or

$$\sum_{j=1}^{3N}\left[(\delta\theta\times\vec{r})_j\frac{\partial H}{\partial r_j}+(\delta\theta\times\vec{p})_j\frac{\partial H}{\partial p_j}\right]=0$$

from which we obtain

$$\delta\vec{\theta}\cdot\left[\sum_{j=1}^{3N}\left\{\left(\vec{r}\times\frac{\partial H}{\partial\vec{r}}\right)_j+\left(\vec{p}\times\frac{\partial H}{\partial\vec{p}}\right)_j\right\}\right]=0 \tag{5.20}$$

where we have used the vector identity $(\vec{A}\times\vec{B})\cdot\vec{C}=(\vec{C}\times\vec{A})\cdot\vec{B}$.

Using Hamilton's equations, Equation 5.20 can be further simplified:

$$\delta\vec{\theta}\cdot\left[\sum_{j=1}^{3N}\left\{(\vec{r}\times\dot{\vec{p}})_j+(\vec{p}\times\dot{\vec{r}})_j\right\}\right]=-\delta\vec{\theta}\cdot\frac{\mathrm{d}}{\mathrm{d}t}\sum_{j=1}^{3N}(\vec{r}\times\vec{p})_j=-\delta\vec{\theta}\cdot\frac{\mathrm{d}\vec{L}}{\mathrm{d}t}=0$$

where $\vec{L}$ is the total angular momentum of the system. Because $\delta\vec{\theta}$ is arbitrary, we have

$$\frac{\mathrm{d}\vec{L}}{\mathrm{d}t}=0,\quad\text{or}\quad\vec{L}=\vec{\alpha}\ \text{(a constant vector)}.$$

5.4 CANONICAL TRANSFORMATIONS

As shown in the previous section, there is some advantage in using cyclic coordinates. However, in general, it is impossible to obtain more than a limited number of such coordinates by means of coordinate transformations. On the other hand, we can employ a more general class of transformations that involve both generalized coordinates and momenta. If the equations of motion are simpler in the set of new variables Q_j and P_j than in the original old set q_j and p_j, we then have a clear gain. We will not be able to consider all possible transformations but only the so-called canonical transformations that preserve the canonical form of Hamilton's equations of motion; that is, given that the q's and p's satisfy Hamilton's equations

$$\dot{q}_j=\frac{\partial H}{\partial p_j},\quad\dot{p}_j=-\frac{\partial H}{\partial q_j}$$

for some H, then the transformation

$$Q_j=Q_j(q_k,p_k,t),\quad P_j=P_j(q_k,p_k,t) \tag{5.21}$$

is canonical if and only if there exists a function K such that the time evolutions of the Q's and P's are still governed by Hamilton's equations

$$\dot{Q}_j=\frac{\partial K}{\partial P_j},\quad\dot{P}_j=-\frac{\partial K}{\partial Q_j}. \tag{5.22}$$

Here, $K(Q, P, t)$ is the new Hamiltonian that may be different from the old Hamiltonian $H(q, p, t)$.

In the old variables q_j and p_j, we can derive Hamilton's equations from the modified Hamilton's principle:

$$\delta\int_{t_1}^{t_2}\left[\sum_j p_j\dot{q}_j - H(p,q,t)\right]\mathrm{d}t = 0. \tag{5.23}$$

In the new variables Q_j and P_j, the modified Hamilton's principle

$$\delta\int_{t_1}^{t_2}\left[\sum_j P_j\dot{Q}_j - H(P,Q,t)\right]\mathrm{d}t = 0 \tag{5.24}$$

should hold. Both requirements can be satisfied if we require a relationship

$$\sum_j p_j\dot{q}_j - H = \alpha\left(\sum_j P_j\dot{Q}_j - K\right) + \frac{\mathrm{d}F}{\mathrm{d}t} \tag{5.25}$$

or

$$\sum_j p_j\mathrm{d}q_j - H\mathrm{d}t = \alpha\left(\sum_j P_j\mathrm{d}Q_j - K\mathrm{d}t\right) + \mathrm{d}F \tag{5.26}$$

where F is some function of the phase space coordinates through continuous second derivatives, and α is a constant independent of coordinates, momenta, and time, and it is related to a simple type of transformation: the scale transformation. It is always possible to select $\alpha = 1$ in Equation 5.25. We shall do so in the following discussion. The function F is termed the generating function, and it may be a function of q_j, p_j, Q_j, P_j, and t.

