Hamilton - Jacobi Theory

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— here, three thrusts:

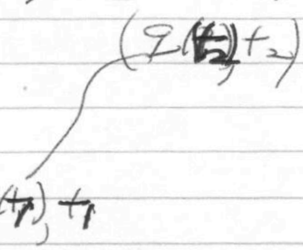
→ how does action evolve ? → $S(q,t)$?
→ semi-classical limit QM ⟺ eikonal equation for Schroedinger Eqn ?
→ when is motion integrable ?

why ?

Now, can see (at least) two perspectives on Action and Principle of Least Action.

① "S as functional" ⟺ fixed end points

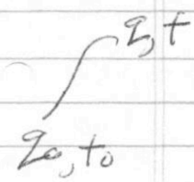
$$S = \int_{t_1}^{t_2} dt\, L(q, \dot{q}, t)$$



$\delta S = 0 \Rightarrow$ Lagrange Eqns.

② $(S = S(q,t))$

"S as function" ⟺ variable upper end point



$S(q,t)$?

Approach by considering increments

i.e. $dS = \left(\frac{\partial S}{\partial q}\right) dq + \left(\frac{\partial S}{\partial t}\right) dt$

seek, for basic parametrization of $S(q,t)$

Outcome: ~~[illegible]~~ $\partial S / \partial q = p$, $\frac{\partial S}{\partial t} = -H$

Now, recall from:

$$\delta S = \delta \int_{t_1}^{t_2} L\,dt$$

$$= \frac{\partial L}{\partial \dot{q}} \delta q \Big|_{t_1}^{t_2} + \int_{t_1}^{t_2} \left(\frac{\partial L}{\partial q} - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}} \right) \right) \delta q \, dt$$

but now:

- $\delta q(t_1) = 0$, but relax constraint on $\delta q(t_2)$ → variable upper endpoint
- continue with trajectories set by Lagrange's equations

so

$$\delta S = \partial L / \partial \dot{q} \; \delta q = p \, \delta q$$

many

$$\delta S = \sum_i p_i \delta q_i$$

$$\delta S = \frac{\partial L}{\partial \dot{q}}\,\delta q \Big|_{t_1}^{t}$$

$$= p(t)\,\delta q \qquad (\delta q(t_1) = 0)$$

so $\boxed{\dfrac{\partial S}{\partial q} = p}$

→ for time dependence; $S = S(q, t)$

$$\frac{dS}{dt} = \frac{\partial S}{\partial q}\dot{q} + \frac{\partial S}{\partial t}$$

but $dS/dt = L$

$\partial S/\partial q = p$

$$L = p\dot{q} + \partial S/\partial t$$

$$\Rightarrow \frac{\partial S}{\partial t} = -(p\dot{q} - L) = -H$$

so $dS = \sum_i p\,dq_i - H\,dt$

Now, to H-J Eqn:

$$H = H(q, p, t) \qquad \left.\begin{aligned} \dot{p} &= -\partial H/\partial q \\ \dot{q} &= \partial H/\partial p \end{aligned}\right\}$$

but also showed:

$$H = H(q, \partial S/\partial q, t) \quad , \quad \text{as} \quad p = \frac{\partial S}{\partial q}$$

and

$$\frac{\partial S}{\partial t} = -H(p, q, t) = -H\left(q, \frac{\partial S}{\partial q}, t\right)$$

$\therefore$

$$\boxed{\frac{\partial S}{\partial t} + H\left(q, \frac{\partial S}{\partial q}, t\right) = 0}$$

$\Bigg\{$ Hamilton-Jacobi Eqn.

! $\Bigg\{$
- $\rightarrow$ contains all info in Hamilton's Eqns.
- $\rightarrow$ full info on dynamics

Now, if $\partial L/\partial t = 0$ so conservative

$$H = E = \text{const.}$$

$$H(p, q) = E = H\left(\frac{\partial S}{\partial q}, q\right)$$

$$S = S_0(q, \frac{\partial S}{\partial q}) - Et$$

$\Rightarrow$ $$\boxed{H\left(\frac{\partial S}{\partial q}, q\right) = E}$$

Time-Independent H-J Eqn. (for conservative system)

why care?:

i.) single, first order pde has full content of system

ii.) solvability (separability) of H-J eqn
$\Leftrightarrow$ integrability of dynamical system
(i.e. via geometrical ~~system~~ structure)

iii.) techniques to solve $S(q,t)$ $\Leftrightarrow$ equiv to solving Hamilton's Eqn.
(integrability)

iv.) H-J eqn. is eikonal equation for Schroedinger Eqn. $\rightarrow$ semi-classical insight

i.e.

