Chapter 5. Hamiltonian Dynamics

(Most of the material presented in this chapter is taken from Thornton and Marion, Chap. 7)

5.1 The Canonical Equations of Motion

As we saw in section 4.7.4, the generalized momentum is defined by

$$\boxed{p_j = \frac{\partial L}{\partial \dot{q}_j}}. \tag{5.1}$$

We can rewrite the Lagrange equations of motion

$$\frac{\partial L}{\partial q_j} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}_j} = 0 \tag{5.2}$$

as follow

$$\boxed{\dot{p}_j = \frac{\partial L}{\partial q_j}}. \tag{5.3}$$

We can also express our earlier equation for the Hamiltonian (i.e., equation (4.89)) using equation (5.1) as

$$H = p_j \dot{q}_j - L. \tag{5.4}$$

Equation (5.4) is expressed as a function of the generalized momenta and velocities, and the Lagrangian, which is, in turn, a function of the generalized coordinates and velocities, and possibly time. There is a certain amount of redundancy in this since the generalized momenta are obviously related to the other two variables through equation (5.1). We can, in fact, invert this equation to express the generalized velocities as

$$\dot{q}_j = \dot{q}_j\left(q_k, p_k, t\right). \tag{5.5}$$

This amounts to making a change of variables from $\left(q_j, \dot{q}_j, t\right)$ to $\left(q_j, p_j, t\right)$; we, therefore, express the Hamiltonian as

$$\boxed{H\left(q_k, p_k, t\right) = p_j \dot{q}_j - L\left(q_k, \dot{q}_k, t\right)}, \tag{5.6}$$

where it is understood that the generalized velocities are to be expressed as a function of the generalized coordinates and momenta through equation (5.5). The *Hamiltonian is, therefore, always considered a function of the* (q_k, p_k, t) *set, whereas the Lagrangian is a function of the* $(q_k, \dot{q}_k, t)$ *set:*

$$\boxed{\begin{aligned} H &= H(q_k, p_k, t) \\ L &= L(q_k, \dot{q}_k, t) \end{aligned}} \tag{5.7}$$

Let's now consider the following total differential

$$dH = \left(\frac{\partial H}{\partial q_k} dq_k + \frac{\partial H}{\partial p_k} dp_k \right) + \frac{\partial H}{\partial t} dt, \tag{5.8}$$

but from equation (5.6) we can also write

$$dH = \left(\dot{q}_k dp_k + p_k d\dot{q}_k - \frac{\partial L}{\partial q_k} dq_k - \frac{\partial L}{\partial \dot{q}_k} d\dot{q}_k \right) - \frac{\partial L}{\partial t} dt. \tag{5.9}$$

Replacing the third and fourth terms of equation (5.9) by inserting equations (5.3) and (5.1), respectively, we find

$$dH = \left(\dot{q}_k dp_k - \dot{p}_k dq_k \right) - \frac{\partial L}{\partial t} dt. \tag{5.10}$$

Equating this last expression to equation (5.8) we get the so-called **Hamilton's** or **canonical equations of motion**

$$\boxed{\begin{aligned} \dot{q}_k &= \frac{\partial H}{\partial p_k} \\ \dot{p}_k &= -\frac{\partial H}{\partial q_k} \end{aligned}} \tag{5.11}$$

and

$$\frac{\partial H}{\partial t} = -\frac{\partial L}{\partial t}. \tag{5.12}$$

Furthermore, if we insert the canonical equations of motion in equation (5.8) we find (after dividing by dt on both sides)

$$\frac{dH}{dt} = \left(\frac{\partial H}{\partial q_k} \frac{\partial H}{\partial p_k} - \frac{\partial H}{\partial p_k} \frac{\partial H}{\partial q_k} \right) + \frac{\partial H}{\partial t}, \tag{5.13}$$

or again

$$\frac{dH}{dt} = \frac{\partial H}{\partial t}. \tag{5.14}$$

Thus, the Hamiltonian is a conserved quantity if it does not explicitly contain time.

We can therefore choose to solve a given problem in two different ways: *i)* solve a set of second order differential equations with the Lagrangian method or *ii)* solve twice as many first order differential equations with the Hamiltonian formalism. It is important to note, however, that it is sometimes necessary to first find an expression for the Lagrangian and then use equation (5.6) to get the Hamiltonian when using the canonical equations to solve a given problem. It is not always possible to straightforwardly find an expression for the Hamiltonian as a function of the generalized coordinates and momenta.

Example

Use the Hamiltonian method to find the equations of motion for a spherical pendulum of mass m and length b.