It is often stated in some textbooks on theoretical mechanics that because both of the variations δq_j and δQ_j vanish at the endpoints t_1 and t_2, the variation of F, δF, would also vanish at t_1 and t_2. So the total time derivative of F in Equation 5.25 will not contribute to the modified Hamilton principle. Caution should be exercised here. The vanishing of δq_j alone would not be sufficient for the vanishing of δQ_j. This follows directly by carrying out the variation in Equation 5.21:

$$\delta Q_j = \sum_k \frac{\partial Q_j}{\partial q_k}\delta q_k + \sum_k \frac{\partial Q_j}{\partial p_k}\delta p_k.$$

In order to make $\delta Q_j = 0$, the variations δq_j and δp_j must all vanish at these endpoints. This is different from the practice employed to obtain canonical equations from the modified Hamilton's principle, where q_j was varied subject to $\delta q_j(t_1) = \delta q_j(t_2) = 0$, but no such restriction was set on the variation of p_j.

Now, as $\delta q_j(t_1) = \delta p_j(t_1) = 0$ and $\delta q_j(t_2) = \delta p_j(t_2) = 0$, Equation 5.21 implies that the variations of the new variables will likewise vanish where $\delta Q_j(t_1) = \delta P_j(t_1) = 0$ and $\delta Q_j(t_2) = \delta P_j(t_2) = 0$. Thus, the total time derivative of F in Equation 5.26 will not contribute to the modified Hamilton's principle because the integral of the total time derivative is just the function evaluated at the endpoints where the variations of all the canonical variables vanish.

The function F must be some function of both the old and the new canonical variables in order for a transformation to be effected. It is obvious that we have the following four choices:

$$F_1(q, Q, t), \quad F_2(q, P, t), \quad F_3(p, Q, t), \quad \text{and} \quad F_4(p, P, t).$$

The circumstances of the problem will dictate which form is the best choice. It may be shown that F_2, F_3, and F_4 can be generated from F_1. As an example, let us consider F_1 and rewrite Equation 5.25) as

$$\sum_i (p_i\dot{q}_i - P_i\dot{Q}_i) + (K - H) = \frac{\mathrm{d}F_1}{\mathrm{d}t} \tag{5.27}$$

which becomes, by multiplying through by dt,

$$\sum_i (p_i\mathrm{d}q_i - P_i\mathrm{d}Q_i) + (K - H)\mathrm{d}t = \sum_i \left(\frac{\partial F_1}{\partial q_i}\mathrm{d}q_i + \frac{\partial F_1}{\partial Q_i}\mathrm{d}Q_i\right) + \frac{\partial F_1}{\partial t}\mathrm{d}t$$

from which it immediately follows that

$$\left.\begin{array}{c} p_i = \dfrac{\partial F_1}{\partial q_i}, \quad P_i = -\dfrac{\partial F_1}{\partial Q_i} \\ K = H + \dfrac{\partial F_1}{\partial t} \end{array}\right\}. \tag{5.28}$$

When F_1 is known, Equation 5.28 gives n relations between q, p and Q, P as well as H and K. The function F_1 thus acts as a bridge between the two sets of canonical variables and is called the "generating function" of the transformation. As an example of such a generating function, we take

$$F_1 = \sum_i q_i Q_i. \tag{5.29}$$

For this special case, Equation 5.28 gives

$$Q_i = p_i, \quad P_i = -q_i, \quad \text{and} \quad K = H \tag{5.30}$$

which shows clearly that generalized coordinates and their conjugate momenta are not distinguishable, and the nomenclature for them is arbitrary. Therefore, q and p should be treated equally, and we simply call them "canonically conjugate variables" or "canonical variables."

