4.5 Canonical Transformations

* For Lagrange function \( L \) recall

\[
L(q, \dot{q}, t) \quad \text{and} \quad L'(q, \dot{q}, t) = L(q, \dot{q}, t) + \frac{df}{dt}(q, t)
\]

are equivalent (mechanical gauge transformation)

Let \( q = (q_i) \) and \( Q = (Q_i) \) be two equivalent sets of generalized coordinates for a system with transformations \( q_i(\dot{q}, t) \) or \( Q_i(Q, t) \) (called "point transformations")

Then

\[
\frac{\partial L}{\partial q_i} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}_i} = 0 \quad \Rightarrow \quad \frac{\partial L}{\partial Q_i} - \frac{d}{dt} \frac{\partial L}{\partial \dot{Q}_i} = 0
\]

\( i = 1, \ldots, s \)

"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. \( \mathcal{Q} = \mathcal{Q}(p, q, t) \) and \( P = P(p, q, t) \)

Such a phase space transformation which leads to

\[
\dot{\mathcal{Q}}_j = \frac{\partial \mathcal{H}}{\partial P_j}, \quad \dot{P}_j = -\frac{\partial \mathcal{H}}{\partial \mathcal{Q}_j} \quad \text{for the new Hamilton func.} \ \mathcal{H}(P, \mathcal{Q}, t)
\]

is called canonical.

Caution: Not all phase space transformations are canonical!
Let $F_1 = F_1(q, \dot{q}, t)$ be a function of the new and old coordinates. The transformation $(q, \dot{q}) \to (p, \dot{p}, \phi, \dot{\phi})$ is canonical if

$$\sum_{j=1}^{n} p_j \dot{q}_j - H = \sum_{j=1}^{n} p_j \dot{q}_j - H + \frac{dT_1}{dt}$$

$H$ is called a generating function of the transformation.

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

$$\delta \int (\sum_j p_j \dot{q}_j - H dt) = 0 \iff \delta \int (\sum_j p_j \dot{q}_j - H dt + dF_1) = 0$$

$$\iff \delta \int (\sum_j p_j \dot{q}_j - H dt) = 0$$

By comparing $dT_1 = \sum_j p_j d\dot{q}_j - \sum_j p_j d\dot{q}_j + (H - H) dt$

and $dT_1 = \sum_j \frac{\partial F_1}{\partial \dot{q}_j} d\dot{q}_j + \sum_j \frac{\partial F_1}{\partial q_j} d\dot{q}_j + \frac{\partial F_1}{\partial t} dt$

we see that

$$p_i = \frac{\partial F_1}{\partial \dot{q}_i}, \quad \dot{p}_i = -\frac{\partial F_1}{\partial q_i}, \quad H = H + \frac{\partial F_1}{\partial t}$$

Canonical transformations can also be generated by generating functions $F_2(q, p, t), F_3(p, \phi, t)$ and $F_4(p, \dot{p}, t)$ with the same condition (x)

E.g. for $F_2$ we get $\dot{p}_i = \frac{\partial F_2}{\partial q_i}, \quad \dot{q}_i = \frac{\partial F_2}{\partial \dot{p}_i}, \quad H = H + \frac{\partial F_2}{\partial t}$

and $\sum_{j=1}^{n} p_j \dot{q}_j - H = \sum_{j=1}^{n} q_j \dot{p}_j - H + \frac{\partial F_2}{\partial t}$

Obviously $F_1 = F_2 - \sum \dot{q}_i p_i$, i.e. $F_1, F_2$ are related by Legendre transformation.
Example: \[ \phi_i = p_i, \quad \psi_i = -q_i; \quad i = 1, \ldots, s \]

is a canonical transformation.

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 coordinates and momenta are invariant under canonical transformations.

Example: \[ \phi_i \mapsto \phi_i(t) = q_i(t + \tau), \quad p_i \mapsto p_i(t) = p_i(t + \tau) \]

is a canonical transformation.

I.e., time evolution of a system can be interpreted as a can. tran.

