

Classical Mechanics

Examples (Canonical Transformation)

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1 Introduction

In classical mechanics, there is no unique prescription for one to choose the generalized coordinates for a problem. As long as the coordinates and the corresponding momenta span the entire phase space, it becomes an acceptable set. However, it turns out in practice that some choices are better than some others as they make a given problem simpler while still preserving the form of Hamilton's equations. Going over from one set of chosen coordinates and momenta to another set which satisfy Hamilton's equations is done by **canonical transformation**.

For instance, if we consider the central force problem in two dimensions and choose Cartesian coordinate, the potential is $-\frac{k}{\sqrt{x^2 + y^2}}$. However, if we choose (r, θ) coordinates,

the potential is $-\frac{k}{r}$ and θ is cyclic, which greatly simplifies the problem. The number of cyclic coordinates in a problem may depend on the choice of generalized coordinates. A cyclic coordinate results in a constant of motion which is its conjugate momentum. The example above where we replace one set of coordinates by another set is known as **point transformation**.

In the Hamiltonian formalism, the coordinates and momenta are given equal status and the dynamics occurs in what we know as the **phase space**. In dealing with phase space dynamics, we need point transformations in the phase space where the new coordinates (Q_i) and the new momenta (P_i) are functions of old coordinates (p_i) and old momenta (p_i):

$$Q_i = Q_i(\{q_j\}, \{p_j\}, t)$$
$$P_i = P_i(\{q_j\}, \{p_j\}, t)$$

Such transformations are called **contact transformations**.

However, in Hamiltonian mechanics, only those transformations are of interest for which the quantities Q_i and P_i are canonically conjugate pairs. This means that there exists some Hamiltonian $K(Q, P, t)$ with respect to which P and Q satisfy Hamilton's equations:

$$\begin{aligned}\dot{Q}_i &= \frac{\partial K}{\partial P_i} \\ \dot{P}_i &= -\frac{\partial K}{\partial Q_i}\end{aligned}$$

Note that Q and P are not specific to a particular mechanical system but are common to all systems having the same degree of freedom. We may, for instance, obtain P and Q for a plane harmonic oscillator and use the same set to solve Kepler's problem. Such transformations, which preserve the form of Hamilton's equations, are known as **canonical transformation**. Though the terms contact transformation is used synonymously with the term canonical transformation, not all contact transformations are canonical, as the following example shows. Let us consider a free particle system with the Hamiltonian $\mathcal{H} = \frac{p^2}{2m}$. Since q is cyclic, the conjugate momentum p is a constant of motion, $\dot{p} = 0$, and we have $\dot{q} = \frac{p}{m}$. Consider now, a contact transformation

$$P = pt; \quad Q = qt \tag{1}$$

Does a Hamiltonian $K(P, Q)$ exist for which P and Q satisfy the Hamilton's equations:

$$\begin{aligned}\dot{P} &= -\frac{\partial K}{\partial Q} \\ \dot{Q} &= \frac{\partial K}{\partial P}\end{aligned}$$

Existence of such a Hamiltonian would imply $\frac{\partial \dot{P}}{\partial P} = -\frac{\partial \dot{Q}}{\partial Q}$ as each of the expressions equals $-\frac{\partial^2 K}{\partial P \partial Q}$. However, Since $\frac{\partial \dot{P}}{\partial P} = \frac{\partial \dot{Q}}{\partial Q} = \frac{1}{t}$, this condition is not satisfied and the modified Hamiltonian K does not exist. Thus the contact transformations (1) are non-canonical, they do not preserve the volume of the phase space.

It may be noted that this does not imply that one cannot find an equation of motion using these variables. Indeed, since p is constant, $dP/dt = p = P/t$, which gives $P = kt$, where k is a constant. Likewise, we have,

$$\frac{d}{dt} \left(\frac{Q}{t} \right) = \frac{dq}{dt} = \frac{p}{m} = \frac{Pt}{m} = \frac{k}{m}$$

so that $Q = \frac{k}{m}t^2 + C$, where C is a constant.

To illustrate a canonical transformation, consider the free particle Hamiltonian again for which $\dot{p} = 0$ and $\dot{q} = p/m$, as before. Consider a linear transformation of (p, q) to a new set (P, Q) , which is given by

$$\begin{aligned} P &= \alpha p + \beta q \\ Q &= \gamma p + \delta q \end{aligned} \quad (2)$$

If the matrix of transformation is non-singular, i.e. if $\Delta = \begin{vmatrix} \alpha & \beta \\ \gamma & \delta \end{vmatrix} \neq 0$, then the above transformation is invertible and we have

$$\begin{aligned} p &= \frac{1}{\Delta}(\delta P - \beta Q) \\ q &= \frac{1}{\Delta}(-\gamma P + \alpha Q) \end{aligned} \quad (3)$$

