H. Hergert
Facility for Rare Isotope Beams
and Department of Physics & Astronomy

PHY422/820: Classical Mechanics

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1 Preparation

- Lemos, Chapter 8 (8.2 / Lagrange brackets, 8.7, 8.9 optional)
- Goldstein, Chapter 9 (Lagrange brackets optional)

2 Canonical Transformations

In our discussion of the Lagrangian formalism, we saw that the Lagrange equations maintain their form under changes of the generalized coordinates in configuration space. In the following, we will study coordinate transformations in *phase space* under which *Hamilton's* equations remain form invariant — the so-called **canonical transformations.** We will see that a suitable transformation can greatly simplify the process of solving the equations of motion (some examples were already discussed in homework problems H26–28.)

2.1 Characteristics of Canonical Transformations

Let us consider a dynamical system described by the Hamiltonian $H(q,p,t)$ and Hamilton's equations

$$\dot{q}_i = \frac{\partial H}{\partial p_i}\,, \qquad \dot{p}_i = -\frac{\partial H}{\partial q_i}\,. \tag{1}$$

We would like to introduce new canonical coordinates (Q,P) by performing an invertible coordinate transformation in phase space,

$$Q_i = Q_i(q,p,t)\,, \qquad P_i = P_i(q,p,t)\,, \tag{2}$$

such that there exists a new Hamiltonian $K(Q,P,t)$ and Hamilton's equations are satisfied:

$$\dot{Q}_i = \frac{\partial K}{\partial P_i}\,, \qquad \dot{P}_i = -\frac{\partial K}{\partial Q_i}\,. \tag{3}$$

Since Hamilton's equations are supposed to hold in both sets of variables, Hamilton's principle implies that

$$\delta \int_{t_1}^{t_2} dt\, \left(\sum_i p_i\dot{q}_i - H(q,p,t)\right) = \delta \int_{t_1}^{t_2} dt\, \left(\sum_i P_i\dot{Q}_i - K(Q,P,t)\right) = 0\,. \tag{4}$$

Thus, we must have

$$\lambda \left(\sum_i p_i \dot{q}_i - H \right) = \sum_i P_i \dot{Q}_i - K + \dot{F} \,, \tag{5}$$

where we have used the invariance of the variation under the addition of a total time derivative, as before:

$$\delta \int_{t_1}^{t_2} dt \, \dot{F} = \delta(F(t_2) - F(t_1)) = 0 \,. \tag{6}$$

Rewriting Eq. (5) in differential form, we obtain

$$\boxed{dF = \sum_i (\lambda p_i dq_i - P_i dQ_i) + K - \lambda H \,. \tag{7}}$$

By integrating this equation, we can obtain a **generating function** F for the desired transformation, and prove that the transformation from the old to the new phase space variables is indeed canonical at the same time. We distinguish several cases:

- For $\lambda = 1$, we have a standard **canonical transformation**, which we will study in the following.
- $\lambda \neq 1$ defines an **extended canonical transformation**. We can rescale the coordinates to obtain the typical case with $\lambda = 1$.
- If $Q_i(q, p)$ and $P_i(q, p)$ do not explicitly depend on time, we call the canonical transformation **restricted**.

2.2 Generating Functions

Since the generating function F of a canonical transformation is supposed to connect the old and new phase space coordinates, it must depend on a mix of these variables. For a system with a single degree of freedom, there are four fundamental classes:

1. Let us take

$$F = F_1(q, Q, t) \tag{8}$$

where the old coordinates q_i and the new coordinates Q_i are independent. According to Eq. (7), we must have

$$dF = \sum_i \left(\frac{\partial F_1}{\partial q_i} dq_i + \frac{\partial F_1}{\partial Q_i} dQ_i \right) + \frac{\partial F_1}{\partial t} = \sum_i (p_i dq_i - P_i dQ_i) + K - H \,, \tag{9}$$

and comparing coefficients, we can identify

$$p_i = \frac{\partial F_1}{\partial q_i} \,, \quad P_i = -\frac{\partial F_1}{\partial Q_i} \,, \quad K = H + \frac{\partial F_1}{\partial t} \,. \tag{10}$$

These equations define the remaining canonical variables as functions of the independent variables,

$$p_i = p_i(q, Q, t) \,, \quad P_i = P_i(q, Q, t) \,, \tag{11}$$

and allow us to connect H and K.

The simplest example of a generating function of type F_1 is

$$F_1(q,Q) = \sum_i q_i Q_i\,. \tag{12}$$

The relations (10) imply that

$$p_i = Q_i\,, \quad P_i = -q_i\,, \tag{13}$$

hence this transformation merely amounts to an exchange of the canonical coordinates and momenta, up to a sign. This shows that in the Hamiltonian formalism, there is really no distinction between the coordinates and momenta.