S.E.: $$i\hbar \frac{\partial \psi}{\partial t} = H\psi$$
$$= -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi$$

now, semi-classical limit appears as $\hbar \rightarrow 0$ limit, so:

$$\psi = \psi_0 \, e^{i\phi(x,t)/\hbar}$$

$\hbar \to 0 \Rightarrow$ classical trajectory emerges as phase stationarity

$\hbar \sim$ action $\Rightarrow \phi \sim$ action

$$+i\hbar \frac{i}{\hbar} \frac{\partial \phi}{\partial t} = \frac{-\hbar^2}{2m} \frac{-1}{\hbar^2} (\nabla\phi)^2 + V$$

$$-\frac{\partial \phi}{\partial t} = \frac{1}{2m} (\nabla\phi)^2 + V$$

$$= H(\nabla\phi, x, t)$$

so, if take $\phi \equiv S$, by classical correspondence (i.e. $\delta S = 0 \Rightarrow$ classical trajectory), then eikonal equation is clearly H-J equation

$$\boxed{\frac{\partial S}{\partial t} = -H\left(\frac{\partial S}{\partial q}, q, t\right)}$$

and eikonal equation for T.I.S.E. is time independent H-J equation

$$H = E \quad , \quad H = H\left(\frac{\partial S}{\partial q}, q\right)$$

→ Additional / Alternative Variational Principle
(Abbreviated Action / Principle of Maupertuis).

Now, for eikonal theory: $\underline{\underline{2}}$ results;

– ray paths ; $\delta \mathcal{T} = 0$ $\quad \mathcal{T} = \int ds\, n(\underline{x})$

i.e. paths trace ray, but dont give any time info.

– ray trajectories : $\delta \Phi = 0$

$$\frac{d\underline{x}}{dt} = \frac{\partial \omega}{\partial \underline{k}} \; ; \; \frac{d\underline{k}}{dt} = -\frac{\partial \omega}{\partial \underline{x}}$$

i.e. trajectories yield time info → at what t does wave packet pass?

Similarly, for particles:

position, trajectory : $\underline{x}(t)$ → usual

path : $r(\ell)$ → curve followed by particle. Does not tell when particle at a particular point.

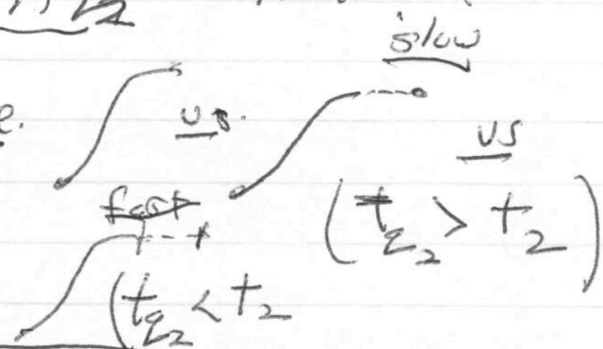
e.g. free particle: paths are geodesics
⇒ contain geometry, only.

now, for $\partial_t L = 0$; $H(p, q) = E$ conservative.

- $\delta \int_{q_1, t_1}^{q_2, t_2} L = 0 \Rightarrow \delta S = 0$ for fixed end points, (usual)

- now, allow t_2 vary; $\underbrace{q_1, q_2}$ fixed

$$\delta \int_{q_1, t_1}^{q_2, t_2} L = -H \delta t$$

i.e. 

$\Rightarrow$ defines virtual paths ...

i.e. particle passes thru q_2 but not necessarily at t_2.