It can be checked that

$$\begin{aligned} \dot{P} &= \alpha \dot{p} + \beta \dot{q} = \beta \dot{q} = \beta \frac{p}{m} = \frac{\beta}{m\Delta}(\delta P - \beta Q) \\ \dot{Q} &= \gamma \dot{p} + \delta \dot{q} = \delta \dot{q} = \delta \frac{p}{m} = \frac{\delta}{m\Delta}(\delta P - \beta Q) \end{aligned} \quad (4)$$

Is there a Hamiltonian K for which P and Q are canonical? It is seen that

$$\begin{aligned} \frac{\partial \dot{P}}{\partial P} &= \frac{\beta\delta}{m\Delta} \\ \frac{\partial \dot{Q}}{\partial Q} &= -\frac{\beta\delta}{m\Delta} \end{aligned}$$

so that K exists. To determine K note that $\dot{P} = -\frac{\partial K}{\partial Q}$ which gives

$$K = - \int \dot{P} dQ = -\frac{\beta\delta}{m\Delta} PQ + \frac{\beta^2}{m\Delta} \frac{Q^2}{2} + f(P)$$

and $\dot{Q} = \frac{\partial K}{\partial P}$ gives

$$K = - \int \dot{Q} dP = -\frac{\beta\delta}{m\Delta} PQ + \frac{\delta^2}{m\Delta} \frac{P^2}{2} + f(Q)$$

These two expressions give

$$K = \frac{1}{2m\Delta}(\delta P - \beta Q)^2$$

Except for the factor Δ , this is just the old Hamiltonian written in terms of the new variables. For $\Delta = 1$, the two Hamiltonians are identical and the transformation corresponds

to a point transformation of Lagrangian mechanics.

Consider a second example where, once again we take the free particle Hamiltonian of the previous example. Consider a transformation

$$P = p \cos q, \quad Q = p \sin q \quad (5)$$

The transformation is invertible and it is easily seen that

$$p = \sqrt{P^2 + Q^2}, \quad q = \tan^{-1} \frac{Q}{P} \quad (6)$$

Using the same algebra as for the previous example, we get

$$\dot{P} = \dot{p} \cos q - \dot{q} p \sin q = -\frac{p^2}{m} \sin q = -\frac{Q}{m} \sqrt{P^2 + Q^2}$$

and

$$\dot{Q} = \frac{P}{m} \sqrt{P^2 + Q^2}$$

It can be seen that $\frac{\partial \dot{P}}{\partial P} = -\frac{\partial \dot{Q}}{\partial Q}$, showing that the Hamiltonian exists. It is easy to show that the Hamiltonian is given by $K = \frac{1}{3m} \sqrt{P^2 + Q^2}$.

However, instead of considering the free particle Hamiltonian, consider the Hamiltonian of a particle in a uniform gravitational field.

$$\mathcal{H} = \frac{p^2}{2m} + mgq$$

In this case $\dot{p} = -mg$ and $\dot{q} = \frac{p}{m}$. We had seen that the transformation is invertible. In this case, we get

$$\begin{aligned} \dot{P} &= \dot{p} \cos q - \dot{q} p \sin q \\ &= -mg \cos q - \frac{p^2}{m} \sin q \\ &= -mg \frac{P}{\sqrt{P^2 + Q^2}} - \frac{1}{m} \frac{Q}{\sqrt{P^2 + Q^2}} \end{aligned}$$

and

$$\begin{aligned} \dot{Q} &= \dot{p} \sin q + \dot{q} p \cos q \\ &= -mg \frac{Q}{\sqrt{P^2 + Q^2}} + \frac{p^2}{m} \cos q \\ &= -mg \frac{Q}{\sqrt{P^2 + Q^2}} - \frac{1}{m} P \sqrt{P^2 + Q^2} \end{aligned}$$

One can check $\frac{\partial \dot{P}}{\partial P} \neq -\frac{\partial \dot{Q}}{\partial Q}$, so that the transformation is not canonical with respect to the given Hamiltonian. This shows that (5) is not a valid canonical transformation. This is because, in order that a transformation may be canonical, it must satisfy Hamilton's equation for all systems having the same number of degrees of freedom.

2 Canonical Transformation & Generating Function

We start with an observation that Hamilton's equations of motion can be derived from the Hamilton's principle by writing action written in the form $S = \int \mathcal{L} dt = \int (p\dot{q} - \mathcal{H}) dt$ and optimizing the action. In deriving the Euler Lagrange equation, we had optimized action subject to the condition that $\delta q(t_i) = \delta q(t_f) = 0$, i.e. there is no variation at the end points. We have

$$\delta S = \delta \int_{t_0}^{t_f} (p_i \dot{q}_i - \mathcal{H}) dt = 0$$

with implied summation on repeated index and we have denoted the initial time as t_0 so as not to confuse with the index i . The variation in the action is then given by