2. Now let the q_i and P_i be the independent variables, and define

$$F = F_2(q,P,t) - \sum_i Q_i P_i\,. \tag{14}$$

Equation (7) now implies that

$$\begin{aligned} dF &= \sum_i \left(\frac{\partial F_2}{\partial q_i} dq_i + \frac{\partial F_2}{\partial P_i} dP_i\right) + \frac{\partial F_2}{\partial t} - \sum_i (P_i dQ_i + Q_i dP_i) \\ &= \sum_i \left(\frac{\partial F_2}{\partial q_i} dq_i + \left(\frac{\partial F_2}{\partial P_i} - Q_i\right) dP_i\right) + \frac{\partial F_2}{\partial t} - \sum_i P_i dQ_i \\ &\overset{!}{=} \sum_i (p_i dq_i - P_i dQ_i) + K - H\,. \end{aligned} \tag{15}$$

The term $\sum_i P_i dQ_i$ cancels, and the comparison of the remaining terms yields

$$p_i = \frac{\partial F_2}{\partial q_i}\,, \quad Q_i = \frac{\partial F_2}{\partial P_i}\,, \quad K = H + \frac{\partial F_2}{\partial t}\,. \tag{16}$$

The simplest generating function of the type F_2 is

$$F_2(q,P) = \sum_i q_i P_i\,, \tag{17}$$

and from Eq. (16) we obtain

$$p_i = P_i\,, \quad q_i = Q_i\,. \tag{18}$$

This is the **identity transformation**.

3. If the independent variables are Q_i and p_i, we set

$$F = F_3(p,Q,t) + \sum_i q_i p_i\,, \tag{19}$$

and

$$\begin{aligned} dF &= \sum_i \left(\frac{\partial F_3}{\partial Q_i} dQ_i + \frac{\partial F_3}{\partial p_i} dp_i\right) + \frac{\partial F_3}{\partial t} + \sum_i (p_i dq_i + q_i dp_i) \\ &= \sum_i \left(\frac{\partial F_3}{\partial Q_i} dQ_i + \left(\frac{\partial F_3}{\partial p_i} + q_i\right) dp_i\right) + \frac{\partial F_3}{\partial t} + \sum_i p_i dq_i \end{aligned}$$

Box 2.1: Summary: Generating Functions

Here we summarize the fundamental classes of generating functions and give the simplest possible examples for each class.

Function	Transformation			Simplest Case	
$F_1(q,Q,t)$	$p_i = \frac{\partial F_1}{\partial q_i}$,	$P_i = -\frac{\partial F_1}{\partial Q_i}$,	$K = H + \frac{\partial F_1}{\partial t}$	$F_1 = \sum_i q_i Q_i$	$Q_i = p_i, \quad P_i = -q_i$
$F_2(q,P,t)$	$p_i = \frac{\partial F_2}{\partial q_i}$,	$Q_i = \frac{\partial F_2}{\partial P_i}$,	$K = H + \frac{\partial F_2}{\partial t}$	$F_2 = \sum_i q_i P_i$	$Q_i = q_i, \quad P_i = p_i$
$F_3(p,Q,t)$	$P_i = -\frac{\partial F_3}{\partial Q_i}$,	$q_i = -\frac{\partial F_3}{\partial p_i}$,	$K = H + \frac{\partial F_3}{\partial t}$	$F_3 = \sum_i p_i Q_i$	$Q_i = -q_i, P_i = -p_i$
$F_4(p,P,t)$	$q_i = -\frac{\partial F_4}{\partial p_i}$,	$Q_i = \frac{\partial F_4}{\partial P_i}$,	$K = H + \frac{\partial F_4}{\partial t}$	$F_4 = \sum_i p_i P_i$	$Q_i = p_i, \quad P_i = -q_i$

$$\stackrel{!}{=} \sum_i (p_i dq_i - P_i dQ_i) + K - H \,. \tag{20}$$

Now $\sum_i p_i dq_i$ cancels, and we obtain

$$P_i = -\frac{\partial F_3}{\partial Q_i}\,, \quad q_i = -\frac{\partial F_3}{\partial p_i}\,, \quad K = H + \frac{\partial F_3}{\partial t}\,. \tag{21}$$

4. Last but not least, we can have P_i and p_i as independent variables, and

$$F = F_4(p, P, t) + \sum_i (p_i q_i - P_i Q_i) \,. \tag{22}$$

From Eq. (7), we have

$$\begin{aligned} dF &= \sum_i \left(\frac{\partial F_4}{\partial p_i} dp_i + \frac{\partial F_4}{\partial P_i} dP_i \right) + \frac{\partial F_4}{\partial t} + \sum_i (p_i dq_i + q_i dp_i - P_i dQ_i - Q_i dP_i) \\ &= \sum_i \left(\left(\frac{\partial F_4}{\partial p_i} + q_i \right) dp_i + \left(\frac{\partial F_4}{\partial P_i} - Q_i \right) dP_i \right) + \frac{\partial F_4}{\partial t} + \sum_i (p_i dq_i - P_i dQ_i) \\ &\stackrel{!}{=} \sum_i (p_i dq_i - P_i dQ_i) + K - H \,, \end{aligned} \tag{23}$$

which yields

$$q_i = -\frac{\partial F_4}{\partial p_i}\,, \quad Q_i = \frac{\partial F_4}{\partial P_i}\,, \quad K = H + \frac{\partial F_4}{\partial t}\,. \tag{24}$$

For convenience, we summarize the four fundamental types of generating functions in Box 2.1.

The extension of the present discussion to dynamical systems with multiple degrees of freedom is straightforward: The most general generating function for a canonical transformation of such systems is a mix of the four fundamental types, e.g., $F = F(q_1, Q_1, p_2, Q_2, \ldots, t)$.