Why? From (10.2) for action with moment and time variable

\[
\frac{dS}{dt} = \sum_{i=1}^{s} \{ p_i \frac{dq_i}{dt} - H(\phi, \psi) \}
\]

If initial point \( (p_i^{(0)}, q_i^{(0)}) \) is also flexible

\[
\frac{dS}{dt} = \sum_{i=1}^{s} \left( p_i^{(0)} \frac{dq_i}{dt} - p_i^{(1)} \frac{dq_i}{dt} \right) - (H^{(0)} - H^{(1)}) \frac{dt}{dt}
\]

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

\[
\Rightarrow \frac{dS}{dt} = \sum_{i=1}^{s} \left( p_i(t + \tau) \frac{dq_i}{dt} - p_i(t) \frac{dq_i}{dt} \right) - (H(t + \tau) - H(t)) \frac{dt}{dt}
\]

Compare with (1) \( \Rightarrow -S \) is generating functional for Kus 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 \( F(q, Q) = \frac{m\omega}{2} q^2 \cot Q \)

\[ \Rightarrow p = \frac{\partial F_i}{\partial q} = m\omega q \cot Q \quad \Rightarrow F_i = \frac{m\omega}{2} q^2 \cot Q \]

\[ \Rightarrow \frac{\partial F_i}{\partial Q} = \frac{m\omega^2 q^2}{2 \sin^2 Q} \]

\[ \Rightarrow \] the solution to these equations is

\[ q = \sqrt{\frac{2P}{m \omega}} \sin Q \quad p = \sqrt{2m \omega^2} \cos Q \]

This is the explicit form of the can. trn. \( q(p, Q), p(p, Q) \)

New Hamiltonian \( H(q, p) = H(q(p, Q), p(q, P)) = \omega P \)

\( Q \) cyclic, \( Q = \omega \quad \dot{Q} = 0 \) from Hamilton equations

Solution: \( Q = \omega t + \alpha \quad P = \frac{H}{\omega} = \frac{E}{\omega} = \text{const.} \)

Much easier in new coord.!

Go back to old coord. to check:

\[ q(t) = \sqrt{\frac{2E}{m \omega^2}} \sin(\omega t + \alpha) \quad \checkmark \]
4.6 The Liouville Theorem

* $d\Gamma = dq_1 dq_2 dp_1 dp_2$ is a volume element in phase space.

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

$$\int d\Gamma(q, p) = \int -\int dq_1 dq_2 dp_1 dp_2 = \int d\Gamma(Q, P) = \int -\int dq_1 dq_2 dp_1 dp_2$$

(invariance of phase space integrals under canonical transformations)

Why? Need to check Jacobian:

$$J = \left| \frac{\partial(q_1, p_1)}{\partial(q_1, p_1)} \right| = \left| \frac{\partial(q_1, p_1)}{\partial(q_1, p_1)} \right| = \left| \frac{\partial q_i}{\partial q_i} \right| \left| \frac{\partial p_i}{\partial p_i} \right| = \left| \frac{\partial q_1}{\partial q_1} \right| \left| \frac{\partial p_1}{\partial p_1} \right|$$

$|\ldots| = \text{det}(\ldots)$

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

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

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 \( \frac{\partial S}{\partial q_i} = p_i, \quad i=1,\ldots,s \)

We can replace the \( p_i \)'s in \( H(p,q) \) to arrive at the Hamilton–Jacobi equation

\[
\frac{\partial S}{\partial t} + H(q_1,\ldots,q_s; \frac{\partial S}{\partial q_1},\ldots,\frac{\partial S}{\partial q_s}; t) = 0
\]

The \( H \) equation is first-order, non-linear partial diff. equation for \( S \).

* The solution is of the general form

\[
S = f(t, q_1, \ldots, q_s; \alpha_1, \ldots, \alpha_s) + \alpha_0
\]

since there are \( s+1 \) integration constants \( \alpha_s \) in such a system. One must be additive (here \( \alpha_0 \)) since the \( H \) equation only depends on derivatives of \( S \).