- for energy conserving virtual paths:

$$\delta S + H \delta t = 0 = \delta S + E \delta t$$

also know:

$$S = \int (p \dot{q} - H) dt$$

$$= \int (p\, dq - H\, dt) = \int (p\, dq - E\, dt)$$

so, in general:

$$\boxed{S = \int \sum_i p_i \, dq_i - E(t - t_0)}$$

define:

$$S_0 = \int \sum_i p_i \, dq_i \equiv \text{abbreviated action}$$

so, for paths:

$$\boxed{\delta S_0' = \delta \int \sum_i p_i \, dq_i = 0}$$ [Principle of Maupertuis

⇒ abbreviated action has minimum (extremum) with respect to all paths which conserve energy and pass thru final point at any t.

⇒ to use S_0', need express momenta in terms q, dq via:

$p_i = \partial L / \partial \dot{q}_i \qquad L = L(q, \dot{q})$

$E(q, \dot{q}) = E$

i.e.

$$L = 1/2 \sum_{i,k} a_{i,k}(q)\,\dot{q}_i \dot{q}_k - U(q)$$

→ generic form (calc' HW)

$$dS_0 = \sum_i p_i \, dq_i$$

but

$$p_i = \frac{\partial L}{\partial \dot{q}_i} = \sum_k a_{i,k}(q)\,\dot{q}_k$$

so

$$dS_0 = \sum_{k,i} a_{ik}(q)\,\dot{q}_k \, dq_i$$

$$= \sum_{k,i} a_{i,k}(q)\,\frac{dq_k}{dt}\,dq_i$$

for dt:

$$E = 1/2 \sum_{i,k} a_{i,k}(q)\,\dot{q}_i \dot{q}_k + U(q)$$

$$1/2 \sum_{i,k} a_{i,k}(q)\,\frac{dq_i \, dq_k}{(dt)^2} = E - U$$

$$\therefore \quad dt = \left[\sum a_{i,k}\, dq_i\, dq_k \,/\, 2(E-U) \right]^{1/2}$$

so using dt:

$$S = \int \Big[2(E-U) \underbrace{\sum_{i,k} a_{i,k}\, dq_i\, dq_k}_{\sim d\ell^2} \Big]^{1/2} \quad *$$

variational for path

For single particle: $T = \frac{1}{2} m (d\ell/dt)^2$

$$\delta S_0 = \delta \int_{q_1}^{q_2} \left[2m(E-U) \right]^{1/2} d\ell$$

- Jacobi's integral $\rightarrow$ { obvious semi-classical correspondence

- if $U = 0$ (free)

$$\delta S_0 = \delta \int d\ell = 0 \quad \rightarrow$$

(extremum) minimal distance path of Least Action is geodesic

Ex. Derive equation for path
(n.b. ray !)

$$\delta \int (E-U)^{1/2} dl$$

$$= -\int \frac{\partial U}{\partial \underline{r}} \cdot \delta \underline{r} \frac{dl}{2(E-U)^{1/2}} + \int (E-U)^{1/2} d\delta l$$

so

$$dl^2 = dr^2$$

$$dl \, d\delta l = d\underline{r} \cdot d\delta \underline{r}$$

$$d\delta l = \frac{d\underline{r}}{dl} \cdot d\delta \underline{r}$$

$$\Rightarrow \delta \int (E-U)^{1/2} dl =$$

$$-\int \left\{ \frac{\partial U}{\partial \underline{r}} \cdot \frac{\delta \underline{r}}{2(E-U)^{1/2}} dl - \sqrt{(E-U)} \frac{d\underline{r}}{dl} \cdot d\delta \underline{r} \right\}$$

$$d\delta \underline{r} = \left(\frac{d}{dl} \delta \underline{r} \right) dl$$

now, e.p.'s fixed, so IBP

$\delta r|_{ep} \Rightarrow$

$$0 = -\int \left\{ \frac{\partial U}{\partial \underline{r}} \cdot \frac{\delta \underline{r}}{2(E-U)^{1/2}}\, d\ell + \frac{d}{d\ell}\left[(E-U)^{1/2} \frac{d\underline{r}}{d\ell} \cdot \delta \underline{r} \, d\ell \right] \right\}$$

$$0 = -\int \delta\underline{r} \cdot \left\{ \partial U/\partial \underline{r} \, \frac{1}{2(E-U)^{1/2}} + \frac{d}{d\ell}\left[(E-U)^{1/2}\frac{d\underline{r}}{d\ell}\right] \right\} d\ell$$