$$\begin{aligned} \delta S &= \int_{t_0}^{t_f} \left[\dot{q}_i \delta p_i + p_i \delta \dot{q}_i - \frac{\partial \mathcal{H}}{\partial q_i} \delta q_i - \frac{\partial \mathcal{H}}{\partial p_i} \delta p_i \right] dt \\ &= \int_{t_0}^{t_f} \left[\left(\dot{q}_i - \frac{\partial \mathcal{H}}{\partial p_i} \right) \delta p_i + \frac{d}{dt} (p_i \delta q_i) - \dot{p}_i \delta q_i - \frac{\partial \mathcal{H}}{\partial q_i} \delta q_i \right] dt \\ &= \int_{t_0}^{t_f} \left[\left(\dot{q}_i - \frac{\partial \mathcal{H}}{\partial p_i} \right) \delta p_i - \left(\dot{p}_i + \frac{\partial \mathcal{H}}{\partial q_i} \right) \delta q_i \right] dt + [p_i \delta q_i]_{t_0}^{t_f} \end{aligned}$$

We have seen earlier that setting $\delta S = 0$ for all variations of q_i gave us Euler Lagrange equation and we expect that setting $\delta S = 0$ for all variations of q_i and p_i will lead to Hamilton's equations. However, there is a subtle difference between the two cases. In the Lagrangian formulation q_i and \dot{q}_i were not independent variables and hence we only needed variation with respect to q_i . In the Hamiltonian formalism, however, we need to vary both q_i and p_i . The last term of the above equation vanishes if $\delta q_i(t_0) = \delta q_i(t_f) = 0$ and it does not requires the corresponding relation for vanishing of the momentum coordinates. Thus, we have an additional degree of freedom and we could define the action as

$$S = \int (p_i \dot{q}_i - \mathcal{H} + \frac{dF(q, p)}{dt}) dt$$

so that for all variations of p_i and q_i , the Hamilton's equations would be valid.

The variational principle requires the function $p\dot{q} - \mathcal{H}$ to satisfy the Euler Lagrange equations. Thus we have

$$\begin{aligned} \frac{d}{dt} \left(\frac{\partial}{\partial \dot{q}} (p\dot{q} - \mathcal{H}) \right) - \frac{\partial}{\partial q} (p\dot{q} - \mathcal{H}) &= 0 \\ \frac{d}{dt} \left(\frac{\partial}{\partial \dot{p}} (p\dot{q} - \mathcal{H}) \right) - \frac{\partial}{\partial p} (p\dot{q} - \mathcal{H}) &= 0 \end{aligned}$$

Since $\mathcal{H} = \mathcal{H}(p, q)$, we get from above, $\frac{d}{dt}p + \frac{\partial \mathcal{H}}{\partial q} = 0$, i.e. $\dot{p} = -\frac{\partial \mathcal{H}}{\partial q}$ and likewise, since $p\dot{q} - \mathcal{H}$ no dependence on \dot{p} , $-\dot{q} + \frac{\partial \mathcal{H}}{\partial p} = 0$, i.e., $\dot{q} = \frac{\partial \mathcal{H}}{\partial p}$. The variational principle satisfied by the old pair of variables (q, p) is

$$\delta S = \delta \int (p\dot{q} - \mathcal{H})dt = 0$$

with no variation at the end points. With respect to the new variables, one then must have

$$\delta S' = \delta \int (P\dot{Q} - \mathcal{H})dt = 0$$

These two forms of S and S' are completely equivalent if the two integrands differ either by a scale factor or by total time differential of a function F , i.e. if

$$\sum_i P_i \dot{Q}_i - K = \lambda \sum_i (p_i \dot{q}_i - \mathcal{H}) \quad (7)$$

known as the **scale transformation** or,

$$\sum_i P_i \dot{Q}_i - K + \frac{dF}{dt} = \sum_i p_i \dot{q}_i - \mathcal{H} \quad (8)$$

known as the **canonical transformation** or by a combination of both

$$\sum_i P_i \dot{Q}_i - K + \frac{dF}{dt} = \lambda \sum_i (p_i \dot{q}_i - \mathcal{H}) \quad (9)$$

which is usually referred to as **extended canonical transformation**. If we rewrite (8) as

$$\sum_i p_i dq_i - \mathcal{H}dt - \sum_i P_i dQ_i + Kdt = dF \quad (10)$$

we notice that the difference between the two differential forms must be an exact differential. Analogous statement can be made regarding (9) as well. It turns out that this condition of exact differentiability is both necessary and sufficient condition for a transformation to be canonical.

2.1 Scale Transformation

Scale transformation is achieved by multiplying the old coordinates and momenta with some scale factors to get the corresponding new quantities, $P_i = \nu p_i$ and $Q_i = \mu q_i$. The scale factors can be different for momenta and the coordinates but must be the same for all coordinates (and all momenta). P and Q are obtainable from the new Hamiltonian K through Hamilton's equations

$$\dot{P}_i = -\frac{\partial K}{\partial Q_i} \quad \dot{Q}_i = \frac{\partial K}{\partial P_i}$$

Thus we have, using $P_i = \nu p_i$ and $Q_i = \mu q_i$,

$$\nu \dot{p}_i = -\frac{\partial K}{\partial \mu q_i}$$

which gives

$$\dot{p}_i = -\frac{1}{\mu\nu} \frac{\partial K}{\partial q_i}$$

Comparing this with the equation $\dot{p}_i = \frac{\partial \mathcal{H}}{\partial q_i}$, we get $K = \mu\nu \mathcal{H}$. This gives

$$\sum_i P_i \dot{Q}_i - K(P, Q, t) = \mu\nu \sum_i (p_i \dot{q}_i - \mathcal{H}(p, q, t))$$

Comparing this with (7) we get $\lambda = \mu\nu$.

