Physical kinetics seminar
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1.2 Canonical transformations

1.2.1 Generating functions

Using Lagrangian formalism, we can change the generalized coordinates $q \to q'$.

The Hamiltonian formalism allows a larger range of transformations:

$$(q, p) \to (q', p')$$

If (q', p') satisfy Hamilton's equations for some H', this kind of transformation is canonical.

Now lets see how to obtain this. We want Hamilton's principle to be satisfied in both frames. Thus

$$\delta \int L(q, \dot{q}, t)\, dt = \delta \int \left(\sum p_i \dot{q}_i - H \right) dt = 0$$

$$\delta \int L'(q', \dot{q}', t)\, dt = \delta \int \left(\sum p_i' \dot{q}_i' - H' \right) dt = 0$$

The equalities hold if

$$\sum_i p_i \dot{q}_i - H = \sum_i p_i' \dot{q}_i' - H' + \frac{dG_1}{dt}$$

Multiplying by dt we obtain

$$\sum_i p_i\, dq_i - \sum_i p_i'\, dq_i' + (H' - H)\, dt = dG_1(q, q', t)$$

From here

$$p_i = \frac{\partial G_1}{\partial q_i}, \quad p_i' = -\frac{\partial G_1}{\partial q_i'}, \quad H' = H + \frac{\partial G_1}{\partial t}$$

Thus function G_1 generates canonical transformation $(q, p) \to (q', p')$.
The procedure to do the canonical transformation is:

1) select suitable $G_1(q, q', t)$.
2) obtain $p_i = p_i(q, q')$ and then invert to $q' = q'(q, p)$
3) obtain $p_i' = p_i'(q, q') = p_i' = p_i'(q, q'(q, p))$
4) transform the Hamiltonian as $H' = H + \frac{\partial G_1}{\partial t}$.

Note that we assume that it is possible to invert $p = p(q, q')$ to $q' = q'(q, p)$. The book says that it is possible if and only if

$$\det \left| \frac{\partial^2 G_1}{\partial q_i \, \partial q'_k} \right| \neq 0$$

For example, $G_1 = f(q) + h(q')$ does not give a canonical transformation, as then $p' = \frac{df(q)}{dq}$, and there is no way to invert this to obtain q'.

As an example that works consider the exchange transformation generated by $G_1 = G_1 - q q'$

Then

$$p = \frac{\partial G_1}{\partial q} = -q', \quad p' = -\frac{\partial G_1}{\partial q'} = q$$

Thus $q' = -p$, $p' = q$ and $H' = H$.

We see that in the Hamiltonian formalism, coordinates and momenta can lose their usual meaning.

1.2.3 Generating other transformations

We can do Legendre transformations to make the generating function depend on some other variables than (q, q').

Note that it will always depend on one set of "new" variables" and one set of "old".

For example, from

$$\sum_i p_i \, dq_i - \sum_i p'_i \, dq'_i + (H' - H) \, dt = dG_1(q, q', t)$$

we can write

$$\sum_i p_i \, dq_i - d\left(\sum_i p'_i q'_i\right) + \sum_i q'_i \, dp'_i + (H' - H) \, dt = dG_1(q, q', t)$$

and

$$\sum_i p_i \, dq_i + \sum_i q'_i \, dp'_i + (H' - H) \, dt = \underbrace{d\left(G_1(q, q', t) + \sum_i p'_i q'_i\right)}_{dG_2(q, p', t)}$$

and we have equations

$$p_i = \frac{\partial G_2}{\partial q_i}, \quad q'_i = \frac{\partial G_2}{\partial p'_i}, \quad H' = H + \frac{\partial G_2}{\partial t}$$

As an example of this type of transformation, we can consider

$$q_i' = f_i(q_1, \dots, q_N)$$

It can be generated using

$$G_2(q, p') = \sum_i p_i' f_i(q)$$

so we have

$$q_i' = \frac{\partial G_2}{\partial p_i'} = f_i(q) \quad , \quad p_i = \frac{\partial G_2}{\partial q_i} = \sum_j p_j' \frac{\partial f_j(q)}{\partial q_i}$$

We would need to invert the last equation to get $p' = p'(q, q')$.