$\Rightarrow$

$$\boxed{2\,(E-U)^{1/2}\frac{d}{d\ell}\left[(E-U)^{1/2}\frac{d\underline{r}}{d\ell}\right] = -\frac{\partial U}{\partial \underline{r}}}$$

now, as for ray case:

$d\underline{r}/d\ell = \underline{t}$ unit tangent to path

so

$$\frac{d^2\underline{r}}{d\ell^2} = \frac{1}{2(E-U)}\left[-\frac{\partial U}{\partial \underline{r}} - \frac{d\underline{r}}{d\ell}\cdot\left(-\frac{\partial U}{\partial \underline{r}}\right)\underline{t} \right]$$

$$= \frac{1}{2(E-U)}\left[\underline{F} - (\underline{t}\cdot\underline{F})\underline{t} \right]$$

but

$$\underline{F} - \underline{t}\cdot\underline{F} = \underline{F}_n$$

normal (to path) force

$$\therefore \quad \frac{d\underline{t}}{d\ell} = \frac{1}{2(E-U)} \underline{F}_n$$

$$E-U = E_{kin} = \frac{1}{2} m V^2$$

$$d\underline{t}/d\ell = \frac{\hat{n}_0}{R_c}$$

$\hat{n}_0 \equiv$ normal to path

$R_c \equiv$ radius of curvature

$$\Rightarrow \boxed{\frac{mV^2}{R_c} \hat{n}_0 = \underline{F}_n}$$

normal acceleration on curved path.

Hamilton-Jacobi II

⇒ Solving the Hamilton-[redacted] Jacobi

a.) Equation... (See L&L: Chapt. VII)

Now goal of classical mechanics is to integrate equations of motion.

What does "integrability" mean?

- can reduce $p_i(t)$, $q_i(t)$ equations to solution by quadrature, each i.
- if N degree of freedom [redacted] system, can find N CoMs (IOMs) s/t $P_{1 \dots N} = \text{const.}$

Now, a sufficient, but not necessary, condition for integrability is that the H-J equation be separable and solvable (N.B. "Solvable" ≡ can reduce pieces of separation to quadrature).

Best to proceed via examples:

i.) trivial - 1D oscillator

$$\frac{p^2}{2m} + \frac{1}{2} k q^2 = E \Rightarrow \frac{1}{2m}\left(\frac{\partial S}{\partial q}\right)^2 + \frac{1}{2} k q^2 = E$$

$$\therefore \quad \frac{1}{2m}\left(\frac{\partial S}{\partial q}\right)^2 = E - \frac{kq^2}{2}$$

$$\boxed{S = \sqrt{2m}\int dq\,\sqrt{E - kq^2/2}} \quad = S(q)$$

but also $\quad \frac{\partial S}{\partial q} = p = m\frac{dq}{dt}$

$$\therefore \quad \frac{dq}{dt} = \frac{\sqrt{2m}}{m}\left(E - kq^2/2\right)^{1/2} \qquad \left\{ t - t_0 = \frac{1}{2}\frac{\partial S}{\partial E} \right\}$$

so $$\boxed{\int dt = \sqrt{m}\int dq \Big/ \sqrt{2}\left(E - kq^2/2\right)^{1/2}}$$ formal solution

Rather clearly, obtaining S is equivalent to a solution for q.

ii.) Non-Trivial – <u>3D Potential</u>

i.e. [What form of $V(r, \theta, \phi)$ allows integrable motion in spherical coordinates?]

$\Rightarrow$ If separable solution of H-J equation can be constructed, motion is integrable.

ie. recall solution of PDE by separation of variables

$$\nabla^2 \psi + \frac{\omega^2}{c^2}\psi = 0$$

c const.

if $c^2(\underline{x})$, what is separable?

$$1/c^2(\underline{x}) = \frac{1}{c^2(x)} + \frac{1}{c^2(y)} + \frac{1}{c^2(z)}$$

and WKB.

$$\psi = X(x)\,Y(y)\,Z(z)$$

$$\frac{X''}{X}\cancel{(x)} + \frac{Y''}{Y}\cancel{(y)} + \frac{Z''}{Z}\cancel{(z)} + \underbrace{\frac{\omega^2}{c^2}}_{\text{cnst}} = 0$$

Now, to each ratio i.e. X''/X, etc assign separation constant k_x^2, k_y^2, k_z^2

then $\frac{X''}{X} = -k_x^2$, etc.

$$-k_x^2 - k_y^2 - k_z^2 + \frac{\omega^2}{c^2} = 0$$

Solutions from separation of variables are not most general.

and determine separation constants by B.C.'s $\Rightarrow$ eigenvalues.

