13 Lecture 13. Canonical transformation

We have already used canonical transformations, but here important facts are collected (point transformation, infinitesimal canonical transformation, Lagrange's bracket, various invariants, Liouville's theorem).

It is important to recognize that time evolution is a canonical transformation.

Classical canonical transformations do not usually correspond to quantum unitary transformations.

13.1 Canonical transformation with generators (review)

The transformation $T : (q, p) \to (Q, P)$ that preserves the form of the canonical equation of motion (10.14) is called a *canonical transformation*. As discussed in **11.3**, we discuss only the canonical transformations with generators F

$$dF = \sum_i p_i dq_i - \sum_i P_i dQ_i + (K - H)dt. \tag{13.1}$$

(13.1) gives

$$\frac{\partial F}{\partial q} = p,\ \frac{\partial F}{\partial Q} = -P,\ \frac{\partial F}{\partial t} = K - H. \tag{13.2}$$

Solving these equations, we can construct the canonical transformation T. In particular, if F is time-independent, then $K = H$ is obtained by replacing q and p in H in terms of Q and P.

Applying a sort of Legendre transformation to generators, we can construct different (perhaps more convenient) transformations:

$$d(F + PQ) = pdq + QdP + (K - H)dt. \tag{13.3}$$

Thus, replacing F with $G = F + \sum_i P_i Q_i$, we obtain

$$dG = \sum_i p_i dq_i + \sum_i Q_i dP_i + (K - H)dt. \tag{13.4}$$

13.2 Canonical transformations make a group

Let us write the generator of the canonical transformation T_i as F_i. The generator of $\prod_i T_i$ is given by $\sum_i F_i$, so the totality of the canonical transformation for a given system makes a(n abelian) group (called the canonical transformation group).

13.3 Point transformations

Through a general canonical transformation position and momentum coordinates are usually mixed up. When we use the spatial coordinate change (say, from the Cartesian to the spherical), no mix-up occurs. Thus, $q \to Q$, $p \to P$ can be described by a subset (subgroup) of canonical transformations called point transformations.

Perhaps, the most convenient generator is the original $G = F + PQ$:

$$dG = p_i dq_i + P_i dQ_i, \tag{13.5}$$

because usually we know q and $Q(q,t)$. Since dG is exact, to obtain G we may use a convenient path: q is constant. Therefore,

$$G = p_i q_i. \tag{13.6}$$

If we write q in terms of Q,

$$P = \frac{\partial G}{\partial Q} \tag{13.7}$$

gives the canonical momentum in the new coordinate system in terms of the old momentum variables. This may be the most mechanical way to get the momentum in the new coordinate system.

Examples:
(1) CM coordinates: $(q_1, q_2) \to Q_1 = (q_1 + q_2)/2, Q_2 = q_1 - q_2$. Since $q_1 = Q_1 + Q_2/2$, $q_2 = Q_1 - Q_2/2$, so (13.6) reads

$$G = p_1(Q_1 + Q_2/2) + p_2(Q_1 - Q_2/2). \tag{13.8}$$

Therefore,

$$P_1 = \frac{\partial G}{\partial Q_1} = p_1 + p_2, \ \ P_2 = \frac{\partial G}{\partial Q_2} = \frac{1}{2}(p_1 - p_2). \tag{13.9}$$

(2) $(x, y, z) \to (r, \theta, \varphi)$: $x = r \sin\theta \cos\varphi$, $y = r \sin\theta \sin\varphi$, $z = r\cos\theta$. The generator reads

$$G = p_x r \sin\theta \cos\varphi + p_y r \sin\theta \sin\varphi + p_z r \cos\theta. \tag{13.10}$$

Its inverse may be generated by

$$G = p_r \|x\| + p_\theta \mathrm{Tan}^{-1} \frac{\sqrt{x^2 + y^2}}{z} + p_\varphi \mathrm{Tan}^{-1} \frac{y}{x}. \tag{13.11}$$

(3) Rotation. We can use an orthogonal transformation to describe it as $x'^i = a^i_j x^j$ (with the summation convention). The generator is $G = a^i_j p_i x^j = p_i x'^i$.
(4) Translation: $x'^k = x^k + \Delta x^k$. Its generator is $G = P(x + \Delta x)$. This gives $P = p$, of course.
(5) Mirror image wrt x^1: $x'^1 = -x^1$, $x'^2 = x^2$, $\cdots$. Its generator is $G = -x_1 P_1 + x^2 P_2 + \cdots$..