2.3 Examples

2.3.1 Finding the Coordinates from a Generating Function

Consider the generating function

$$F_1 = -\frac{Q}{q}\,. \tag{25}$$

The old and new canonical momenta are defined by (cf. Eq. (10) or Box 2.1):

$$p = \frac{\partial F_1}{\partial q} = \frac{Q}{q^2}\,, \quad P = -\frac{\partial F_1}{\partial Q} = \frac{1}{q}\,. \tag{26}$$

Writing the new coordinates as function of the old ones, we have

$$Q = pq^2\,, \quad P = \frac{1}{q}\,. \tag{27}$$

2.3.2 Construction of a Generating Function to Test Canonicity

Given a coordinate transformation

$$Q = \ln\left(\frac{p}{q}\right)\,, \quad P = -\left(\frac{q^2}{2}+1\right)\frac{p}{q} \tag{28}$$

we can attempt to construct a generating function in order to prove that the transformation is canonical. From the definition of the new coordinates, we know that

$$\frac{\partial F_1}{\partial q} = p = qe^Q\,. \tag{29}$$

We can integrate this relation to obtain

$$F_1 = \int dq\; qe^Q = \frac{q^2}{2}e^Q + g(Q)\,. \tag{30}$$

The definition of P and its relation to the generating function imply

$$P = -\frac{\partial F_1}{\partial Q} = -\frac{q^2}{2}e^Q - \frac{dg}{dQ} \overset{!}{=} -\left(\frac{q^2}{2}+1\right)\frac{p}{q} = -\left(\frac{q^2}{2}+1\right)e^Q\,, \tag{31}$$

which is solved by

$$g(Q) = e^Q\,. \tag{32}$$

Thus, F_1 is given by

$$F_1 = \left(\frac{q^2}{2}+1\right)e^Q\,, \tag{33}$$

and we find that the coordinate transformation is indeed canonical.

3 Poisson Brackets

In Sec. 2, we saw that the existence of a generating function that links two given sets of phase space coordinates (q, p) and (Q, P) will imply that the transformation between these coordinates is canonical. However, in order to verify its existence, we need to perform an explicit construction by integrating the equations relating the old and new coordinates (cf. Box 2.1). This quickly becomes a tedious task, especially for systems with multiple degrees of freedom or nonlinear coordinate transformations. Fortunately, there is a more efficient test of the canonicity of a coordinate transformation that only requires differentiation: It is based on considering the impact of a coordinate transformation on the **symplectic invariants** (see below) of the dynamical system. The specific invariant we will consider in the following are the **Poisson brackets**.

3.1 Definition and Properties

For a dynamical system with generalized coordinates and canonical momenta $(q_i, p_i), i = 1, \ldots, n$ that is described by the Hamiltonian $H(q, p, t)$, we define the Poisson bracket of two functions $f(q, p, t), g(q, p, t)$ as

$$\big\{f, g\big\} \equiv \sum_{i=1}^{n} \left(\frac{\partial f}{\partial q_i} \frac{\partial g}{\partial p_i} - \frac{\partial g}{\partial q_i} \frac{\partial f}{\partial p_i} \right) . \tag{34}$$

The Poisson brackets satisfy the following algebraic properties (see problem G33):

- **Antisymmetry**:

$$\big\{f, g\big\} = -\big\{g, f\big\} . \tag{35}$$

  Note that this also implies

$$\big\{f, f\big\} = \big\{g, g\big\} = 0 . \tag{36}$$

- **Linearity**:

$$\big\{\alpha f + \beta g, h\big\} = \alpha\big\{f, h\big\} + \beta\big\{g, h\big\} . \tag{37}$$

  The combination of this property with Eq. (35) implies that the Poisson brackets are also linear in the second argument.

- **Leibniz' rule**:

$$\big\{fg, h\big\} = \big\{f, h\big\}g + f\big\{g, h\big\} , \tag{38}$$

  which follows from the product rule for the derivatives.

- **Jacobi identity**:

$$\big\{f, \big\{g, h\big\}\big\} + \big\{g, \big\{h, f\big\}\big\} + \big\{h, \big\{f, g\big\}\big\} = 0 , \tag{39}$$

  which encodes the non-associativity of the algebra of Poisson bracket: i.e., repeated applications of the bracket operation depend on the order of evaluation[1].

For the special case where $f = q_i$, $g = p_i$, we find the **fundamental Poisson brackets**

$$\big\{q_i, q_j\big\} = 0 , \quad \big\{p_i, p_j\big\} = 0 , \quad \big\{q_i, p_j\big\} = \delta_{ij} \tag{40}$$

[1] Other nonassociative operations that satisfy this identity are the cross product or the quantum-mechanical commutator.

since the coordinates and canonical momenta are independent variables. Furthermore, noting that we can use the Poission brackets to write the total time derivative of a function $f(q, p, t)$ as

$$\frac{df}{dt} = \big\{f, H\big\} + \frac{\partial f}{\partial t} \tag{41}$$

(see problem G34), we see that Hamilton's equations can also be written as

$$\dot{q}_i = \big\{q_i, H\big\}\,, \quad \dot{p}_i = \big\{p_i, H\big\}\,. \tag{42}$$

Using the fundamental brackets and the properties (35)– (39), we can evaluate the right-hand sides of these equations in an *algebraic* way. This is useful for making the transition from classical to quantum mechanics, because the quantum-mechanical commutators have essentially the same algebraic structure as the Poisson brackets.