We can interpret \( S \) as the generating function of a canonical transformation to new coordinates \( \beta_1, \ldots, \beta_s \) with momenta \( \alpha_1, \ldots, \alpha_s \) since

\[
p_i = \frac{\partial S}{\partial q_i}; \quad \beta_i = \frac{\partial S}{\partial \alpha_i}; \quad \bar{H} = H + \frac{\partial S}{\partial t}
\]

definition

However, due to the \( H \)

\[
\bar{H} = 0, \quad \text{i.e. the mechanical problem is trivial,}
\]

all new coordinates \( \beta_i \) are cyclic! In particular

\[
\alpha_i = \text{const.} \quad \beta_i = \text{const} \quad i=1,\ldots,s
\]

* Application: find \( H \) \( \rightarrow \) solve Hamilton–Jacobi for \( S \) \( \rightarrow \) solve set of

equations

\[
\frac{\partial S}{\partial \alpha_i} = \beta_i; \quad i=1,\ldots,s
\]

for the \( q_i \) as pts. of \( \alpha_i, \beta_i, t \).
Example: Harmonic Oscillator

\[ H = \frac{p^2}{2m} + \frac{1}{2} \mu w^2 q^2 \]

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

\[ \frac{1}{2m} \left( \frac{\partial S}{\partial q} \right)^2 + \frac{1}{2} \mu w^2 q^2 + \frac{\partial S}{\partial t} = 0 \]

Try separation ansatz \( S(q, p, t) = W(q, p) + V(t) \):

\[ \Rightarrow \frac{1}{2m} \left( \frac{\partial W}{\partial q} \right)^2 + \frac{1}{2} \mu w^2 q^2 = -\frac{\partial V}{\partial t} \]

\( \text{indep of } t \)

\[ \Rightarrow \frac{1}{2m} \left( \frac{\partial W}{\partial q} \right)^2 = \kappa \Rightarrow \left( \frac{\partial W}{\partial q} \right)^2 = m \mu w^2 \left( \frac{\partial W}{\partial q} - \kappa \right) \]

\[ \Rightarrow \frac{\partial V}{\partial t} = -\kappa \Rightarrow V(t) = -\kappa t + \text{const.} \]

\[ \Rightarrow S(q, p, t) = m \mu w^2 \int dq \sqrt{\mu} \sqrt{\frac{\partial W}{\partial q} - \kappa} - \kappa t + \text{const.} \]

\[ \text{We have const. } \beta = \frac{\partial S}{\partial p} = \frac{1}{\mu w^2} \int dq \sqrt{\frac{\partial W}{\partial q} - \kappa} \]

\[ = \frac{1}{\mu w^2} \arcsin \left( \frac{\mu w^2}{\sqrt{\mu}} \frac{\partial W}{\partial q} \right) - \kappa t \] (1)

This can be used to determine \( q \):

\[ q = \frac{1}{\mu w^2} \sqrt{\frac{\partial W}{\partial q}} \sin \sqrt{\frac{\partial W}{\partial q} - \kappa} \]

On the other hand,

\[ p = \frac{\partial S}{\partial q} = \frac{\partial W}{\partial q} = m \mu w^2 \sqrt{\frac{\partial W}{\partial q} - \kappa} = m \mu w^2 \cos \sqrt{\frac{\partial W}{\partial q} - \kappa} = p(\alpha, \beta, t) \]

\[ \alpha, \beta \text{ conserved conjugate variables with dimensions of energy and time resp.} \]

\[ \alpha, \beta \text{ fixed by initial conditions, e.g. } p(t=0) = 0, q(t=0) = q_0 \]

\[ p(t=0) \Rightarrow \alpha = \frac{1}{2} m \mu w^2 q_0^2 \]

\[ \Rightarrow \beta = \frac{1}{\mu w^2} \arcsin \left( \frac{\mu w^2}{\sqrt{\mu}} \frac{\partial W}{\partial q} \right) = \frac{1}{\mu w^2} \]

Finally plug \( \alpha, \beta \) back into solutions:

\[ q(t) = \sqrt{\frac{\mu w^2}{\mu w^2} \cos \omega t} = q_0 \cos \omega t \]

\[ p(t) = -\sqrt{E m} \sin \omega t = -m \mu w^2 q_0 \sin \omega t \]

As we already know!
*Action Waves:*

From here on: particle of mass $m$ in 3-D space, self-motion system with

$$\frac{\partial \mathbf{r}}{\partial t} = 0; \quad (q_1, q_2, q_3) = (x, y, z) = \mathbf{r}; \quad (p_1, p_2, p_3) = \mathbf{p}$$