13.4 Infinitesimal canonical transformation

A canonical transformation $(q, p) \to (Q, P)$ is said to be an infinitesimal canonical transformation, if $Q - q$ and $P - p$ are infinitesimal.

Let G be its generator:

$$dG = pdq + QdP \tag{13.12}$$

Notice that

$$d(G - qP) = (p - P)dq + (Q - q)dP, \tag{13.13}$$

so $G - qP$ may be written as εS, where ε is an infinitesimal parameter. Therefore, any infinitesimal canonical transformation has the following generator

$$G(q, P) = qP + \varepsilon S(q, p), \tag{13.14}$$

where P in S has been replaced by p because of ε in front of it. S is called the generator of the infinitesimal canonical transformation. We have

$$p = \frac{\partial G}{\partial q} = P + \varepsilon \frac{\partial S}{\partial q}, \tag{13.15}$$

$$Q = \frac{\partial G}{\partial P} = q + \varepsilon \frac{\partial S}{\partial p}. \tag{13.16}$$

That is,

$$Q = q + \varepsilon \frac{\partial S}{\partial p}, \;\; P = p - \varepsilon \frac{\partial S}{\partial q}. \tag{13.17}$$

13.5 Infinitesimal canonical transformation of mechanical variables

A mechanical variable $F = F(q, p)$ changes, according to the infinitesimal canonical transformation with generator S, as

$$F(Q, P) - F(q, p) = \varepsilon \left(\frac{\partial F}{\partial q} \frac{\partial S}{\partial p} - \frac{\partial F}{\partial p} \frac{\partial S}{\partial q} \right) = \varepsilon [F, S]_{PB}. \tag{13.18}$$

13.6 Time evolution is canonical transformation

We know the time evolution of a mechanical variable according to the natural motion of the system obeys

$$\frac{dF}{dt} = [F, H]_{PB}. \tag{13.19}$$

$\varepsilon \to \delta t$ and $S \to H$ in (13.18) just gives this equation. Thus we may conclude that time evolution is a canonical transformation.

13.7 One form of Noether's theorem

Suppose the Hamiltonian is invariant under the infinitesimal canonical transformation with the generator W that changes a mechanical variable $f \to f + df$. Then (13.18) implies

$$dH = df[H, W] = 0. \tag{13.20}$$

That is, W is an invariant of motion.

13.8 What is the relation between classical canonical and quantum unitary transformations?

As point transformations tell us, any coordinate transformation is canonical classically. However, it is well known that the canonical quantization using the correspondence between the commutator and the Poisson bracket must choose (basically) the Cartesian coordinates; if the formalism is naively applied to the system described with the aid of the spherical coordinates, the resultant quantum mechanics are not at all equivalent. Thus, it is clear that the usual canonical quantization and canonical transformations are usually not compatible.

If a transformation gives an equivalent quantum mechanical system, and if there is a corresponding classical system, there is a corresponding canonical transformation. However, the converse is not usually true.

13.9 Lagrange bracket

Let f and g be differentiable mechanical quantities. The Lagrange bracket between them is defined as

$$(f,g) = \frac{\partial q}{\partial f}\frac{\partial p}{\partial g} - \frac{\partial q}{\partial g}\frac{\partial p}{\partial f}. \tag{13.21}$$

13.10 Poisson vs Lagrange brackets

Let $2n$ canonical variables be denoted as $\{u_j\}_{j=1}^{2n}$. Then

$$\sum_k [u_k, u_i]_{PB}(u_k, u_j) = \delta_{ij}. \tag{13.22}$$

This is shown by explicit calculation:[136]

$$\sum_k \left(\frac{\partial u_k}{\partial q}\frac{\partial u_i}{\partial p} - \frac{\partial u_k}{\partial p}\frac{\partial u_i}{\partial q}\right)\left(\frac{\partial q}{\partial u_k}\frac{\partial p}{\partial u_j} - \frac{\partial p}{\partial u_k}\frac{\partial q}{\partial u_j}\right) = \frac{\partial u_i}{\partial p}\frac{\partial p}{\partial u_j} + \frac{\partial u_i}{\partial q}\frac{\partial q}{\partial u_j} = \frac{\partial u_i}{\partial u_j}. \tag{13.23}$$