2.2 Generating Function

The function F in (8) or (9) is, in principle, a function of p_i, q_i, P_i, Q_i and t . It is known as the **generating function** of canonical transformation. We will illustrate it with a couple of examples. *We will use Einstein summation convention according to which a repeated index in a single term implies a sum, i.e. $f_i g_i = \sum_i f_i g_i$.*

Example : Identity Transformation:

Consider a transformation $F = q_i P_i - Q_i P_i$ in which the dependence on time is implicit. We have

$$\begin{aligned} P_i Q_i - K + \frac{dF}{dt} &= P_i Q_i - K + \dot{q}_i P_i + q_i \dot{P}_i - \dot{Q}_i P_i - Q_i \dot{P}_i \\ &= -K + (q_i - Q_i) \dot{P}_i + P_i \dot{q}_i \\ &\equiv p_i \dot{q}_i - \mathcal{H} \end{aligned}$$

The equation is satisfied by identity transformation $p_i = P_i, q_i = Q_i$ and $K = \mathcal{H}$.

Example: Swapping Coordinates and Momenta

We can generalize the above example and consider a generating function of the following type (summation convention used)

$$F = f_i(q_1, q_2, \dots, q_n; t) P_i - Q_i P_i$$

where f_i is a function of the arguments q_1, q_2, \dots, q_n and t . We then have

$$\begin{aligned} P_i \dot{Q}_i - K + \frac{dF}{dt} &= P_i \dot{Q}_i - K + \left(\frac{\partial f_i}{\partial q_j} \dot{q}_j P_i + \frac{\partial f_i}{\partial t} P_i \right) + f_i \dot{P}_i - (\dot{Q}_i P_i + Q_i \dot{P}_i) \\ &= -K + (f_i - Q_i) \dot{P}_i + \frac{\partial f_i}{\partial q_j} \dot{q}_j P_i + \frac{\partial f_i}{\partial t} P_i \\ &\equiv p_i \dot{q}_i - \mathcal{H} \end{aligned}$$

The set of equations above can be satisfied by taking $Q_i = f_i$, $K = \mathcal{H} + \frac{\partial f_i}{\partial t} P_i$ and requiring $p_i \dot{q}_i = \frac{\partial f_i}{\partial q_j} \dot{q}_j P_i$ which can be rearranged as follows:

$$p_i \dot{q}_i = \frac{\partial f_i}{\partial q_j} \dot{q}_j P_i = \frac{\partial f_j}{\partial q_i} \dot{q}_i P_j$$

where in the last term we have interchanged the sum over i and j . This gives

$$p_i = \sum_j \frac{\partial f_j}{\partial q_i} P_j$$

where we have explicitly reintroduced the sum for clarity. These are n equations which must be inverted to get P_i . It may be noted that the choice of F is not unique corresponding to a particular canonical transformation. For instance, if we add any $g(t)$ to F it does not affect the action integral, because $\frac{dF}{dt} \rightarrow \frac{dF}{dt} + \frac{dg}{dt}$ does not change the Lagrangian equations.

Let us illustrate how to find generator. Let $K(Q, P, t) = \mathcal{H}(q, p, t)$. Plugging this into (8), we get

$$\frac{dF}{dt} = \sum_i (p_i \dot{q}_i - P_i \dot{Q}_i)$$

This is not very interesting because there is no time dependence. The simplest way to satisfy it is

$$F = F(q, Q)$$

We have

$$\begin{aligned} \frac{dF}{dt} &= \sum_i \frac{\partial F}{\partial q_i} \dot{q}_i + \frac{\partial F}{\partial Q_i} \dot{Q}_i \\ &= \sum_i (p_i \dot{q}_i - P_i \dot{Q}_i) \end{aligned}$$

This gives with $\frac{\partial F}{\partial q_i} = p_i$; $\frac{\partial F}{\partial Q_i} = -P_i$. A trivial way to satisfy the equations is to take $F(q_i, Q_i) = \sum_i q_i Q_i$ so that

$$\begin{aligned} \frac{\partial F}{\partial q_i} &= Q_i = p_i \\ \frac{\partial F}{\partial Q_i} &= q_i = -P_i \end{aligned}$$

which simply requires us to swap the coordinates and the momenta in the Hamiltonian formalism (but for a sign).