Then from

$$S = \int \left( \frac{1}{2} \mathbf{r} \cdot \mathbf{r} \, dq_i - \mathbf{r} \cdot \mathbf{p} \, dt \right) \Rightarrow S(\mathbf{r}, \mathbf{p}, t) = W(\mathbf{r}, \mathbf{p}) - Et$$

(Separation of $\mathbf{r}$ and $t$)

$W$ independent of $t \Rightarrow W = \text{const.}$ defines a surface in configuration space $\mathbb{R}^3$

since also $\mathbf{p} = \text{const.}$

$\Rightarrow$ The condition $S = \text{const.}$ defines surfaces $W = \text{const.}$ moving as a set of finite

![Wave Front](image)

$S(t_1)$ $S(t_2)$ $S(t_3)$ $S(t_4) = C$

$\Rightarrow W = C + Et$

What is the velocity of the action waves?

$$0 = S(t+\Delta t) - S(t) = \frac{\partial S}{\partial t} \Delta t + \frac{\partial S}{\partial x} \Delta x + \frac{\partial S}{\partial y} \Delta y + \frac{\partial S}{\partial z} \Delta z = -E \Delta t + \nabla W \cdot d\mathbf{r}$$

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

$\nabla W$ orthogonal to surface $W = \text{const.} \Rightarrow \text{wave velocity} \quad \frac{\mathbf{p}}{E} \quad W = \text{const.}$ surface

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

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

Magnitudes: $a = |\mathbf{a}| = \frac{|E|}{|\nabla W|} = \frac{|E|}{|\mathbf{p}|} \quad (*)$

$v = \frac{|\mathbf{v}|}{m} = \frac{|E|}{m}$

$\Rightarrow u v = \frac{|E|}{m^2} = \text{const.}$
1. E. particle and action wave velocities are both perpendicular to the wave front and their magnitudes are inversely proportional.

Free particle \( E = T; \quad u = \frac{1}{2} v \)

Particle at rest \( E = V; \quad u = \infty \)

* Connection with quantum mechanics:

In the previous case Hamilton - Jacobi can be written as

\[
\left( \frac{1}{2m} \left( \nabla W \right)^2 + u = E \right) \quad \Rightarrow \left( \frac{1}{2m} \left( \nabla W \right)^2 = \frac{E^2}{u^2} \right)
\]

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

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

\( \Rightarrow \left( \nabla S \right)^2 = \frac{1}{u^2} \left( \frac{\partial S}{\partial t} \right)^2 \) * Wave equation for action

This is formally similar to eikonal approximation in optics

wave optics

\( \nabla^2 - \frac{x^2}{c^2} \frac{\partial^2}{\partial t^2} = 0 \)

\( \text{geom. optics} \quad \left( \nabla \Gamma (\mathbf{r}) \right)^2 = n^2 = \frac{c^2}{u^2} \)

(\text{wave in } z\text{-direction})

time-rep. Schrödinger Equation

\( \Delta \psi + \frac{2mV}{\hbar^2} (E-V) \psi = 0 \quad \Rightarrow \quad \left( \nabla W(\mathbf{r}) \right)^2 = \frac{E^2}{u^2} = 2m(E-U) \)

\( S = W - ET \left\leftrightarrow \right k_0 (L - ct) \Rightarrow E \sim ck_0 \sim V \)

Planck's constant!
\[ \Delta \psi + \frac{2m}{\hbar^2} (E-V) \psi = 0 \]

use ansatz \( \psi(\mathbf{r}) = e^{i \frac{\mathbf{p} \cdot \mathbf{r}}{\hbar}} \)

\[ \Rightarrow \frac{i}{\hbar} \Delta W e^{i \frac{\mathbf{p} \cdot \mathbf{r}}{\hbar}} + \left( \frac{i}{\hbar} \nabla W \right) e^{i \frac{\mathbf{p} \cdot \mathbf{r}}{\hbar}} + \frac{2m}{\hbar^2} (E-V) e^{i \frac{\mathbf{p} \cdot \mathbf{r}}{\hbar}} \psi = 0 \]

\[ \Rightarrow (\nabla W)^2 = 2m (E-V) + i \hbar \Delta W \]

\[ \rightarrow 0 \quad \text{for} \quad \hbar \rightarrow 0 \quad \text{(classical limit)} \]

Similarly: time-independent Schrödinger eq. leads to (\( \ast \))