $\underline{p} = \frac{\partial \mathcal{L}}{\partial \dot{\underline{q}}} = \underline{\underline{M}} \cdot \dot{\underline{q}} + \underline{N} \rightarrow \dot{\underline{q}} = \underline{\underline{M}}^{-1} \cdot (\underline{p} - \underline{N})$.

$$H = \underline{p}^T \cdot \dot{\underline{q}} - L$$

$$= \underline{p}^T \cdot \underline{\underline{M}}^{-1} (\underline{p} - \underline{N}) - \frac{1}{2} (\underline{p} - \underline{N})^T M^{-1} \cancel{M M^{-1}} (p - N)$$

$$- (p - N)^T M^{-1} N - R + U$$

$$= \frac{1}{2} p^T M^{-1} p - p^T M^{-1} N - \cancel{\frac{1}{2} p^T M^{-1} p} + \frac{1}{2} p^T M^{-1} N$$

$$+ \frac{1}{2} N^T M^{-1} p - \cancel{\frac{1}{2} N^T M^{-1} N} - p^T M^{-1} N$$

$$+ \frac{1}{2} N^T M^{-1} N - R + U$$

$$= \frac{1}{2} (\underline{p} - \underline{N})^T \cdot \underline{\underline{M}}^{-1} \cdot (\underline{p} - \underline{N}) - R + U \neq E \text{ generally}$$

using the fact that $M = M^T \Rightarrow M^{-1} = M^{-1\,T}$

$$\Rightarrow p^T M^{-1} N = N^T M^{-1} p \qquad \Rightarrow$$

e.g. particle in EM field

$$L = \frac{1}{2} m \dot{\underline{x}}^2 - q \varphi(\underline{x}) + \frac{q}{c} \underline{A} \cdot \dot{\underline{x}}$$

$$\underline{p} = m \dot{\underline{x}} + \frac{q}{c} \underline{A}, \quad \underline{N} = \frac{q}{c} \underline{A} \;\&\; \underline{\underline{M}} = \underline{\underline{1}}, \; \underline{\underline{R}} = \underline{\underline{0}}$$

$$H = \frac{1}{2} m \left| \underline{p} - \frac{q}{c} \underline{A} \right|^2 + q \varphi \quad \left(= \frac{m}{2} \dot{\underline{x}}^2 + q \varphi \right)$$

Example 1: mass m moves on wire $y=f(x)$ w/o friction

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

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

so $p = m\dot x\left[1+f'(x)^2\right]$ or $\dot x = \dfrac{p}{m\left[1+f'^2\right]}$

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

$$= \frac{p^2}{2m(1+f'^2)} + mgf \quad = \text{energy} \quad \left(= \tfrac{1}{2} p M^{-1} p + V,\ M = \tfrac{1}{1+f'^2}\ N=0\right)$$

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

cf Lagrange eq

$$0 = \frac{d}{dt}\left[m\dot x(1+f'^2)\right] - m\dot x^2 f' f'' + mgf'$$

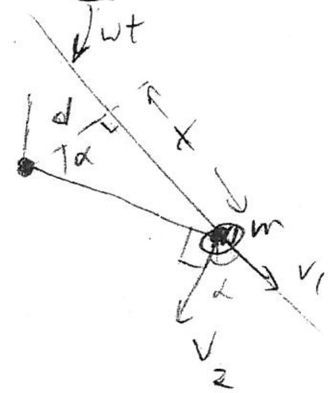
$$= \ddot x(1+f'^2) + \dot x^2 f' f'' + g f'$$

hard to solve in general either way

Ex 2: Bead on a wire rotating at const. ω at d from axis

$t=0$

$t>0$



$$v_1 = \dot{x}$$

$$v_2 = \sqrt{d^2+x^2}\,\omega$$

$$\underline{v}^2 = v_1^2 + v_2^2 + 2v_1v_2\cos\alpha\,, \qquad \cos\alpha = \frac{d}{\sqrt{d^2+x^2}}$$

