4.5 Canonical Transformations

* For Lagrange function L recall

$$L(q,\dot{q},t) \quad \text{and} \quad L'(q,\dot{q},t) = L(q,\dot{q},t) + \frac{d}{dt} f(q,t)$$

are equivalent (mechanical gauge transformation)

Let $q = (q_i)_{i=1}^{s}$ and $Q = (q_i)_{i=1}^{s}$ be two equivalent sets of generalized coordinates for a system with transformations $q(Q,t)$ or $Q(q,t)$ (called "point transformations")

Then

$$\frac{\partial L}{\partial q_i} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}_i} = 0 \quad \Longleftrightarrow \quad \frac{\partial L}{\partial Q_i} - \frac{d}{dt}\frac{\partial L}{\partial \dot{Q}_i} = 0$$

$$i = 1, \dots, s \qquad\qquad i = 1, \dots, s$$

"Form invariance of Lagrange equations under point transformations".

* The Hamilton equations are invariant under a much wider range of transformations in phase space.

Consider new phase space coord. $Q = Q(p,q,t)$ and $P = P(p,q,t)$

Such a phase space transformation which leads to

$$\dot{Q}_j = \frac{\partial \bar{H}}{\partial P_j} \qquad \dot{P}_j = -\frac{\partial \bar{H}}{\partial Q_j}$$

$j = 1, \dots, s$ for the new Hamilton fct. $\bar{H}(P,Q,t)$

is called canonical.

Caution: Not all phase space transformations are canonical!

* Let $F_1 \equiv F_1(q, Q, t)$ be a function of the new and old coordinates. The transformation $(p,q) \to (P,Q)$ is canonical if

$$\boxed{\sum_{j=1}^{s} p_j \dot{q}_j - H = \sum_{j=1}^{s} P_j \dot{Q}_j - \overline{H} + \frac{dF_1}{dt}} \qquad (*)$$

F_1 is called a generating function of the transformation.

Why? The left and right hand side lead to the same Hamilton principle:

$$\delta \int \Big(\sum_j p_j dq_j - H dt\Big) = 0 \iff \delta \int \Big(\sum_j P_j dQ_j - \overline{H}\, dt + dF_1\Big) = 0$$

total differential doesn't affect variation

$$\iff \delta \int \Big(\sum_j P_j dQ_j - \overline{H} dt\Big) = 0$$

* By comparing $dF_1 = \sum_j p_j dq_j - \sum_j P_j dQ_j + (\overline{H} - H) dt$

and $dF_1 = \sum_j \frac{\partial F_1}{\partial q_j} dq_j + \sum_j \frac{\partial F_1}{\partial Q_j} dQ_j + \frac{\partial F_1}{\partial t} dt$

we see that

$$\boxed{p_i = \frac{\partial F_1}{\partial q_i} \qquad P_i = -\frac{\partial F_1}{\partial Q_i} \qquad \overline{H} = H + \frac{\partial F_1}{\partial t}}$$

$i = 1, \dots, s$

i.e. Hamiltonian changes not just through plugging in transformation!

* Canonical transformations can also be generated by generating functions $F_2(q, P, t)$, $F_3(p, Q, t)$ and $F_4(p, P, t)$

~~with the same condition (*)~~

E.g. for F_2 we get $p_i = \frac{\partial F_2}{\partial q_i}$, $Q_i = \frac{\partial F_2}{\partial P_i}$, $\overline{H} = H + \frac{\partial F_2}{\partial t}$

and $\sum_{j=1}^{s} p_j \dot{q}_j - H = -\sum_{j=1}^{s} Q_j \dot{P}_j - \overline{H} + \frac{dF_2}{dt}$

Obviously $F_1 = F_2 - \sum_{j=1}^{s} Q_j P_j$

i.e. F_1, F_2 are related by Legendre transformation

$\bar{H} = H$

* Example: $Q_i = p_i$, $P_i = -q_i$ $i = 1, .., s$
is a canonical transformation
Why? Canonical equations obviously invariant

Thus there is a symmetry between p_i and q_i in phase space which makes the distinction between coordinates and momenta arbitrary.
Pairs (p_i, q_i) are called "canonically conjugate" quantities

Note that Poisson brackets between coord. and momenta are invariant under canonical transformations.