For completeness, I list the remaining two generating functions

$$G_3(p, q') = G_1 - \sum_i p_i q_i \Rightarrow q_i = -\frac{\partial G_3}{\partial p_i} \, , \; p_i' = -\frac{\partial G_3}{\partial q_i'} \quad , \quad H' = H + \frac{\partial G_3}{\partial t}$$

$$G_4(p, p', t) = G_1 - \sum_i p_i q_i + \sum_i p_i' q_i' \Rightarrow q_i = -\frac{\partial G_4}{\partial p_i} \, , \; q_i' = \frac{\partial G_4}{\partial p_i'} \quad , \quad H' = H + \frac{\partial G_4}{\partial t}$$

Note that not all canonical transformations can be obtained from generating functions. Also, it is possible to have mixed canonical transformations, with only a part of coordinates and momenta changed to new ones.

1.2.3 Canonical invariants

A canonical invariant is a dynamical quantity that remains invariant under a canonical transformation.

Poisson brackets of two dynamical functions is a canonical invariant. That is, if

$$A(q, p) \xrightarrow{C} A'(q', p')$$

$$B(q, p) \xrightarrow{C} B'(q', p')$$

then

$$[A, B]_{q,p} \xrightarrow{C} [A', B']_{q',p'} = [A, B]_{q,p}$$

The book provides somewhat handwaving arguments, but this can be proven rigorously.

One of the most important things that follow is the invariance of the fundamental Poisson brackets:

$$[q_i', q_j']_{q,p} = 0$$

$$[p_i', p_j']_{q,p} = 0$$

$$[q_i', p_j']_{q,p} = \delta_{ij}$$

These could be taken as conditions for the transformation to be canonical.

1.2.4 Group property of Canonical transformations.

Lets assume that canonical transformation $(q,p) \xrightarrow{C_1} (q',p')$ arises from generating function $G(q,q')$:

$$\sum_i p_i \, dq_i - \sum_i p_i' \, dq_i' = dG(q,q')$$

We further assume that $(q',p') \xrightarrow{C_2} (q'',p'')$ arises from $K(q,q')$:

$$\sum_i p_i' \, dq_i' - \sum_i p_i'' \, dq_i'' = dK(q,q')$$

Adding, we have

$$\sum_i p_i \, dq_i - \sum_i p_i'' \, dq_i'' = d\varphi(q,q') = d(G+K)$$

This means that $(q,p) \xrightarrow{C_3} (q'',p'')$ is also canonical. Thus

$$C_3 = C_1 \otimes C_2$$

Canonical transformations obey the group property - the product of any two canonical transformations is canonical.

1.2.5 Constants of Motion and Symmetry

Constants of motion of a system may be associated with its symmetries. Remember that if $\frac{\partial H}{\partial q_j} = 0$, then $p_j = \text{const}$. If a system is symmetric with respect to displacements of a given coordinate, the momentum conjugate to that coordinate is constant.

Noether's theorem: if the Lagrangian is invariant under a continuous symmetry transformation, there are conserved quantities associated with that symmetry, one for each parameter of the transformation.

Invariance under time translations gives conservation of energy.

Invariance under spatial ~~rotations~~ translations gives conservation of total momentum, which is equal to the center-of-mass momentum.

Invariance under spatial rotations gives conservation of total angular momentum.

For a system of particles, we can write

$$\vec{J} = \underbrace{[\vec{R} \times \vec{P}]}_{\substack{\text{center of} \\ \text{mass motion}}} + \underbrace{\sum_i [\vec{r}_i^{\,\prime} \times \vec{p}_i^{\,\prime}]}_{\substack{\text{motion relative} \\ \text{to center of mass}}}$$

If we rotate all the particles together, the second term is clearly constant, and thus if total angular momentum is constant, then the center of mass angular momentum is also constant.

We can also analyze the constants of motion by using the Poisson bracket formalism:

$$\frac{du}{dt} = [u, H]$$

We could introduce generators and infinitesimal canonical transformations...

1.3 Liouville theorem

1.3.1 Proof

The Liouville theorem states that the Jacobian of a canonical transformation is unity. Thus

$$\mathcal{J}\left(\frac{q',p'}{q,p}\right) = \frac{\partial(q',p')}{\partial(q,p)} = \begin{vmatrix} \frac{\partial q'_1}{\partial q_1} & \frac{\partial q'_2}{\partial q_1} & \cdots & \frac{\partial p'_1}{\partial q_1} & \cdots & \frac{\partial p'_N}{\partial q_1} \\ \vdots & \vdots & & \vdots & & \vdots \\ \frac{\partial q'_1}{\partial p_N} & \frac{\partial q'_2}{\partial p_N} & \cdots & \frac{\partial p'_1}{\partial p_N} & \cdots & \frac{\partial p'_N}{\partial p_N} \end{vmatrix} = 1$$

Now we will prove this.