$$L = T = \frac{1}{2}m\underline{v}^2 = \frac{m}{2}\left(\dot{x}^2 + \omega^2(d^2+x^2) + 2d\omega\dot{x}\right)$$

$$p = \frac{\partial L}{\partial \dot{x}} = m\dot{x} + md\omega \qquad (\neq m\dot{x} \text{ alone})$$

$$H = p\left(\frac{p}{m} - d\omega\right) - \left[\frac{1}{2m}(m\dot{x} + md\omega)^2 + \frac{m\omega^2x^2}{2}\right]$$

$$= \frac{p^2}{2m} - d\omega p - \frac{m\omega^2x^2}{2}$$

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

but $E = T \neq H$ & is not conserved.

(because the rotating wire does work on the mass.)

Lagrange eqs $\quad \dot{p} = \frac{\partial L}{\partial x}$ or $m\ddot{x} = m\omega^2 x$

$$\rightarrow x = \alpha e^{\omega t} + \beta e^{-\omega t}$$

Hamilton eqs: $\quad \dot{x} = \frac{\partial H}{\partial p} = \frac{p}{m} - d\omega$

$$\dot{p} = -\frac{\partial H}{\partial x} = m\omega^2 x$$

$$\rightarrow \ddot{p} = m\omega^2 \dot{x} = \omega^2 p - m\omega^3 d$$

$$\text{or} \quad \frac{d^2}{dt^2}\left(p - m\omega d\right) = \omega^2 \left(p - m\omega d\right)$$

$$\rightarrow \quad p = m\omega d + \hat{\alpha} e^{\omega t} + \hat{\beta} e^{-\omega t}.$$

$$\rightarrow \quad x = \frac{\hat{\alpha}}{m\omega} e^{\omega t} - \frac{\hat{\beta}}{m\omega} e^{-\omega t}$$

Hamiltonian action principle:

first consider action as a fn of the upper limit:

$$A(q,t) = \int_{t_0}^{t} dt' \, L(q(t'), \dot q(t'), t')$$

with $q(t_0) = q_0$ $\quad q(t) = q$.

$$\delta A = \int_{t_0}^{t} dt' \Big[\sum_i \frac{\partial L}{\partial q_i} \delta q_i + \frac{\partial L}{\partial \dot q_i} \underbrace{\delta \dot q_i}_{\frac{d}{dt}\delta q_i} \Big]$$

$$= \sum_i \frac{\partial L}{\partial \dot q_i} \delta q_i \Big|_{t_0}^{t} + \sum_i \int dt' \, \delta q_i \Big[\frac{\partial L}{\partial q_i} - \frac{d}{dt} \frac{\partial L}{\partial \dot q_i} \Big]$$

$$= \sum_i p_i \, \delta q_i \Big|_{t_0}^{t}$$

$$\rightarrow \quad \frac{\partial A}{\partial q_i(t)} = p_i(t)$$

when $q_i(t)$ is the physical trajectory satisfying Lagrange's eq.

Also
$$\frac{dA}{dt} = \frac{\partial A}{\partial t} + \sum_i \frac{\partial A}{\partial q_i} \dot q_i = \frac{\partial A}{\partial t} + \sum_i p_i \dot q_i$$

also $= L(q(t), \dot q(t), t)$ from def of A

$$\rightarrow \quad \frac{\partial A}{\partial t} = -H$$

$$\rightarrow \quad dA = \Big(\sum_i p_i \dot q_i - H \Big) dt = L \, dt$$

Example: $L = \frac{m}{2}\dot{\underline{r}}^2 - U(\underline{r}) = m\dot{\underline{r}}^2 - E$

so $A = \int_{t_0}^{t} dt\, m\left|\frac{d\underline{r}}{dt}\right|^2 - E(t-t_0)$

(on the physical trajectory where $E = \text{const.}$)

$+ \quad A = \int_{\underline{r}(0)}^{\underline{r}(T)} d\underline{r} \cdot \left(m \frac{d\underline{r}}{dt}\right) - E(t-t_0)$

$\therefore \quad \frac{\partial A}{\partial \underline{r}} = m\dot{\underline{r}} = \underline{p} \quad , \quad \frac{\partial A}{\partial t} = -E$

Since in the Lagrange formulation $\delta A = 0$, this suggests the new action principle

$$\delta \int_{t_1}^{t_2} dt \left[\sum p_i \dot{q}_i - H(q, p) \right] = 0$$

where q_i and p_i are varied independently.