* Example: $q_i \mapsto Q_i(t) = q_i(t+\tau)$; $p_i \mapsto P_i(t) = p_i(t+\tau)$
is a canonical transformation.
I.e. time evolution of a system can be interpreted as a can. trans.

Why? From (4.4.2) for action with endpoint $(p_i^{(2)}, q^{(2)})$ and time variable

$$dS = \sum_{i=1}^{s} p_i^{(2)} dq_i^{(2)} - H^{(2)}dt.$$ If initial point $(p^{(1)}, q^{(1)})$ is also flexible

$$dS = \sum_{i=1}^{s} \left(p_i^{(2)} dq_i^{(2)} - p_i^{(1)} dq_i^{(1)}\right) - \left(H^{(2)} - H^{(1)}\right)dt$$

H taken at (2) and (1) resp.

$$\Rightarrow dS = \sum_i \left(p(t+\tau)\, dq(t+\tau) - p(t)\, dq(t)\right) - \left(H(t+\tau) - H(t)\right)dt$$

Compare with (*) $\Rightarrow -S$ is generating functional for this transformation and it is canonical.

* Example: Harmonic Oscillator

Start with usual coord. and $H = \frac{p^2}{2m} + \frac{m\omega^2}{2} q^2$

Consider generating function $F_1(q, Q) = \frac{m\omega}{2} q^2 \cot Q$

$\Rightarrow \quad p = \frac{\partial F_1}{\partial q} = m\omega q \cot Q \qquad P = -\frac{\partial F_1}{\partial Q} = \frac{m\omega q^2}{2 \sin^2 Q}$

$\Rightarrow$ the solution to these equations is

$$q = \sqrt{\frac{2P}{m\omega}} \sin Q \qquad p = \sqrt{2m\omega P} \cos Q$$

this is the explicit form of the can. trans. $q(P,Q)$, $p(P,Q)$

New Hamiltonian $\bar{H}(Q,P) = H(q(Q,P), p(Q,P)) = \omega P$!

Q cyclical, $\dot{Q} = \omega \qquad \dot{P} = 0$ from Hamilton equations

Solutions. $Q = \omega t + \alpha \qquad P = \frac{H}{\omega} = \frac{E}{\omega}$ = const.

Much easier in new coord.!

Go back to old coord. to check:

$$q(t) = \sqrt{\frac{2E}{m\omega^2}} \sin(\omega t + \alpha) \qquad \checkmark$$

4.6 The Liouville Theorem

* $d\Gamma = dq_1 \dots dq_s \, dp_1 \dots dp_s$ is a volume element in phase space.

Let (p,q) and (P,Q) be variables related by a canonical transformation. Then

$$\int d\Gamma(p,q) = \int \dots \int dq_1 \dots dq_s \, dp_1 \dots dp_s = \int d\Gamma(P,Q) = \int \dots \int dQ_1 \dots dQ_s \, dP_1 \dots dP_s$$

(invariance of phase space integrals under canonical transformations)

Why? Need to check Jacobian J

$$J = \left| \frac{\partial(Q,P)}{\partial(q,p)} \right| \underset{\substack{\uparrow \\ \text{write as} \\ \text{two subsequent} \\ \text{transformations}}}{=} \frac{\left| \frac{\partial(Q,P)}{\partial(q,P)} \right|}{\left| \frac{\partial(q,p)}{\partial(q,P)} \right|} \underset{\substack{\uparrow \\ \text{use block} \\ \text{structure of} \\ \text{determinant}}}{=} \frac{\left| \frac{\partial Q}{\partial q} \right|}{\left| \frac{\partial p}{\partial P} \right|} = \frac{\left| \left(\frac{\partial^2 F_2}{\partial P_i \partial q_k} \right)_{i,k=1}^{s} \right|}{\left| \left(\frac{\partial^2 F_2}{\partial q_k \partial P_i} \right)_{i,k=1}^{s} \right|} = 1$$

$|\dots| = \det(\dots)$

matrices in num. and denom. related through transposition, det is the same.