Another immediate consequence of Eq. (41) is that any quantity $I(q, p)$ that has a vanishing Poisson bracket with the Hamiltonian will be conserved:

$$\dot{I} = \big\{I, H\big\} = 0 \quad \Rightarrow \quad I = \text{const.} \tag{43}$$

As an example, assume that q_i is a cyclic coordinate, i.e., $\frac{\partial H}{\partial q_i} = 0$. Then it is easy to see that the associated canonical momentum p_i is conserved:

$$\dot{p}_i = \big\{p_i, H\big\} = -\frac{\partial H}{\partial q_i} = 0 \quad \Rightarrow \quad p_i = \text{const.} \tag{44}$$

Moreover, the conserved quantities form a *closed algebra* under the Poisson bracket: If $I(q, p)$ and $J(q, p)$ are conserved quantities, then

$$\big\{\big\{I, J\big\}, H\big\} = \big\{I, \big\{J, H\big\}\big\} + \big\{J, \big\{I, H\big\}\big\} = 0\,, \tag{45}$$

and $\big\{I, J\big\}$ is conserved as well.

3.2 Symplectic Invariance

3.2.1 Symplectic Notation

To study the invariance of symplectic invariants, we first introduce a more convenient notation for the phase space variables (q, p) by combining them into $2n$-dimensional vectors[2]:

$$\vec{\xi} = \big(q_1, \ldots, q_n, p_1, \ldots, p_m\big)^T\,. \tag{46}$$

Analogously, we can combine the partial derivatives of the Hamiltonian into a "gradient" vector,

$$\frac{\partial H}{\partial \vec{\xi}} = \left(\tfrac{\partial H}{\partial q_1}, \ldots, \tfrac{\partial H}{\partial q_n}, \tfrac{\partial H}{\partial p_1}, \ldots, \tfrac{\partial H}{\partial p_m}\right)^T\,, \tag{47}$$

which allows us to write Hamilton's equations as

$$\dot{\vec{\xi}} = \boldsymbol{J}\frac{\partial H}{\partial \vec{\xi}}\,. \tag{48}$$

[2]In general, phase space is a **symplectic manifold** that could also be curved, but we will focus on "flat" manifolds here. That means the tangent spaces at all points can be identified with each other, as well as the manifold itself.

Here, we have defined the skew-symmetric matrix

$$\boldsymbol{J} = \begin{pmatrix} 0_{n\times n} & \mathbb{1}_{n\times n} \\ -\mathbb{1}_{n\times n} & 0_{n\times n} \end{pmatrix}\,, \tag{49}$$

which has the properties

$$\boldsymbol{J}^2 = -\mathbb{1}_{2n\times 2n}\,, \tag{50}$$

$$\boldsymbol{J}^T = -\boldsymbol{J} \qquad \text{(skew-symmetry)}\,, \tag{51}$$

$$\boldsymbol{J}^T\boldsymbol{J} = \boldsymbol{J}\boldsymbol{J}^T = \mathbb{1}_{2n\times 2n} \qquad \text{(orthogonality)}\,, \tag{52}$$

$$\det \boldsymbol{J} = 1\,. \tag{53}$$

Using the vector notation, the Poisson bracket of two functions $f(\vec{\xi})$ and $g(\vec{\xi})$ can be written as

$$\{f,g\}_{\vec{\xi}} = \frac{\partial f}{\partial \vec{\xi}}\cdot \boldsymbol{J}\cdot \frac{\partial g}{\partial \vec{\xi}} = \sum_{jk} \frac{\partial f}{\partial \xi_j} J_{jk} \frac{\partial g}{\partial \xi_k} \tag{54}$$

and the fundamental brackets become

$$\{\xi_i, \xi_j\} = J_{ij}\,. \tag{55}$$

3.2.2 Canonicity

We are now ready to state the following theorem on the canonicity of a coordinate transformation:

Theorem: Canonicity of a Coordinate Transformation

A coordinate transformation

$$\vec{\xi} = (q_1,\ldots,q_n,p_1,\ldots,p_n) \quad\longrightarrow\quad \vec{\eta} = (Q_1,\ldots,Q_n,P_1,\ldots,P_n) \tag{56}$$

is canonical if and only if

$$\{\eta_i, \eta_j\}_{\vec{\xi}} = J_{ij} \tag{57}$$

or in the traditional notation

$$\{Q_i, Q_j\}_{(q,p)} = 0, \quad \{P_i, P_j\}_{(q,p)} = 0, \quad \{Q_i, P_j\}_{(q,p)} = \delta_{ij}\,. \tag{58}$$

To prove it, we start by assuming that Eq. (48) holds for the original coordinates. Then

$$\dot{\eta}_i = \sum_j \frac{\partial \eta_i}{\partial \xi_j}\dot{\xi}_j = \sum_{jk} \frac{\partial \eta_i}{\partial \xi_j} J_{jk} \frac{\partial H}{\partial \xi_k} = \sum_{jkl} \frac{\partial \eta_i}{\partial \xi_j} J_{jk} \frac{\partial \eta_l}{\partial \xi_k}\frac{\partial H}{\partial \eta_l}\,. \tag{59}$$

We define the Jacobian of the coordinate transformation as

$$M_{ij} \equiv \frac{\partial \eta_i}{\partial \xi_j}\,, \tag{60}$$

hence we can write

$$\dot{\eta}_i = \sum_{jkl} M_{ij}J_{jk}M_{lk}\frac{\partial H}{\partial \eta_l} = \sum_l \left(MJM^T\right)_{il}\frac{\partial H}{\partial \eta_l} \tag{61}$$

or in vectorial form

$$\dot{\vec{\eta}} = \left(\boldsymbol{M}\boldsymbol{J}\boldsymbol{M}^T\right)\frac{\partial H}{\partial \vec{\eta}}\,. \tag{62}$$