N.B. Separation constants $\rightarrow$ [b.c.'s, symmetry

Now;

$$H = \frac{p_r^2}{2m} + \frac{p_\theta^2}{2mr^2} + \frac{p_\phi^2}{2m\sin^2\theta\, r^2} + V =$$

a $H\left(\frac{\partial S}{\partial q}, q, E\right) = E$ $\qquad S = S_0 - Et$

is T.I. H-J eqn.

$\Rightarrow$

$$\boxed{\frac{1}{2m}\left\{\left(\frac{\partial S}{\partial r}\right)^2 + \frac{1}{r^2}\left(\frac{\partial S}{\partial \theta}\right)^2 + \frac{1}{r^2\sin^2\theta}\left(\frac{\partial S}{\partial \phi}\right)^2\right\} + V(r,\theta,\phi) = E}$$

Here, separation is <u>additive</u>:

$$S = S_1(r) + S_2(\theta) + S_3(\phi)$$

$\Rightarrow$

$$\frac{1}{2m}\left\{\left(\frac{\partial S_1(r)}{\partial r}\right)^2 + \frac{1}{r^2}\left[\left(\frac{\partial S_2(\theta)}{\partial \theta}\right)^2 + \frac{1}{\sin^2\theta}\left(\frac{\partial S_3}{\partial \phi}\right)^2\right]\right\} + V(r,\theta,\phi) = E.$$

Now:

$\rightarrow$ structure of V must match the factors in kinetic energy.

→ integrability set by metric ⇒ determines KE via $d\ell^2/dt^2$. ✳

so, evident that:

$$\boxed{V(r,\theta,\phi) = a(r) + \frac{b(\theta)}{r^2} + \frac{c(\phi)}{r^2\sin^2\theta}}$$

will allow solution by separation.

Now, to solve:

$$E = \left\{\frac{1}{2m}\left(\frac{\partial S_1(r)}{\partial r}\right)^2 + a(r)\right\} + \frac{1}{r^2}\left[\left\{\frac{1}{2m}\left(\frac{\partial S_2(\theta)}{\partial\theta}\right)^2 + b(\theta)\right\} + \frac{1}{\sin^2\theta}\left\{\frac{1}{2m}\left(\frac{\partial S_3(\phi)}{\partial\phi}\right)^2 + c(\phi)\right\}\right]$$

or

$$E = f_1(r) + \frac{1}{r^2}\left\{f_2(\theta) + \frac{1}{\sin^2\theta}f_3(\phi)\right\}$$

and can separate and solve f:

$$f_3(\phi) = C_\phi^2 \rightarrow \text{const}$$

$$f_2(\theta) + \frac{C_\phi}{\sin^2\theta} = C_\theta^2 \rightarrow \text{const}$$

$$f_1(r) + \frac{C_\theta}{r^2} = E \rightarrow \text{const}$$

then:

- can solve azimuthal, polar, radial EOMs.

- separate and solve H-J.

Key points:

- in separation of H-J eqn., separation constants C_ϕ, C_θ, E
  - related to COMs p_ϕ, L^2, E
  - related to symmetry.

separation solution related to ability to identify C.O.Ms.