13.11 Integral invariant

Take a smooth closed curve C in the phase space (q,p). If a canonical transformation $(q,p) \to (Q,P)$ is applied to this curve, we get a closed curve C' in the phase space

[136] If you do not like the following shorthand, do explicit calculation with summation convention. For example, one cross term reads

$$\frac{\partial u_k}{\partial p_f}\frac{\partial u_i}{\partial q_f}\frac{\partial q_g}{\partial u_k}\frac{\partial p_g}{\partial u_j} = \frac{\partial q_q}{\partial p_f}\frac{\partial u_i}{\partial q_f}\frac{\partial p_g}{\partial u_j} = 0$$

The surviving terms read

$$\frac{\partial u_k}{\partial q_f}\frac{\partial u_i}{\partial p_f}\frac{\partial q_g}{\partial u_k}\frac{\partial p_g}{\partial u_j} + \frac{\partial u_k}{\partial p_f}\frac{\partial u_i}{\partial q_f}\frac{\partial p_g}{\partial u_k}\frac{\partial q_g}{\partial u_j} = \frac{\partial q_g}{\partial q_f}\frac{\partial u_i}{\partial p_f}\frac{\partial p_g}{\partial u_j} + \frac{\partial p_g}{\partial p_f}\frac{\partial u_i}{\partial q_f}\frac{\partial q_g}{\partial u_j} = \delta_{fg}\left(\frac{\partial u_i}{\partial p_f}\frac{\partial p_g}{\partial u_j} + \frac{\partial u_i}{\partial q_f}\frac{\partial q_g}{\partial u_j}\right)$$

That is,

$$\sum_f \left(\frac{\partial u_i}{\partial p_f}\frac{\partial p_f}{\partial u_j} + \frac{\partial u_i}{\partial q_f}\frac{\partial q_f}{\partial u_j}\right) = \frac{\partial u_i}{\partial u_j}.$$

which is the sum over all the independent variables (recall u are understood as a function of (q,p); just as $\frac{\partial F(G_i(x))}{\partial x} = \frac{\partial F}{\partial G_i}\frac{\partial G_i}{\partial x}$)

spanned by (Q, P). Since $pdQ - PdQ = dF$,[137]

$$\oint_C pdq - \oint_{C'} PdQ = 0. \tag{13.24}$$

This is called a relative integral invariant. Applying the Stokes' theorem, we get

$$\int_A dqdp = \int'_A dQdP \tag{13.25}$$

where $\partial A = C$ and $\partial A' = C'$. This is called the absolute integral invariant. This is true for any area A floating in the phase space.

Suppose A has a coordinate system (u, v). Then, on A q and p are functions of (u, v). After the canonical transformation Q and P depend on (u, v) through the original variable, so (13.26) reads (with the summation convention)

$$\int_A \frac{\partial(q^r, p^r)}{\partial(u, v)} dudv = \int'_A \frac{\partial(Q^r, P^r)}{\partial(u, v)} dudv \tag{13.26}$$

This is true for any A, so we must conclude that

$$\frac{\partial(q^r, p^r)}{\partial(u, v)} \tag{13.27}$$

is invariant (do not forget the summation convention).

13.12 Lagrange brackets are invariant of canonical transformation

The invariance of (13.27) implies

$$\frac{\partial(q^r, p^r)}{\partial(u, v)} dudv = dq^r d'p^r - d'q^r dp^r \tag{13.28}$$

is invariant. Here, d and d' are independent infinitesimal changes. Therefore, Lagrange brackets are invariant.

As we will see soon the converse is true: if a transformation keeps Lagrange brackets invariant, it is a canonical transformation.

[137] pdQ is a shorthand notation of $\sum_r p_r dQ_r$ as usual.