First we note that Jacobians can be treated like fractions, so

$$\mathcal{J} = \frac{\partial(q',p')}{\partial(q,p')} \Big/ \frac{\partial(q,p')}{\partial(q,p)}$$

This is related to the fact that Jacobians are constructed from partial derivatives, thus combination of chain rule and properties of matrices and determinants give this.

Now we say that when the same quantities appear in both partial derivatives, the Jacobian reduces to one in fewer variables, with repeated variables taken as constant.

An illustrative example of this is Jacobian related to transformation from Cartesian to cyllindrical coordinates:

$$\frac{\partial(x,y,z)}{\partial(\rho,\varphi,z)} = \begin{vmatrix} \frac{\partial x}{\partial \rho} & \frac{\partial y}{\partial \rho} & \frac{\partial z}{\partial \rho} \\ \frac{\partial x}{\partial \varphi} & \frac{\partial y}{\partial \varphi} & \frac{\partial z}{\partial \varphi} \\ \frac{\partial x}{\partial z} & \frac{\partial y}{\partial z} & \frac{\partial z}{\partial z} \end{vmatrix} = \begin{vmatrix} \frac{\partial x}{\partial \rho} & \frac{\partial y}{\partial \rho} & 0 \\ \frac{\partial x}{\partial \varphi} & \frac{\partial y}{\partial \varphi} & 0 \\ 0 & 0 & 1 \end{vmatrix} = \begin{vmatrix} \frac{\partial x}{\partial \rho} & \frac{\partial y}{\partial \rho} \\ \frac{\partial x}{\partial \varphi} & \frac{\partial y}{\partial \varphi} \end{vmatrix}$$

This allows us to write

$$J = \frac{\partial(q_i')}{\partial(q_r)}\bigg|_{p'} \bigg/ \frac{\partial(p_i')}{\partial(p_r)}\bigg|_{q_r} = \frac{J_n}{J_d}$$

Now, if we treat the Jacobian as a matrix, we can write

$$J_n^{ik} = \frac{\partial q_i'}{\partial q_k} \qquad \text{[though this is transposed if compared to before]}$$

We also have $q' = q'(q, p')$, $q_i' = \frac{\partial G_2}{\partial p_i'}$, thus

$$J_n^{ik} = \frac{\partial^2 G_2}{\partial p_i' \, \partial q_k}$$

In the denominator we have $J_d^{ik} = \frac{\partial p_i}{\partial p_k'} = \frac{\partial G_2}{\partial q_i \, \partial p_k'}$

Thus, $J_n^{ik} = J_d^{ki}$

Remembering that determinant doesn't change if we transpose the matrix, we obtain

$$J = \frac{J_n}{J_d} = 1$$

Liouville theorem is proven.

1.3.2 Geometric Significance

From Liouville's theorem it follows that volume elements in Γ-space are canonical invariants

$$\Omega = \iint_{\Omega} dq\, dp = \iint_{\Omega'} J\left(\frac{q, p}{q', p'}\right) dq'\, dp' = \iint_{\Omega'} dq'\, dp' = \Omega'$$

1.3.3

We now consider action integral corresponding to motion from t to $t+T$. This should correspond to going from point 1 to point 2.

Thus

$$S(t,T) = \int_t^{t+T} \mathcal{L}(q,\dot{q})\,d\tau = \int_0^{t+T} \left(\sum_i p_i \dot{q}_i - H\right) d\tau - \int_0^t \left(\sum_i p_i \dot{q}_i - H\right) d\tau$$

$$\frac{d}{dt}\int_{a(t)}^{b(t)} F(t,\tau)\,d\tau = \int_{a(t)}^{b(t)} \frac{\partial F(t,\tau)}{\partial t}\,d\tau + \frac{db(t)}{dt} F(t, b(t)) - \frac{da(t)}{dt} F(t, a(t))$$

Differentiating, we obtain

$$\frac{dS}{dt} = \frac{d(t+T)}{dt}\left(\sum_i p_i \dot{q}_i - H\right)_{t+T} - \frac{dt}{dt}\left(\sum_i p_i \dot{q}_i - H\right)_t =$$

$$= \sum_i p_i' \dot{q}_i' - \sum_i p_i \dot{q}_i + (H - H')$$

Here prime denotes variables at $t+T$:

$$\dot{q}' = \dot{q}(t+T), \quad p' = p'(t+T), \quad H' = H(t+T)$$

If we assume that H is time independent, we obtain

$$dS = \sum_i p_i' dq_i' - \sum_i p_i dq_i$$

Therefore:

1. Action is a generating function for actual physical motion.
2. Differential motion in time is a canonical transformation.
3. Extended motion in time is also a canonical transformation (due to the group property of canonical transformations).