* Follow time evolution of a volume in phase space. We have

$$\boxed{\int d\Gamma = \text{const.}}$$

i.e. phase space curves behave like incompressible flow.

Why? Time evolution is canonical transformation, then use invariance from above.

This is the starting point of statistical mechanics.

4.7 The Hamilton - Jacobi Equation

* From (4.4.2) we know $\frac{\partial S}{\partial t} + H = 0$ and $\frac{\partial S}{\partial q_i} = p_i$ $i=1,..,s$

We can replace the p_i in $H(p,q)$ to arrive at the Hamilton-Jacobi equation

$$\boxed{\frac{\partial S}{\partial t} + H\left(q_1,..,q_s;\frac{\partial S}{\partial q_1},..,\frac{\partial S}{\partial q_s};t\right) = 0}$$

The HJ equation is first-order, non-linear partial diff. equation for S

* The solution is of the general form

$$S = f(t;q_1,..,q_s;\alpha_1,..,\alpha_s) + \alpha_0$$

since there are $s+1$ integration constants α_i in such a system. One must be additive (here α_0) since the HJ equation only depends on derivatives of S.

We can interpret S as the generating function of a can. transformation to new coordinates $\beta_1,..,\beta_s$ with momenta $\alpha_1,..,\alpha_s$ since

$$p_i = \frac{\partial S}{\partial q_i} \quad ; \quad \underset{\text{definition!}}{\beta_i \equiv \frac{\partial S}{\partial \alpha_i}} \quad ; \quad \underset{\text{definition}}{\bar{H} \equiv H + \frac{\partial S}{\partial t}}$$

However, due to HJ $\bar{H} = 0$, i.e. the mechanical problem is trivial, all new coordinates β_i are cyclical! In particular

$$\alpha_i = \text{const.} \qquad \beta_i = \text{const} \qquad i=1,..,s$$

* Application: find H → solve Hamilton-Jacobi for S → solve set of equations $\frac{\partial S}{\partial \alpha_i} = \beta_i$ $i=1,..,s$ for the q_i as fcts. of α_i, β_i, t

* Example: Harmonic Oscillator

find HJ

$$H = \frac{p^2}{2m} + \frac{1}{2} m \omega_0^2 q^2$$

We want to find $S(q,\alpha,t)$ with $p = \frac{\partial S}{\partial q}$ which fulfills the Hamilton-Jacobi equation

$$\frac{1}{2m}\left(\frac{\partial S}{\partial q}\right)^2 + \frac{1}{2} m\omega_0^2 q^2 + \frac{\partial S}{\partial t} = 0$$

solve HJ

Try separation ansatz $S(q,\alpha,t) = W(q,\alpha) + V(t,\alpha)$

$$\Rightarrow \underbrace{\frac{1}{2m}\left(\frac{\partial W}{\partial q}\right)^2 + \frac{1}{2} m\omega_0^2 q^2}_{\text{indep. of } t} = \underbrace{-\frac{\partial V}{\partial t}}_{\text{indep. of } q} \rightarrow \text{i.e. l.h.s} = \text{const.} = \text{r.h.s.}$$

$$\Rightarrow \begin{cases} \frac{1}{2m}\left(\frac{\partial W}{\partial q}\right)^2 + \frac{1}{2} m\omega_0^2 q^2 = \alpha & \Rightarrow \left(\frac{\partial W}{\partial q}\right)^2 = m^2\omega_0^2\left(\frac{2\alpha}{m\omega_0^2} - q^2\right) \\ \frac{dV}{dt} = -\alpha & \Rightarrow V(t) = -\alpha t + \text{const.} \end{cases}$$