Thus, the new coordinates will obey Hamilton's equation iff

$$\boldsymbol{M}\boldsymbol{J}\boldsymbol{M}^T = \boldsymbol{J}\,. \tag{63}$$

Now consider the fundamental Poisson brackets. We have

$$\left\{\eta_i, \eta_j\right\}_{\vec{\xi}} = \sum_{kl}\frac{\partial \eta_i}{\partial \xi_k}J_{kl}\frac{\partial \eta_j}{\partial \xi_l} = \sum_{kl} M_{ik}J_{kl}M^T_{lj} = \left(MJM^T\right)_{ij}\,, \tag{64}$$

hence the new coordinates will satisfy

$$\left\{\eta_i, \eta_j\right\}_{\vec{\xi}} = J_{ij} \tag{65}$$

if and only if Eq. (63) holds, which in turn is true if and only if the transformation is canonical. Writing this relation for the pair of canonical variables (Q_i, P_i) (i.e., $j = i + n$), we have

$$\begin{pmatrix} \left\{Q_i, Q_j\right\}_{(q,p)} & \left\{Q_i, P_j\right\}_{(q,p)} \\ \left\{P_i, Q_j\right\}_{(q,p)} & \left\{P_i, P_j\right\}_{(q,p)} \end{pmatrix} = \begin{pmatrix} 0 & \delta_{ij} \\ -\delta_{ij} & 0 \end{pmatrix}\,. \tag{66}$$

Invariance of the Poisson Bracket

There are two important corollaries of this theorem. First, we see that for a general Poisson bracket

$$\begin{aligned}\left\{f, g\right\}_{\xi} &= \sum_{ij}\frac{\partial f}{\partial \xi_i}J_{ij}\frac{\partial g}{\partial \xi_j} = \sum_{ijkl}\frac{\partial f}{\partial \eta_k}\frac{\partial \eta_k}{\partial \xi_i}J_{ij}\frac{\partial \eta_l}{\partial \xi_j}\frac{\partial g}{\partial \eta_l} = \sum_{ijkl}\frac{\partial f}{\partial \eta_k}\left(M_{ki}J_{ij}M_{lj}\right)\frac{\partial g}{\partial \eta_l} \\ &= \sum_{kl}\frac{\partial f}{\partial \eta_k}\left(MJM^T\right)_{kl}\frac{\partial g}{\partial \eta_l}\,. \end{aligned} \tag{67}$$

Under a canonical transformation, Eq. (63) implies that

$$\boxed{\left\{f, g\right\}_{\vec{\xi}} = \left\{f, g\right\}_{\vec{\eta}}\,.} \tag{68}$$

Thus, the Poisson brackets are **invariant under canonical transformations**, and they can be evaluated in any set of canonical coordinates.

Invariance of the Phase Space Volume

Second, consider a region $\mathcal{R}$ of the phase space (q, p) that is mapped onto the region $\mathcal{R}'$ of the phase space (Q, P) by a canonical transformation. Its original volume is given by

$$V = \int_{\mathcal{R}} dq_1 \ldots dq_n dp_1 \ldots dp_n = \int_{\mathcal{R}} d^{2n}\xi\,, \tag{69}$$

while the volume after the mapping is

$$V' = \int_{\mathcal{R}'} dQ_1 \ldots dQ_n dP_1 \ldots dP_n = \int_{\mathcal{R}'} d^{2n}\eta\,. \tag{70}$$

Under a change of coordinates, the volume element transforms as

$$d^{2n}\eta = \left|\frac{\partial\left(\eta_1,\ldots,\eta_{2n}\right)}{\partial\left(\xi_1,\ldots,\xi_{2n}\right)}\right| d^{2n}\xi = |\det \boldsymbol{M}|\, d^{2n}\xi\,. \tag{71}$$

If the transformation is canonical, we must have

$$\det \boldsymbol{M}\boldsymbol{J}\boldsymbol{M}^T = \det \boldsymbol{M}\cdot\det \boldsymbol{J}\det \boldsymbol{M}^T = (\det \boldsymbol{M})^2\det \boldsymbol{J} \stackrel{!}{=} \det \boldsymbol{J}\,, \tag{72}$$

which means

$$|\det \boldsymbol{M}| = 1\,. \tag{73}$$

Thus, the volume element is invariant under a canonical transformation, and so is the volume:

$$\boxed{V' = \int_{\mathcal{R}'} d^{2n}\eta = \int_{\mathcal{R}} d^{2n}\xi = V\,.} \tag{74}$$

3.3 Infinitesimal Canonical Transformations

3.3.1 Generators

Let us now consider an infinitesimal canonical transformation

$$q_i \longrightarrow Q_i = q_i + \delta q_i \equiv q_i + \epsilon f(q,p)\,, \tag{75}$$

$$p_i \longrightarrow P_i = p_i + \delta p_i \equiv p_i + \epsilon g(q,p)\,. \tag{76}$$

The Jacobian of this transformation will consist of blocks

$$M_{ij} = \begin{pmatrix} \delta_{ij} + \epsilon\frac{\partial f_i}{\partial q_j} & \epsilon\frac{\partial f_i}{\partial p_j} \\ \epsilon\frac{\partial g_i}{\partial q_j} & \delta_{ij} + \frac{\partial g_i}{\partial p_j} \end{pmatrix}\,. \tag{77}$$