3 Different types of Generating Functions

We have remarked that the generating function F is a function of the old coordinates (and momenta) q, p , the new coordinates Q, P and time t . However, since Q and P themselves are functions of q and p (and vice-versa), only two of the four variables are needed in the description of the generating function. We need one each from the old pair and the new pair to describe the generating function, in addition to time. There are four possibilities and depending on the combination that we choose, the generating functions are classified as type 1, 2, 3 or 4.

3.1 Type 1 Generator

Type 1 generator, denoted by F_1 is a function of q_i and Q_i . We denote

$$F = F_1(q_i, Q_i, t) \quad (11)$$

Since $F_1 = F_1(q, Q, t)$, we can write

$$\begin{aligned} \frac{dF}{dt} &= \frac{\partial F_1}{\partial q_i} \dot{q}_i + \frac{\partial F_1}{\partial Q_i} \dot{Q}_i + \frac{\partial F_1}{\partial t} \\ &\equiv \sum_i p_i \dot{q}_i - \sum_i P_i \dot{Q}_i + K - \mathcal{H} \end{aligned} \quad (12)$$

where the last expression is from (8). We can compare the last two expressions for $\frac{dF_1}{dt}$ to get

$$\begin{aligned} p_i &= \frac{\partial F_1}{\partial q_i} \\ P_i &= -\frac{\partial F_1}{\partial Q_i} \\ K &= \mathcal{H} + \frac{\partial F_1}{\partial t} \end{aligned} \quad (13)$$

Note that (12) can be rewritten as

$$dF_1 = p_i dq_i - P_i dQ_i + (K - \mathcal{H})dt \quad (14)$$

If the Hamiltonian has no explicit time dependence, the generating function will also not have an explicit time dependence and in such a case $K = \mathcal{H}$. In such a situation (8) can be written as (summation convention used)

$$\frac{dF}{dt} = p_i \dot{q}_i - P_i \dot{Q}_i$$

For instantaneous transformation, we can write the above as

$$dF = p_i \delta q_i - P_i \delta Q_i$$

Since the left hand side is a perfect differential, so is the right hand side. In order that this may be so, we require

$$\frac{\partial p_i}{\partial Q_i} = \frac{\partial P_i}{\partial q_i} \quad (15)$$

When the functional dependence are given, one can always use (15) to test whether the transformation is canonical.

As shown earlier, one of the simplest examples of a F_1 type transformation is $F_1(q_i, Q_i) = q_i Q_i$, which gives the swapping transformation $p_i = Q_i$ and $P_i = -q_i$. Let us see what it does to the Hamiltonian of the Harmonic oscillator for which $\mathcal{H} = \frac{p^2}{2m} + \frac{1}{2}kq^2$. Since the Hamiltonian has no explicit time dependence, we have $K = \mathcal{H}$. In such a case

$$K = \frac{Q^2}{2m} + \frac{1}{2}kP^2$$

The new equations of motion are

$$\begin{aligned} \dot{Q} &= \frac{\partial K}{\partial P} = kP \\ \dot{P} &= -\frac{\partial K}{\partial Q} = -\frac{Q}{m} \end{aligned}$$

Thus we get

$$\ddot{Q} = k\ddot{P} = -\frac{Q}{m}$$

which has the solution $Q = Q_0 \cos(\omega t + \delta)$. We can obtain P from the equation $P = \frac{\dot{Q}}{k}$ which gives $P = -\frac{Q_0\omega}{k} \sin(\omega t + \delta)$. Since this is equal to $-q$, we can identify $q_0 = Q_0\omega/k$. We then can write

$$q = q_0 \cos(\omega t + \delta')$$

where $\delta' - \delta = \pi/2$.

3.2 Type 2 Generator

Type 2 generators, denoted by $F_2(q, P, t)$ can be obtained from the type 1 generator $F_1(q, Q, t)$ by means of a Legendre transformation. Since we have, in view of (13)

$$P_i = -\frac{\partial F_1}{\partial Q_i}$$

and we wish to replace the variable Q_i by the new variable P_i , we define

$$F_2(q_i, P_i, t) = F_1(q_i, Q_i, t) + \sum_i P_i Q_i \quad (16)$$

Note that starting with the equation (14) for F_1 can be written (use summation convention) by observing

$$\frac{dF_1}{dt} = p_i \dot{q}_i - P_i \dot{Q}_i + K - \mathcal{H} \quad (17)$$

Using (16), we have

$$\begin{aligned} \frac{dF_2}{dt} &= \frac{dF_1}{dt} + P_i \dot{Q}_i + \dot{P}_i Q_i \\ &= p_i \dot{q}_i + \dot{P}_i Q_i + (K - \mathcal{H}) \end{aligned} \quad (18)$$

Since F_2 depends on q and P , we can write

$$\frac{dF_2}{dt} = \frac{\partial F_2}{\partial q_i} \dot{q}_i + \frac{\partial F_2}{\partial P_i} \dot{P}_i + \frac{\partial F_2}{\partial t} dt$$