$$\Rightarrow S(q,\alpha,t) = m\omega_0 \int dq \sqrt{\frac{2\alpha}{m\omega_0^2} - q^2} - \alpha t + \text{const.}$$

integral doable but not needed here

find q,p as functions of α,β

We have $\text{const.} = \beta = \frac{\partial S}{\partial \alpha} = \frac{1}{\omega_0}\int dq \frac{1}{\sqrt{\frac{2\alpha}{m\omega_0^2} - q^2}} - t$

$$= \frac{1}{\omega_0} \arcsin\left(q\omega_0\sqrt{\frac{m}{2\alpha}}\right) - t \qquad (*)$$

This can be used to determine q: $q = \frac{1}{\omega_0}\sqrt{\frac{2\alpha}{m}} \sin\omega_0(t+\beta) \equiv q(\alpha,\beta,t)$

On the other hand $p = \frac{\partial S}{\partial q} = \frac{\partial W}{\partial q} = m\omega_0\sqrt{\frac{2\alpha}{m\omega_0^2} - q^2} \underset{\text{pluging}}{=} \sqrt{2\alpha m}\cos\omega_0(t+\beta) \equiv p(\alpha,\beta,t)$

fix α,β from initial cond.

α,β conserved conjugate variables with dimensions of energy and time resp.

α,β fixed by initial conditions, e.g. $p(t=0)=0$, $q(t=0)=q_0$

$p(t=0) \Rightarrow \alpha = \frac{1}{2} m\omega_0^2 q_0^2$ i.e. $\alpha = E$ is the energy of the oscillator

$(*) \Rightarrow \beta = \frac{1}{\omega_0}\arcsin(1) = \frac{\pi}{2\omega_0}$

Finally plug α,β back into solutions: $q(t) = \sqrt{\frac{2E}{m\omega_0^2}}\cos\omega_0 t = q_0\cos\omega_0 t$

$p(t) = -\sqrt{2Em}\sin\omega_0 t = -m\omega_0 q_0 \sin\omega t$ as we already know!

* Action Waves:

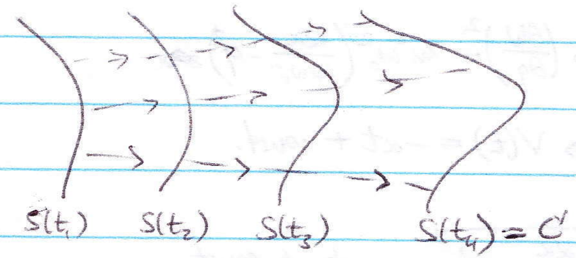
From here on: particle of mass m in 3-D space, scleronomic system with $\frac{\partial H}{\partial t}=0$; $(q_1,q_2,q_3)=(x,y,z)=\vec{r}$; $(\alpha_1,\alpha_2,\alpha_3)\equiv(P_1,P_2,P_3)=\vec{P}$

Then from $S=\int\left(\sum_{i=1}^{3} p_i\,dq_i - H\,dt\right) \Rightarrow S(\vec{r};\vec{P},t)=W(\vec{r},\vec{P})-Et$

(separation of $\vec{r}$ and t)

W indep. of t $\Rightarrow$ $W=$ const. defines a surface in configuration space $\mathbb{R}^3$ since also $\vec{P}=$ const.

$\Rightarrow$ The condition $S=$ const. defines surfaces $W=$ const. moving as a fct. of time



can be interpreted as a moving wave front.