Since the canonical transformation must satisfy

$$\begin{aligned}
(MJM^T)_{ik} &= \sum_j \begin{pmatrix} \delta_{ij} + \epsilon\frac{\partial f_i}{\partial q_j} & \epsilon\frac{\partial f_i}{\partial p_j} \\ \epsilon\frac{\partial g_i}{\partial q_j} & \delta_{ij} + \epsilon\frac{\partial g_i}{\partial p_j} \end{pmatrix} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} \delta_{jk} + \epsilon\frac{\partial f_j}{\partial q_k} & \epsilon\frac{\partial g_j}{\partial q_k} \\ \epsilon\frac{\partial f_j}{\partial p_k} & \delta_{jk} + \epsilon\frac{\partial g_j}{\partial p_k} \end{pmatrix} \\
&= \sum_j \begin{pmatrix} \delta_{ij} + \epsilon\frac{\partial f_i}{\partial q_j} & \epsilon\frac{\partial f_i}{\partial p_j} \\ \epsilon\frac{\partial g_i}{\partial q_j} & \delta_{ij} + \epsilon\frac{\partial g_i}{\partial p_j} \end{pmatrix} \begin{pmatrix} \epsilon\frac{\partial f_j}{\partial p_k} & \delta_{jk} + \epsilon\frac{\partial g_j}{\partial p_k} \\ -\delta_{jk} - \epsilon\frac{\partial f_j}{\partial q_k} & -\epsilon\frac{\partial g_j}{\partial q_k} \end{pmatrix} + O(\epsilon^2) \\
&= J_{ik} + \epsilon \begin{pmatrix} 0 & \frac{\partial f_i}{\partial q_k} + \frac{\partial g_i}{\partial p_k} \\ -\frac{\partial f_i}{\partial q_k} - \frac{\partial g_i}{\partial p_k} & 0 \end{pmatrix} + O(\epsilon^2) \\
&\stackrel{!}{=} J_{ik}\,,
\end{aligned} \tag{78}$$

we must have

$$\frac{\partial f_i}{\partial q_k} = -\frac{\partial g_i}{\partial p_k} \tag{79}$$

through order $O(\epsilon^2)$. This condition is satisfied if

$$f_i = \frac{\partial G}{\partial p_i}\,, \quad g_i = -\frac{\partial G}{\partial q_i}\,, \tag{80}$$

where the function $G(q,p)$ is the **generator** of the transformation. Switching back to the variations of the coordinates, we have

$$\delta q_i = \epsilon \frac{\partial G}{\partial p_i}\,, \quad \delta p_i = -\epsilon \frac{\partial G}{\partial q_i}\,, \tag{81}$$

which can be written in terms of the Poisson brackets as

$$\boxed{\delta q_i = \epsilon \big\{ q_i, G \big\}\,, \quad \delta p_i = -\epsilon \big\{ p_i, G \big\}\,. \tag{82}}$$

In symplectic vector notation, these equations can be combined into the relation

$$\boxed{\delta \vec{\xi} = \epsilon \big\{ \vec{\xi}, G \big\}. \tag{83}}$$

Using Eq. (82) we can express the change of any dynamical quantity $u(q,p,t)$ under an infinitesimal canonical transformation generated by G as

$$\begin{aligned} \delta u &= \sum_i \left(\frac{\partial u}{\partial q_i}\delta q_i + \frac{\partial u}{\partial p_i}\delta p_i \right) = \epsilon \sum_i \left(\frac{\partial u}{\partial q_i}\big\{ q_i, G \big\} + \frac{\partial u}{\partial p_i}\big\{ p_i, G \big\} \right) \\ &= \epsilon \sum_{ij} \left(\frac{\partial u}{\partial q_i}\frac{\partial q_i}{\partial q_j}\frac{\partial G}{\partial p_j} - \frac{\partial u}{\partial p_i}\frac{\partial p_i}{\partial p_j}\frac{\partial G}{\partial q_j} \right) = \epsilon \sum_i \left(\frac{\partial u}{\partial q_i}\frac{\partial G}{\partial p_i} - \frac{\partial u}{\partial p_i}\frac{\partial G}{\partial q_i} \right)\,, \end{aligned} \tag{84}$$

and therefore

$$\boxed{\delta u = \epsilon \big\{ u, G \big\}\,. \tag{85}}$$

The equations (82) look a lot like (rearranged) Hamilton's equations, with ϵ playing the role of time, and G that of the Hamiltonian. This observation suggests an alternative way of interpreting canonical transformations: So far, we treated them from a *passive* perspective, where (q,p) and (Q,P) are merely different coordinates describing the same point in phase space. Instead, we can view the transformation from an *active* perspective, where the canonical transformation takes us from one point in phase space to another.

3.3.2 Fundamental Examples

Time Evolution

As a counterpoint to viewing canonical transformations as active evolutions, we can view the time evolution generated by the Hamiltonian as a canonical transformation of the coordinates. Choosing $G = H$ and $\epsilon = dt$ in Eq. (83), we have

$$d\vec{\xi} = \big\{ \vec{\xi}, H \big\} dt \tag{86}$$

and therefore

$$\dot{\vec{\xi}} = \big\{ \vec{\xi}, H \big\}\,. \tag{87}$$

A *finite* time evolution of the coordinates can be viewed as a succession of infinitesimal canonical transformations.

Translations

Setting $G = p_k$ in Eq. (85), we see that

$$\delta p_i = \epsilon \big\{ p_i, p_k \big\} = 0 \,, \tag{88}$$

and

$$\delta q_i = \epsilon \big\{ q_i, p_k \big\} = \epsilon \delta_{ik} \,. \tag{89}$$

Thus, the *canonical* momentum p_k generates a constant shift in the *canonical* coordinate q_k.