Comparing it with (17), we get

$$\begin{aligned} \frac{\partial F_2}{\partial q_i} &= p_i \\ \frac{\partial F_2}{\partial P_i} &= Q_i \\ \frac{\partial F_2}{\partial t} &= K - \mathcal{H} \end{aligned} \quad (19)$$

3.3 Type 3 Generator

In a similar way as above, we can define $F_3(p, Q, t)$ through a Legendre transform on F_1 . Referring to (13), we have, since the variable q_i is being replaced by p_i , and, $p_i = \frac{\partial F_1}{\partial q_i}$

$$F_3(p, Q, t) = F_1(q, Q, t) - p_i q_i$$

We then have

$$\begin{aligned} \frac{dF_3}{dt} &= \frac{dF_1}{dt} - p_i \dot{q}_i - q_i \dot{p}_i \\ &= -q_i \dot{p}_i - P_i \dot{Q}_i + (K - \mathcal{H}) \end{aligned} \quad (20)$$

On the other hand, since F_3 depends on (p_i, Q_i, t) , we can write,

$$\frac{dF_3}{dt} = \frac{\partial F_3}{\partial p_i} \dot{p}_i + \frac{\partial F_3}{\partial Q_i} \dot{Q}_i + \frac{\partial F_3}{\partial t}$$

Comparing this with (20) we get

$$\begin{aligned} \frac{\partial F_3}{\partial Q_i} &= -P_i \\ \frac{\partial F_3}{\partial p_i} &= -q_i \\ \frac{\partial F_3}{\partial t} &= K - \mathcal{H} \end{aligned} \quad (21)$$

3.4 Type 4 Generator

Finally we would like to define $F_4(p, P, t)$. In this case it is better to start with F_2 or F_3 and do a Legendre transformation. Starting with F_3 , we have to replace Q_i with P_i . In view of (21), we have

$$F_4(p, P, t) = F_3(p, Q, t) - Q_i P_i$$

We then have

$$\begin{aligned} \frac{dF_4}{dt} &= \frac{dF_3}{dt} + Q_i \dot{P}_i + P_i \dot{Q}_i \\ &= -q_i \dot{p}_i + Q_i \dot{P}_i + (K - \mathcal{H}) \end{aligned}$$

Since $F_4 = F_4(p, P, t)$, we have

$$\frac{dF_4}{dt} = \frac{\partial F_4}{\partial p_i} \dot{p}_i + \frac{\partial F_4}{\partial P_i} \dot{P}_i + \frac{\partial F_4}{\partial t}$$

Comparing with the preceding relation, we have we get

$$\begin{aligned} \frac{\partial F_4}{\partial p_i} &= -q_i \\ \frac{\partial F_4}{\partial P_i} &= Q_i \\ \frac{\partial F_4}{\partial t} &= K - \mathcal{H} \end{aligned} \tag{22}$$

3.5 Summary of the different types of Generators

The following table gives a summary of relationships for different types of generators.

Generators	Derivatives	Relationship
$F_1(q, Q, t)$	$p_i = \frac{\partial F_1}{\partial q_i}; P_i = -\frac{\partial F_1}{\partial Q_i}$	$\frac{\partial p_i}{\partial Q_j} = -\frac{\partial P_j}{\partial q_i}$
$F_2(q, P, t)$	$p_i = \frac{\partial F_2}{\partial q_i}; Q_i = \frac{\partial F_2}{\partial P_i}$	$\frac{\partial p_i}{\partial P_j} = \frac{\partial Q_j}{\partial q_i}$
$F_3(p, Q, t)$	$P_i = -\frac{\partial F_3}{\partial Q_i}; q_i = -\frac{\partial F_3}{\partial p_i}$	$\frac{\partial P_i}{\partial p_j} = \frac{\partial q_j}{\partial Q_i}$
$F_4(p, P, t)$	$q_i = -\frac{\partial F_4}{\partial p_i}; Q_i = \frac{\partial F_4}{\partial P_i}$	$\frac{\partial Q_i}{\partial p_j} = -\frac{\partial q_j}{\partial P_i}$

4 Invariance of Poisson's Bracket

A canonical transformation preserves the Poisson's bracket. This property can be used to verify whether a transformation is indeed canonical. Let $(q, p) \rightarrow (Q, P)$ be a transformation. The set (q, p) satisfies Poisson's bracket relationship, i.e.

$$\{q_i, p_j\} = \delta_{ij} \quad (23)$$

What we need to show is that Poisson's bracket calculated using either basis is the same, i.e.,

$$\{Q_i, P_j\}_{QP} = \{Q_i, P_j\}_{qp} \quad (24)$$

Clearly, since $\{Q_i\}, \{P_i\}$ are canonically conjugate pairs, they satisfy

$$\{Q_i, P_j\}_{QP} = \delta_{ij} \quad (25)$$

To prove (24), we note

$$\begin{aligned} \{Q_i, P_j\}_{qp} &= \sum_k \left[\frac{\partial Q_i}{\partial q_k} \cdot \frac{\partial P_j}{\partial p_k} - \frac{\partial Q_i}{\partial p_k} \cdot \frac{\partial P_j}{\partial q_k} \right] \\ &= \sum_k \left[\frac{\partial Q_i}{\partial q_k} \cdot \frac{\partial q_k}{\partial Q_j} - \frac{\partial Q_i}{\partial p_k} \cdot \left(-\frac{\partial p_k}{\partial Q_j} \right) \right] = \frac{\partial Q_i}{\partial Q_j} = \delta_{ij} \end{aligned} \quad (26)$$

In proving the above, we have used (15).