13.13 Poisson brackets are invariant of canonical transformation

(13.22) implies that if Lagrange bracket is invariant, then so is Poison bracket. Thus, a necessary and sufficient condition for $(q, p) \to (Q, P)$ is canonical is that

$$[P, P]_{PB} = [Q, Q]_{PB} = 0, [Q, P]_{PB} = 1. \tag{13.29}$$

13.14 Invariance of Lagrange bracket implies canonical nature of the transformation

Looking at **13.11**, we see we have only to show that $pdq - PdQ$ is exact. That is, there is a function W such that

$$dW = pdq - PdQ. \tag{13.30}$$

If there is such W, it must satisfy, as a function of P and Q

$$\frac{\partial W}{\partial P} = p\frac{\partial q}{\partial P}, \ \frac{\partial W}{\partial Q} = p\frac{\partial q}{\partial P} - P. \tag{13.31}$$

Also we need $\partial^2 W/\partial P\partial Q = \partial^2 W/\partial Q\partial P$: we have

$$\frac{\partial^2 W}{\partial Q\partial P} = \frac{\partial p}{\partial Q}\frac{\partial q}{\partial P} + p\frac{\partial^2 q}{\partial Q\partial P}, \tag{13.32}$$

$$\frac{\partial^2 W}{\partial P\partial Q} = \frac{\partial p}{\partial P}\frac{\partial q}{\partial Q} + p\frac{\partial^2 q}{\partial P\partial Q} - 1. \tag{13.33}$$

Equating these formulas, we get

$$(Q, P) = 1. \tag{13.34}$$

That is,[138] if we have the invariance of Lagrange's brackets, then $(q, p) \to (Q, P)$ is canonical.

13.15 Liouville's theorem

The phase volume is invariant under canonical transformations. That is

$$\int_V d^n p d^n q = \int_{V'} d^n P d^n Q, \tag{13.35}$$

[138] Needless to say, we must also demand $(P, P) = (Q, Q) = 0$ as well for dW to be exact. Check this.

where V is a ($2n$-)subset of the phase space, and V' its image due to the canonical transformation $(q,p) \to (Q,P)$. To demonstrate this we have only to show that following Jacobian to be ± 1:

$$J = \frac{\partial(q,p)}{\partial(Q,P)}. \tag{13.36}$$

We compute this as

$$J = \frac{\partial(q,p)}{\partial(Q,p)}\frac{\partial(Q,p)}{\partial(Q,P)} = \left.\frac{\partial q}{\partial Q}\right|_p \left.\frac{\partial p}{\partial P}\right|_Q = \left.\frac{\partial p}{\partial P}\right|_Q \Bigg/ \left.\frac{\partial Q}{\partial q}\right|_p. \tag{13.37}$$

Now, in terms of the generator $dG = pdq - QdP$, we have

$$\left.\frac{\partial Q}{\partial q}\right|_p = \frac{\partial^2 G}{\partial q \partial P}, \tag{13.38}$$

$$\left.\frac{\partial p}{\partial P}\right|_Q = \frac{\partial^2 G}{\partial P \partial q}. \tag{13.39}$$

Thus, $J = 1$.

13.6 implies that the phase volume is invariant of motion.

13.16 Integration by quadratures

Integration by quadrature is the search of the solutions by a finite number of algebraic operations (including inversion of functions) and 'quadratures' = calculation of integrals of known functions. T

If n first integrals are commutative (the classical involution case), the system is solvable by quadrature.

13.17 Jacobi's method of complete integral[139]

Jacobi showed that for a system with n degrees of freedom of motion if we can find a complete solution (solution with $n+1$ arbitrary and independent constants) for the Hamilton-Jacobi equation, we can determine the motion completely.

The Hamilton-Jacobi equation has the following form

$$\frac{\partial A}{\partial t} + H = 0, \tag{13.40}$$

[139] See Landau-Lifshitz Section 47.

so a complete solution can have the form $A = C + f(q, \alpha, t)$, where C and α (n-vector) are the arbitrary constants. We can introduce a canonical transformation whose generator is f that makes α as the new momentum (f corresponds to G)

$$p_i = \frac{\partial f}{\partial q_i}, \; \beta_j = \frac{\partial f}{\partial \alpha_j}, \; K = \frac{\partial f}{\partial t} + H = \frac{\partial A}{\partial t} + H = 0. \tag{13.41}$$

Thus, the new coordinates are β. Since the Hamiltonian in this coordinate system vanishes, the canonical equation of motion tells us that β are constants. Solving n equations $\beta = \frac{\partial f}{\partial \alpha}$, we can determine q as a function of t.

13.18 Separation of variables

If the action A (or called Hamilton's principal function) may be written as a sum of two functions without common coordinates: $A = A_1(a_1, t) + A_2(q_2, t)$, we can separately find complete solutions. Especially when A_2 depends only on one coordinate q_n, we say this coordinate is separated from the rest, and the 1D problem may be solved.