Rotations

Consider a system with multiple particles in three dimensions, with

$$q = (x_1, y_1, z_1, \ldots, x_n, y_n, z_n) \,, \tag{90}$$

$$p = (p_{1x}, p_{1y}, p_{1z}, \ldots, p_{nx}, p_{ny}, p_{nz}) \,. \tag{91}$$

A rotation around the z axis is generated by the z component of the total angular momentum (cf. worksheet #4)

$$G = L_z = \sum_{i=1}^{A} \left(x_i p_{iy} - y_i p_{ix} \right) \,. \tag{92}$$

For an infinitesimal rotation angle $\epsilon = \delta\phi$, Eq. (85) then implies

$$\begin{aligned}
\delta x_i = \big\{ x_i, G \big\} \delta\phi &= \sum_j \left\{ x_i, x_j p_{jy} - y_j p_{jx} \right\} \delta\phi = \sum_j \Big(\underbrace{\left\{ x_i, x_j p_{jy} \right\}}_{=0} - \left\{ x_i, y_j p_{jx} \right\} \Big) \delta\phi \\
&= - \sum_j y_j \underbrace{\left\{ x_i, p_{jx} \right\}}_{=\delta_{ij}} \delta\phi = - y_i \delta\phi \,,
\end{aligned} \tag{93}$$

where we have used that Poisson brackets of the positions and momenta of *different* particles vanish. Analogously,

$$\begin{aligned}
\delta y_i = \big\{ y_i, G \big\} \delta\phi &= \sum_j \left\{ y_i, x_j p_{jy} - y_j p_{jx} \right\} \delta\phi = \sum_j \Big(\left\{ y_i, x_j p_{jy} \right\} - \underbrace{\left\{ y_i, y_j p_{jx} \right\}}_{=0} \Big) \delta\phi \\
&= \sum_j x_j \delta_{ij} \delta\phi = x_i \delta\phi \,,
\end{aligned} \tag{94}$$

and

$$\delta z_i = \big\{ z_i, G \big\} \delta\phi = \sum_j \left\{ z_i, x_j p_{jy} - y_j p_{jx} \right\} = 0 \,, \tag{95}$$

where we have used that p_{iz} does not appear in the generator. For the momenta, we find

$$\delta p_{ix} = - p_{iy} \delta\phi \,, \qquad \delta p_{iy} = p_{ix} \delta\phi \,, \qquad \delta p_{iz} = 0 \,. \tag{96}$$

It is easy to verify that we would get the same changes in the variables if we applied a rotation matrix $\boldsymbol{R}_z(\delta\phi)$ to $\vec{r}_i = (x_i, y_i, z_i)^T$ and performed an expansion for small angles.

3.3.3 Symmetries and Constants of the Motion

We can use the formalism of canonical transformations to revisit the connection between symmetries and conservation laws. To this end, we consider Eq. (85) with $u = H$ for a generator that does not explicitly depend on time. We have

$$\delta H = \epsilon\big\{H, G\big\} = -\epsilon\dot{G}\,, \tag{97}$$

where we have also used Eq. (41). This relationship implies that if H is invariant under an canonical transformation, then H and the generator G commute, and G is a constant of the motion.

4 The Liouville and Poincaré Theorems

4.1 Liovuille's Theorem and Liouville's Equation

In Section 3.2, we saw that the phase space volume is a symplectic invariant. Since we can view the time evolution of the system as a canonical transformation, this implies the following important result:

Liouville's Theorem

The volume of any phase space region is invariant under Hamiltonian time evolution.

Liouville's theorem allows us to deal with applications in which we are either unwilling or unable to treat the trajectories of individual particles in phase space, but an ensemble that is described by a density distribution $\rho(q,p,t)$. For example, we may only be able to specify the state of our system with a certain likelihood due to theoretical or measurement uncertainties, so that

$$\int\prod_i dq_i dp_i\;\rho(q,p,t) = 1\,, \tag{98}$$

or we might be studying a system consisting of a large number of particles ($N \approx 10^{23}$) using techniques from classical statistical mechanics, where

$$\int\prod_i dq_i dp_i\;\rho(q,p,t) = N\,. \tag{99}$$

In these applications both the total probability of finding the system in phase space or the total number of particles must be conserved. Since the phase space volume remains invariant under time evolution, we must have

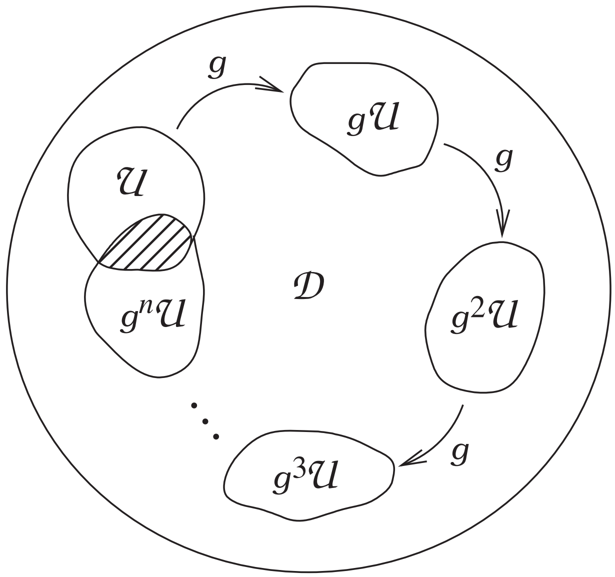
$$\boxed{\frac{d\rho}{dt} = \big\{\rho, H\big\} + \frac{\partial\rho}{\partial t} = 0\,,} \tag{100}$$

which is known as **Liovuille's equation**. Note that this equation holds even if $\frac{\partial H}{\partial t} \neq 0$, as long as the time evolution is governed by a Hamiltonian.