If so, $\quad 0 = \int dt \left\{ \sum_i \delta p_i \left(\dot{q}_i - \frac{\partial H}{\partial p_i} \right) + \sum_i \left(p_i \delta \dot{q}_i - \frac{\partial H}{\partial q_i} \delta q_i \right) \right\}$

$p_i \delta q_i \Big|_{t_1}^{t_2} - \dot{p}_i \delta q_i$

$$\text{or} \quad 0 = \sum p_i \delta q_i \Big|_{t_1}^{t_2} + \int_{t_1}^{t_2} dt \left\{ \sum_i \delta p_i \left(\dot{q}_i - \frac{\partial H}{\partial p_i} \right) - + \sum_i \delta q_i \left(\dot{p}_i + \frac{\partial H}{\partial q_i} \right) \right\}$$

require $\delta q(t_1) = \delta q(t_2) = 0$ $\rightarrow$

$$\dot{q}_i = \frac{\partial H}{\partial p_i} \qquad \dot{p}_i = -\frac{\partial H}{\partial q_i}$$

Notice $\delta p_i(t)$ are not specified, due to absence of $\dot{p}_i$ in $\sum p\dot{q} - H$. Often convenient to specify $\delta p(t_i) = 0$.

Other way of looking at this:

extremize $\int dt \; F(q, \dot{q}, p, \dot{p}, t)$ wrt $\{q, \dot{q}, p, \dot{p}\}$

$$\rightarrow \frac{d}{dt}\frac{\partial F}{\partial \dot{q}} - \frac{\partial F}{\partial q} = 0 \quad ; \quad \frac{d}{dt}\frac{\partial F}{\partial \dot{p}} - \frac{\partial F}{\partial p} = 0$$

provided $\delta q = \delta p = 0$ at the endpoints

If $F \rightarrow \sum p_i \dot{q}_i - H(q_i, p_i)$ this $\rightarrow$

$$\dot{p}_i + \frac{\partial H}{\partial q_i} = 0 \qquad -\dot{q}_i + \frac{\partial H}{\partial p_i} = 0 \quad \text{again}$$

Remark: if $\dfrac{\partial A}{\partial q_i} = p_i$ is $\dfrac{\partial A}{\partial p_i}$ related to q_i?

not quite – if $p_i \to p_i + \delta p_i$ then

$$A = \int dt \left[\sum p_i \dot{q}_i - H(q_i p_i) \right]$$

$$\to A + \int dt \left[\sum_i \delta p_i \left(\cancel{\dot{q}_i - \frac{\partial H}{\partial p_i}} \right) + \sum_{ij} \frac{1}{2} \frac{\partial^2 H}{\partial p_i \partial p_j} \delta p_i \delta p_j + \cdots \right]$$

whereas $q_i \to q_i + \delta q_i$ has 1st order endpoint terms.

However, an equally good action principle is

$$\delta \hat{A} \equiv \delta \int_{t_1}^{t_2} dt \left(-\sum q_i \dot{p}_i - H(q_i p_i) \right) = 0$$

because

$$\delta \hat{A} = -\int dt \left(\sum_i \delta q_i \left(\dot{p}_i + \frac{\partial H}{\partial q_i} \right) + \dot{q}_i \delta p_i + \frac{\partial H}{\partial p_i} \delta p_i \right)$$

$$= -\sum_i q_i \delta p_i \Big|_{t_1}^{t_2} + (\text{terms} = 0 \text{ on trajectory})$$

$$\to \frac{\partial \hat{A}}{\partial p_i} = -q_i$$