Earlier, we mentioned that F_2, F_3, and F_4 may be generated from F_1. Now let us consider a simple example in which the independent arguments of F are to be q_i and P_i. Then, the generating function is of the type F_2. Equation 5.28 will give us help for the transition from q, Q as independent variables to q, P because

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

This suggests that the generating function F_2 can be defined in terms of F_1 according to the relationship

$$F_2(q, P, t) = F_1(q, Q, t) + \sum_i P_i Q_i. \tag{5.31}$$

We now rewrite Equation 5.25 in terms of F_1:

$$\sum_j p_j \dot{q}_j - H = \left(\sum_j P_j \dot{Q}_j - K\right) + \frac{\mathrm{d}F_1}{\mathrm{d}t}.$$

Solving Equation 5.31 for F_1 and substituting, the last equation becomes

$$\sum_j p_j \dot{q}_j - H = \sum_j P_j \dot{Q}_j - K + \frac{\mathrm{d}}{\mathrm{d}t}\left(F_2(q,P,t) - \sum_i Q_i P_i\right)$$
$$= -\sum_i Q_i \dot{P}_i - K + \frac{\mathrm{d}}{\mathrm{d}t} F_2(q,P,t)$$

where

$$\frac{\mathrm{d}F_2}{\mathrm{d}t} = \sum_i \left(\frac{\partial F_2}{\partial q_i}\dot{q}_i + \frac{\partial F_2}{\partial P_i}\dot{P}_i\right) + \frac{\partial F_1}{\partial t}\mathrm{d}t.$$

Combining the last two equations and collecting coefficients of $\dot{q}_i$, $\dot{P}_i$ we obtain the transformation equations:

$$p_i = \frac{\partial F_2}{\partial q_i} \tag{5.32a}$$

$$Q_i = \frac{\partial F_2}{\partial P_i} \tag{5.32b}$$

$$K = H + \frac{\partial F_2}{\partial t}. \tag{5.32c}$$

As an example of such a generating function, we take

$$F_2 = \sum_i q_i P_i. \tag{5.33a}$$

For this special case, Equations 5.32a through 5.32c gives

$$p_i = \frac{\partial F_2}{\partial q_i} = P_i, \quad Q_i = \frac{\partial F_2}{\partial P_i} = q_i, \quad K = H. \tag{5.33b}$$

The new and old coordinates are the same; hence, F_2 merely generates the identity transformation from Equations 5.28 and 5.32 and observing that the difference $K - H$ is the partial derivative of the generating function F with respect to time. This is also true for the other two generating functions F_3 and F_4. Thus, if the generating function does not contain the time explicitly, then $K = H$.

We also note that time t is unchanged by the transformation and that it may be regarded as an independent parameter. Because t is not directly involved, we may consider a contemporaneous variation with dt set equal to zero. Then, Equation 5.26 with $\alpha = 1$ becomes

$$\sum_i (p_i \delta q_i - P_i \delta Q_i) = \delta F \tag{5.34}$$

which is a criterion for a canonical transformation without reference to the Hamiltonian function. Thus, it is more convenient to use Equation 5.34 in testing whether or not a given transformation is canonical. The functions Q_j and P_j from Equation 5.21 are used in expressing each P_j, Q_j in terms of the old variables. If the differential form on the left-hand side of Equation 5.34 is exact and if the functions $Q_j(q, p, t)$, $P_j(q, p, t)$ are at least twice differentiable, then the given transformation is canonical, and a function $\phi(q, p, t) = F$ exists such that

$$\delta\phi = \sum_j p_j \delta q_j - \sum_j P_j \delta Q_j$$

or equivalently

$$\left. \begin{aligned} p_j - \sum_j P_j \frac{\partial Q_j}{\partial q_j} &= \frac{\partial \phi}{\partial q_j} \\ -\sum_j P_j \frac{\partial Q_j}{\partial P_j} &= \frac{\partial \phi}{\partial P_j} \end{aligned} \right\}. \tag{5.35}$$

Upon integrating to obtain $\phi(q, p, t)$, the new Hamiltonian K is found by equating the coefficients of dt in Equation 5.26. This leads to

$$K = H + \frac{\partial \phi}{\partial t} + \sum_j P_j \frac{\partial Q_j}{\partial t}. \tag{5.36}$$

It is different in form from the expression $K = H + \partial F/\partial t$. This is because different variables are held constant in the two cases when taking partial derivatives with respect to time.