Stationary Distributions

In many applications we are interested in **stationary distributions** for which

$$\frac{\partial\rho}{\partial t} = 0 \quad\Rightarrow\quad \big\{\rho, H\big\} = 0\,, \tag{101}$$



which describe systems in thermodynamic equilibrium. In general, we can guarantee that ρ is stationary if we construct if from the constants of the motion of the system. For conservative systems, an obvious choice is the (time-independent) Hamiltonian, because $\rho(H(q,p))$ is guaranteed to have a vanishing Poisson bracket with H:

$$\begin{aligned}\{\rho, H\} &= \sum_i \left(\frac{\partial \rho}{\partial q_i} \frac{\partial H}{\partial p_i} - \frac{\partial \rho}{\partial p_i} \frac{\partial H}{\partial q_i} \right) = \sum_i \left(\frac{\partial \rho}{\partial H} \frac{\partial H}{\partial q_i} \frac{\partial H}{\partial p_i} - \frac{\partial \rho}{\partial H} \frac{\partial H}{\partial p_i} \frac{\partial H}{\partial q_i} \right) \\ &= \frac{\partial \rho}{\partial H} \{H, H\} = 0 \,. \end{aligned} \tag{102}$$

A well-known example is the **canonical ensemble** for a system in equilibrium with an external heat bath. It is described by the Boltzmann distribution

$$\boxed{\rho = \exp\left(-\frac{H(q,p)}{k_B \mathcal{T}} \right) ,} \tag{103}$$

where k_B is the Boltzmann constant and $\mathcal{T}$ the temperature. For instance, the Boltzmann distribution of a system of free non-interacting particles is

$$\rho = \frac{1}{Z} \exp\left(-\frac{H(q,p)}{k_B \mathcal{T}} \right) = \frac{1}{Z} \exp\left(-\sum_i \frac{\vec{p}_i^{\,2}}{2 m k_B \mathcal{T}} \right) = \frac{1}{Z} \exp\left(-\sum_i \frac{m \dot{\vec{r}}_i^{\,2}}{2 k_B \mathcal{T}} \right) \tag{104}$$

with a normalization factor $1/Z$, which is a Gaussian distribution in velocities.

4.2 Poincaré's Recurrence Theorem

[...]

5 Group Exercises

Problem G33 – Algebraic Properties of the Poisson Brackets

Prove the following properties of the Poisson Brackets, where f, g, h are functions of the canonical variables and α, β are arbitrary constants:

1. $\big\{f, g\big\} = -\big\{g, f\big\}$,
2. $\big\{\alpha f + \beta g, h\big\} = \alpha\big\{f, h\big\} + \beta\big\{g, h\big\}$,
3. $\big\{fg, h\big\} = \big\{f, h\big\}g + f\big\{g, h\big\}$.
4. Show that the Poisson brackets satisfy the **Jacobi identity**
$$\big\{f, \big\{g, h\big\}\big\} + \big\{g, \big\{h, f\big\}\big\} + \big\{h, \big\{f, g\big\}\big\} = 0\,. \tag{105}$$
Hint: Compute the sum of two of the three terms, e.g., $\big\{f, \big\{g, h\big\}\big\} + \big\{g, \big\{h, f\big\}\big\}$, and compare your result to the remaining term of the identity.

Problem G34 – Poisson Brackets and Dynamics

The Poisson brackets can be used to formulate the dynamics of Hamiltonian systems in a compact way. (In the following, keep in mind that $q = (q_1, \ldots, q_n), p = (p_1, \ldots, p_n)$).

1. Prove the fundamental relation $\big\{q_i, p_j\big\} = \delta_{ij}$.
2. Show that the Poisson brackets can be used to write Hamilton's equations as
$$\dot{q}_i = \big\{q_i, H\big\}\,, \quad \dot{p}_i = \big\{p_i, H\big\}\,. \tag{106}$$
3. Use Hamilton's equations to show that the total time derivative of an arbitrary function $f(q, p, t)$ can be written as
$$\frac{df}{dt} = \big\{f, H\big\} + \frac{\partial f}{\partial t}\,. \tag{107}$$
What happens if f is a conserved quantity?
4. Show that the Poisson bracket of two conserved quantities is also a conserved quantity.

Problem G35 – Poisson Brackets for the Angular Momentum

Show that the Poisson brackets of the angular momentum components $l_i = \sum_{jk} \epsilon_{ijk} x_j p_k$ $(i, j, k = 1, \ldots, 3)$ satisfiy the following relation:

$$\{l_i, l_j\} = \epsilon_{ijk} l_k \,. \tag{108}$$

Conclude that a system with Hamiltonian H that is invariant under rotations around the x and y axes must also be invariant under rotations around the z axis.

HINT: First, use the algebraic properties of the Poisson brackets to prove the relation

$$\{AB, CD\} = AC\{B, D\} + A\{B, C\}D + C\{A, D\}B + \{A, C\}DB \,. \tag{109}$$

Problem G36 – Canonicity of Coordinate Transformations

Use the Poisson brackets to prove that the following transformations are canonical:

1. $Q = q \cdot \tan p$, $P = \ln \sin p$
2. $Q = \sqrt{2q} \cdot e^{\alpha} \cos p$, $P = \sqrt{2q} \cdot e^{-\alpha} \sin p$