In a similar way, we can prove that the Poisson's brackets of the old variables are preserved in the new basis,

$$\{q_i, p_j\}_{qp} = \{q_i, p_j\}_{QP}$$

In general, for any two dynamical variables X and Y , one can show that the Poisson's bracket relationship remains the same in either basis

$$\{X, Y\}_{QP} = \{X, Y\}_{qp} \quad (27)$$

5 Illustrative Problems

Example 1: Harmonic Oscillator The Hamiltonian for the Harmonic oscillator is $\mathcal{H}(p, q) = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 q^2$. Let us carry out a transformation

$$\begin{aligned} p &= f(P) \cos Q \\ q &= \frac{f(P)}{m\omega} \sin Q \end{aligned} \quad (28)$$

This converts the Hamiltonian to a function of P alone with $K = \mathcal{H} = \frac{f(P)^2}{2m}$. Note that the Hamiltonian is cyclic in Q so that P is constant. The problem is to find $f(P)$ such

that the transformation is canonical.

Let us try an F_1 type transformation for which, as per eqn. (13)

$$\begin{aligned} p &= \frac{\partial F_1}{\partial q} \\ P &= -\frac{\partial F_1}{\partial Q} \\ K &= \mathcal{H} + \frac{\partial F_1}{\partial t} = \mathcal{H} \end{aligned} \tag{29}$$

the last equality because the Hamiltonian is time independent. From (28), we get,

$$p = m\omega q \cot Q = \frac{\partial F_1}{\partial q}$$

Integrating, we get

$$F_1 = \frac{m\omega q^2}{2} \cot Q$$

The momenta conjugate to Q is then given by

$$\begin{aligned} P &= -\frac{\partial F_1}{\partial Q} \\ &= \frac{m\omega q^2}{2} \operatorname{cosec}^2 Q \\ &= \frac{p^2}{2m\omega} \frac{1}{\cos^2 Q} \end{aligned}$$

which gives

$$p = \sqrt{2Pm\omega} \cos Q$$

so that $f(P) = \sqrt{2Pm\omega}$. This in turn gives the new Hamiltonian to be $K = \frac{f(P)^2}{2m} = \omega P$.

Thus the transformation (28) is equivalent to

$$\begin{aligned} p &= \sqrt{2Pm\omega} \cos Q \\ q &= \sqrt{\frac{2}{m\omega}} \sin Q \end{aligned}$$

Inverting, we get

$$\begin{aligned} P &= \frac{1}{2m\omega} (q^2 m^2 \omega^2 + p^2) \\ Q &= \tan^{-1} \left(\frac{m\omega q}{p} \right) \end{aligned}$$

Note that

$$\begin{aligned}\frac{\partial Q}{\partial q} &= \frac{m\omega p}{p^2 + m^2\omega^2 q^2} \\ \frac{\partial P}{\partial p} &= \frac{p}{m\omega} \\ \frac{\partial Q}{\partial p} &= -\frac{m\omega q}{p^2 + m^2\omega^2 q^2} \\ \frac{\partial P}{\partial q} &= qm\omega\end{aligned}$$

which shows that

$$\{Q, P\}_{qp} = 1$$

i.e. as expected, the transformation preserves Poisson's bracket.

As the energy is constant we have $P = \frac{E}{\omega}$. The Hamilton's equations for the new variables then gives

$$\dot{Q} = \frac{\partial K}{\partial P} = \omega$$

yielding $Q = \omega t + \alpha$ The original problem is now solved,

$$\begin{aligned}p &= \sqrt{2mE} \cos Q = \sqrt{2mE} \cos(\omega t + \alpha) \\ q &= \sqrt{\frac{2P}{m\omega}} \sin Q = \sqrt{\frac{2E}{m\omega^2}} \sin(\omega t + \alpha)\end{aligned}$$

Example 2:

Consider the Hamiltonian $\mathcal{H} = \frac{1}{2}(p^2 + q^2)$. Determine if the transformation $Q = \frac{1}{2}(q^2 + p^2)$ and $P = -\tan^{-1}(q/p)$ is canonical. If so, find a generating function of type F_1 .