Proceeding:

$$\frac{1}{2m}\left(\frac{\partial S_3}{\partial \phi}\right)^2 + C(\phi) = C_\phi^2$$

Simplifying assumption: take $C(\phi) = 0$
i.e. no azimuthal symmetry breaking in potential.

so

$$\frac{1}{2m}\left(\frac{\partial S_3}{\partial \phi}\right)^2 = C_\phi^2$$

so,

$$\frac{\partial S_3}{\partial \phi} = \text{const} = p_\phi$$

↳ azimuthal momentum

$$S_3 = p_\phi \phi + C_3$$

$$C_\phi^2 = \frac{p_\phi^2}{2m}$$

so, plugging in S_3 bit:

$$E = \left\{\frac{1}{2m}\left(\frac{\partial S_1}{\partial r}\right)^2 + a(r)\right\} + \frac{1}{r^2}\left\{\frac{1}{2m}\left(\frac{\partial S_2}{\partial \theta}\right)^2 + b(\theta) + \frac{p_\phi^2}{2m\sin^2\theta}\right\}$$

Observe:

$$f_2'(\theta) = f_2(\theta) + \frac{p_\phi^2}{2m\sin^2\theta}$$

now $f_2'(\theta) \to \underbrace{C_\theta^2}_{\text{sep const. for } \theta}$

$\therefore$

can relate to L_θ

$$\frac{1}{2m}\left(\frac{\partial S_2}{\partial \theta}\right)^2 + b(\theta) + \frac{p_\phi^2}{2m\sin^2\theta} = C_\theta^2$$

$\Rightarrow$

$$\frac{\partial S_2}{\partial \theta} = \sqrt{2m}\left(C_\theta^2 - b(\theta) - \frac{p_\phi^2}{2m\sin^2\theta}\right)^{1/2}$$

$$S_2(\theta) = \sqrt{2m}\int d\theta \left(C_\theta^2 - b(\theta) - \frac{p_\phi^2}{2m\sin^2\theta}\right)^{1/2} + C_2$$

observe:

$\rightarrow$ $C_\theta^2 = L^2$ <u>if</u> $b(\theta) = 0$ (i.e. C_θ^2 = angular momentum <u>if</u> central potential)

→ Reality $\mathcal{S}$ constrains P_ϕ relative to C_Θ

→ Note have: $\left.\begin{matrix} P_\phi \\ C_\Theta \end{matrix}\right\}$ consts. (~ mom.)

and C_2, C_3 (i.c.'s)

Then for last step absorb C_Θ^2/r^2 into radial piece $f_1(r)$

$$\boxed{E = \frac{1}{2m}\left(\frac{\partial S_1}{\partial r}\right)^2 + a(r) + \frac{C_\Theta^2}{2mr^2}}$$

from f_2'/r^2
(centrifugal bit of radial motion)

so

$$S_1(r) = \sqrt{2m}\int dr \left(E - a(r) - \frac{C_\Theta^2}{2mr^2}\right)^{1/2} + C_1$$

so

$$\mathcal{S} = S_1(r) + S_2(\theta) + S_3(\phi)$$

where:

COM, sep const ↓   sep const ↓

$$S = \int dr \left[\sqrt{2m}\left(E - a(r) - \frac{C_\theta^2}{2mr^2}\right)^{1/2}\right]$$

sep const

$$+ \int d\theta \left[\left(C_\theta^2 - b(\theta) - \frac{p_\phi^2}{2m\sin^2\theta}\right)\sqrt{2m}\right]^{1/2}$$

$$+ p_\phi \phi + C_1 + C_2 + C_3$$

N.B.: 3D $\Rightarrow$ 6 const. $\begin{cases} 3 \text{ non-trivial} \\ 3 \text{ trivial} \end{cases}$

$= S(r, \theta, \phi)$

is separation solution of H-J equation

$$U = a(r) + \frac{b(\theta)}{r^2} + \frac{C(\phi)}{r^2\sin^2\theta}$$

Sep. constants:

$C_\phi^2 \rightarrow$ sep const for ϕ
$\Rightarrow p_\phi^2/2m$ for $C(\phi) = 0$

$C_\theta^2 \rightarrow$ sep const for θ
$\Rightarrow \frac{L^2}{2m}$ if $b(\theta) = 0$.

E → Sep constant for r
→ Energy

Finally, if seek time dependence, obtain explicit $q(t)$ for r, θ, ϕ from

$$p_i = \frac{\partial S}{\partial q_i} \quad \text{and} \quad p_i = \frac{\partial L}{\partial \dot{q}_i} = \begin{cases} m\dot{r} \\ mr^2\dot{\theta} \\ m\sin^2\phi\, r^2\dot{\phi} \end{cases}$$