We can get a better understanding of the usefulness of canonical transformations by examining a specific problem. We choose the simple harmonic oscillator. Of course, using such a powerful method as canonical transformation is scarcely necessary for such a simple problem. But an example with familiar physics and uncomplicated algebra will help us to gain a better understanding of the procedures employed.

Example 5.4: Simple Harmonic Oscillator

Consider a linear harmonic oscillator for which we have the Hamiltonian

$$H = \frac{1}{2m} p^2 + \frac{1}{2} k q^2$$

and the Hamilton equations of motion

$$\dot{q} = \partial H/\partial p = p/m, \ \dot{p} = -\partial H/\partial q = -kq.$$

Suppose that we do not know the solution to these equations and that we wish to simplify them by a canonical transformation. For the generating function, we select a function of the type

$$F_1 = \mu\, q^2 \cot Q. \tag{5.37}$$

Then, from Equation 5.28, we find that

$$p = \partial F_1/\partial q = 2\,\mu q \cot Q, \quad P = -\partial F_1/\partial Q = \mu q^2 \operatorname{cos} ec^2\, Q.$$

Hence,

$$p=\sqrt{4\mu P}\cos Q,\quad q=\sqrt{P/\mu}\ \sin Q. \tag{5.38}$$

Now, we can evaluate the new Hamiltonian K. Because the generating function F_1 does not depend on time explicitly, we have

$$\begin{aligned} K=H&=\frac{1}{2m}p^2+\frac{1}{2}kq^2 \\ &=\frac{kP}{2\mu}\left(\sin^2 Q+\frac{4\mu^2}{mk}\cos^2 Q\right). \end{aligned}$$

If $\mu=\sqrt{mk}/2$, this reduces to

$$K=kP/2\mu=P\sqrt{k/m} \tag{5.39}$$

which is of a particularly simple form. Because the new coordinate Q is a cyclic coordinate, the new momentum P conjugated to Q is a constant of the motion:

$$\dot{P}=-\partial K/\partial Q=0$$

and

$$P=\beta \text{ (a constant of the motion)}. \tag{5.40}$$

Hamilton's equations of motion for the new coordinate Q gives

$$\dot{Q}=\partial K/\partial P=\sqrt{k/m}$$

from which we obtain

$$Q=\sqrt{k/mt}+\alpha \tag{5.41}$$

where α is the integration of the constant. The desired expression for p and q can be obtained by substituting Equations 5.40 and 5.41 into Equation 5.38.

You might wonder where we obtained the generating function F_1. Unfortunately, it is not always easy to find a generating function that leads to a convenient solution, and there is no simple standard procedure for doing so. Sometimes, the desired transformation can be found by an intuitive method or by solving Equation 5.28 that connects the generating function to the old and new Hamiltonians. However, there are two unknown functions in Equation 5.28: One of the two is F, which is needed to generate the coordinate transformation equations. The other is K, which is needed to provide the equations of motion. Thus, given K, we can work backward with Equation 5.28 until the generating function F is reached. A detailed discussion goes beyond our syllabus. Fortunately, the generating function for a linear harmonic oscillator $F_1=\mu\, q^2\cot Q$ can be constructed by the recognition that F_1 transforms oscillatory motion into uniform rectilinear motion. See Chow (1997).

It should be pointed out that, in practice, we rarely solve a dynamic problem by canonical transformations but rather study these transformations as a means of gaining a deeper understanding of the Hamiltonian formalism and of phase space.

5.5 POISSON BRACKETS

The Poisson brackets were originally introduced into the framework of theoretical mechanics in 1809 by Simeon Denis Poisson (1781–1840) in the study of planetary motion. The Poisson brackets