$\Leftrightarrow W=C+Et_4$

What is the velocity of the action waves?

$$0 \stackrel{!}{=} S(t+dt)-S(t)=\frac{\partial S}{\partial t}dt+\frac{\partial S}{\partial x}dx+\frac{\partial S}{\partial y}dy+\frac{\partial S}{\partial z}dz=-E\,dt+\nabla W\cdot\underbrace{d\vec{r}}_{\vec{u}\,dt}$$

$$\Rightarrow \nabla W\cdot\vec{u}=E$$

∇W orthogonal to surface $W=$ const. $\Rightarrow$ wave velocity $\vec{u}$ $\perp$ $W=$ const. surface

on the other hand $p_i=\frac{\partial S}{\partial r_i}=\frac{\partial W}{\partial r_i}$ or $\vec{p}=\nabla W$

$\Rightarrow$ Particle velocity $\vec{v}$ also perpendicular to wave front.

Magnitudes: $u=|\vec{u}|=\frac{|E|}{|\nabla W|}=\frac{|E|}{|\vec{p}|}$ (*)

$v=|\vec{v}|=\frac{|\vec{p}|}{m}$

$$\Rightarrow uv=\frac{|E|}{m}=\text{const.}$$

i.e. particle and action wave velocities are both perpendicular to the wave front and their magnitudes are inversely proportional

Free particle $E = T$: $u = \frac{1}{2} v$

Particle at rest $E = V$: $u = \infty$

* Connection with quantum mechanics:

In the previous case Hamilton-Jacobi can be written as

$$\frac{1}{2m}(\nabla W)^2 + \mathcal{U} = E$$

$$\Rightarrow (\nabla W)^2 = 2m(E - \mathcal{U})$$

$$u^2 = \frac{E^2}{p^2} = \frac{E^2}{2mT} = \frac{E^2}{2m(E-\mathcal{U})}$$

$$\Rightarrow (\nabla W)^2 = \frac{E^2}{u^2}$$

on the other hand (*) $\Rightarrow (\nabla W)^2 = \frac{E^2}{u^2}$

plug back in $\nabla W = \nabla S$, $E = -\frac{\partial S}{\partial t}$

$$\Rightarrow (\nabla S)^2 = \frac{1}{u^2}\left(\frac{\partial S}{\partial t}\right)^2 \qquad \binom{*}{*}$$ wave equation for action!

This is formally similar to eikonal approximation in optics

wave optics $\qquad\qquad$ geom. optics

$$\nabla^2\phi - \frac{n^2}{c^2}\frac{\partial^2\phi}{\partial t^2} = 0 \quad \xrightarrow[\text{eikonal appr.}]{} \quad (\nabla L(\vec r))^2 = n^2 = \frac{c^2}{u^2}$$

$\phi = e^{(A(\vec r) + ik_0(L(\vec r) - ct))}$

(wave in z-direction)

time-indep. Schrödinger Equation $\qquad\qquad$ Hamilton-Jacobi

$$\Delta\psi + \frac{2m}{\hbar^2}(E-V)\psi = 0 \quad \longrightarrow \quad (\nabla W(\vec r))^2 = \frac{E^2}{u^2} = 2m(E-\mathcal{U})$$

$S = W - Et \iff k_0(L - ct) \Rightarrow E \sim ck_0 \sim \nu$

need constant with dimension of action

$E \equiv h\nu$

Planck's constant!

116b

$$\Delta\psi + \frac{2m}{\hbar^2}(E-V)\psi = 0 \qquad \text{use ansatz } \psi(\vec r) = e^{\frac{i}{\hbar}W(\vec r)}$$

$$\Rightarrow \frac{i}{\hbar}\Delta W e^{i/\hbar W} + \left(\frac{i}{\hbar}\nabla W\right)^2 e^{i/\hbar W} + \frac{2m}{\hbar^2}(E-V)\, e^{i/\hbar W} = 0$$

$$\Rightarrow (\nabla W)^2 = 2m(E-V) + \underbrace{i\hbar\,\Delta W}_{\to 0 \text{ for } \hbar \to 0 \text{ (classical limit)}}$$

Similarly: time-dep. Schrödinger eq. leads to (**)