In order that the given transformation is canonical, $p\delta q - P\delta Q = dF$ must be an exact differential. Note that

$$\begin{aligned}p\delta q - P\delta Q &= p\delta q + \tan^{-1} \frac{q}{p} \delta \left(\frac{q^2 + p^2}{2} \right) \\ &= \left(p + q \tan^{-1} \frac{q}{p} \right) \delta q + p \tan^{-1} \frac{q}{p} \delta p\end{aligned}$$

In order that the above is an exact differential,

$$\frac{\partial}{\partial p} \left(p + q \tan^{-1} \frac{q}{p} \right) = \frac{\partial}{\partial q} \left(p \tan^{-1} \frac{q}{p} \right)$$

It can be easily seen that both sides of the above condition equals $\frac{p^2}{p^2 + q^2}$ so that the transformation is canonical.

The Poisson's brackets can be shown to be preserved:

$$\begin{aligned}\{Q, P\} &= \frac{\partial}{\partial q} \left(\frac{1}{2}(q^2 + p^2) \right) \frac{\partial}{\partial p} \left(-\tan^{-1} \frac{q}{p} \right) - \frac{\partial}{\partial p} \left(\frac{1}{2}(q^2 + p^2) \right) \frac{\partial}{\partial q} \left(-\tan^{-1} \frac{q}{p} \right) \\ &= q \frac{(q/p^2)}{1 + q^2/p^2} - p \left(-\frac{1/p}{1 + q^2/p^2} \right) = 1\end{aligned}$$

We can obtain F by integrating either of the factors. For instance, a bit of exercise in integration gives

$$\begin{aligned}F &= \int \left(p + q \tan^{-1} \frac{q}{p} \right) dq \\ &= \frac{pq}{2} + \frac{q^2 + p^2}{2} \tan^{-1} \frac{q}{p}\end{aligned}$$

However, the above form cannot be a generating function as it has no dependence on the new variables. Since we wish it to be of form F_1 , we need to eliminate p . This is done by substitution $p = \sqrt{2Q - q^2}$ so that $\tan^{-1} \frac{q}{p} = \tan^{-1} \frac{q}{\sqrt{2Q - q^2}} = \sin^{-1} \frac{q}{\sqrt{2Q}}$. With these substitutions, we get

$$F = Q \sin^{-1} \frac{q}{\sqrt{2Q}} + \frac{1}{2} q \sqrt{2Q - q^2}$$

The Hamiltonian $K = \frac{1}{2}(q^2 + p^2) = Q$, so that $\dot{Q} = \frac{\partial K}{\partial P} = 0$, i.e. Q is constant, and $\dot{P} = -\frac{\partial K}{\partial Q} = -1$. Since Q is constant, so is the Hamiltonian and P decreases with time.

Example 3:

Prove that the transformation $Q = \ln \frac{\sin p}{q}$ and $P = q \cot p$ is canonical and derive all the different forms of generating functions.

We have, for the given transformation

$$\delta Q = \cot p \delta p - \frac{1}{q} \delta q$$

Thus

$$\begin{aligned}p \delta q - P \delta Q &= p \delta q - q \cot p \left(\cot p \delta p - \frac{1}{q} \delta q \right) \\ &= (p + \cot p) \delta q - q \cot^2 p \delta p\end{aligned}$$

This is an exact differential if

$$\frac{\partial}{\partial p} (p + \cot p) = \frac{\partial}{\partial q} (-q \cot^2 p)$$

It can be seen that both sides equal $-\cot^2 p$ and hence the transformation is canonical. It is also easy to see that Poisson's bracket is preserved.

The structure of generating function is

$$F = \int (p + \cot p) dq = pq + q \cot p$$

(We can also integrate the other factor over p and show that both the forms are the same if the constant integration is taken to be zero). We will now express this in terms of different forms of the generating function. Note that for the given transformation, $\sin p = qe^Q$ which gives $\cos p = \sqrt{1 - q^2 e^{2Q}}$ and $q \cot p = \sqrt{e^{-2Q} - q^2}$. Substituting these, we get

$$F_1 = q \cos^{-1} \sqrt{1 - q^2 e^{2Q}} + \sqrt{e^{-2Q} - q^2}$$

Suppose we wish to find the generator form F_2 . In such a case, we need to replace p by P , which is quite straightforward. We can find F_2 by a Legendre transformation. Since $P = -\frac{\partial F_1}{\partial Q}$, we have $F_2(q, P) = F_1(q, Q) + PQ$. Thus

$$F_2(q, P) = F_1(q, Q) = q \sin^{-1}(qe^Q) + \frac{1}{e^Q} \sqrt{1 - q^2 e^{2Q}} + PQ$$

However, as F_2 must be expressed as a function of q and P , we must accordingly express the variables. We had shown that $P = \frac{\sqrt{1 - q^2 e^{2Q}}}{e^Q}$, which gives $e^Q = \frac{1}{\sqrt{P^2 + q^2}}$. Thus

$$F_2(q, P) = q \sin^{-1} \left(\frac{q}{\sqrt{P^2 + q^2}} \right) + P - \frac{P}{2} \ln(P^2 + q^2)$$