Solution. The generalized coordinates are θ and ϕ. The kinetic energy is therefore

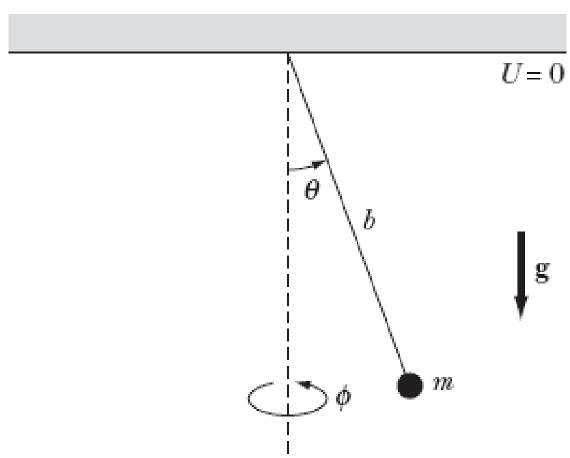

Figure 5.1 – A spherical pendulum with generalized coordinates θ and ϕ.

$$
\begin{aligned}
T &= \frac{1}{2}m\left(\dot{x}^2+\dot{y}^2+\dot{z}^2\right) \\
&= \frac{1}{2}m\left\{\left[\frac{d}{dt}\left(b\sin(\theta)\cos(\phi)\right)\right]^2+\left[\frac{d}{dt}\left(b\sin(\theta)\sin(\phi)\right)\right]^2+\left[\frac{d}{dt}\left(b\cos(\theta)\right)\right]^2\right\} \\
&= \frac{1}{2}mb^2\left\{\left[\dot{\theta}\cos(\theta)\cos(\phi)-\dot{\phi}\sin(\theta)\sin(\phi)\right]^2\right. \\
&\quad \left.+\left[\dot{\theta}\cos(\theta)\sin(\phi)+\dot{\phi}\sin(\theta)\cos(\phi)\right]^2+\left[\dot{\theta}\sin(\theta)\right]^2\right\} \\
&= \frac{1}{2}mb^2\left(\dot{\theta}^2+\dot{\phi}^2\sin^2(\theta)\right),
\end{aligned}
\tag{5.15}
$$

with the usual definition for x, y, and z. The potential energy is

$$
U = -mgb\cos(\theta). \tag{5.16}
$$

The generalized momenta are then

$$
\begin{aligned}
p_\theta &= \frac{\partial L}{\partial\dot{\theta}} = mb^2\dot{\theta} \\
p_\phi &= \frac{\partial L}{\partial\dot{\phi}} = mb^2\sin^2(\theta)\dot{\phi},
\end{aligned}
\tag{5.17}
$$

and using these two equations we can solve for $\dot{\theta}$ and $\dot{\phi}$ as a function of the generalized momenta.

Since the system is conservative and that the transformation from Cartesian to spherical coordinates does not involve time, we have

$$
\begin{aligned}
H &= T+U \\
&= \frac{1}{2}mb^2\left(\frac{p_\theta}{mb^2}\right)^2+\frac{1}{2}mb^2\sin^2(\theta)\left(\frac{p_\phi}{mb^2\sin^2(\theta)}\right)^2-mgb\cos(\theta) \\
&= \frac{p_\theta{}^2}{2mb^2}+\frac{p_\phi{}^2}{2mb^2\sin^2(\theta)}-mgb\cos(\theta).
\end{aligned}
\tag{5.18}
$$

Finally, the equations of motion are

$$\begin{aligned}
\dot{\theta} &= \frac{\partial H}{\partial p_\theta} = \frac{p_\theta}{mb^2} \\
\dot{\phi} &= \frac{\partial H}{\partial p_\phi} = \frac{p_\phi}{mb^2 \sin^2(\theta)} \\
\dot{p}_\theta &= -\frac{\partial H}{\partial \theta} = \frac{{p_\phi}^2 \cos(\theta)}{mb^2 \sin^3(\theta)} - mgb\sin(\theta) \\
\dot{p}_\phi &= -\frac{\partial H}{\partial \phi} = 0.
\end{aligned} \tag{5.19}$$

Because ϕ is cyclic (or *ignorable*), the generalized momentum p_ϕ about the symmetry axis is a constant of motion. p_ϕ is actually the component of the angular momentum along the z-axis.

5.2 The Modified Hamilton's Principle

In the preceding chapter we derived Lagrange's equation from Hamilton's Principle

$$\delta \int_{t_1}^{t_2} L\left(q_j, \dot{q}_j, t\right) dt = 0. \tag{5.20}$$

As it turns out, it is also possible to obtain the canonical equations of motions using the same variational principle. To do so, we start from equation (5.6) to express the Lagrangian as a function of the Hamiltonian

$$L\left(q_j, \dot{q}_j, t\right) = p_k \dot{q}_k - H\left(q_j, p_j, t\right). \tag{5.21}$$

Inserting equation (5.21) in (5.20) we have

$$\delta \int_{t_1}^{t_2} \left[p_k \dot{q}_k - H\left(q_j, p_j, t\right) \right] dt = 0, \tag{5.22}$$

and carrying the variation on the integrand

$$\int_{t_1}^{t_2} \left(p_k \delta \dot{q}_k + \dot{q}_k \delta p_k - \frac{\partial H}{\partial q_k} \delta q_k - \frac{\partial H}{\partial p_k} \delta p_k \right) dt = 0. \tag{5.23}$$

But since $\delta \dot{q}_k = d\left(\delta q_k\right)/dt$, we can write

$$
\begin{aligned}
\int_{t_1}^{t_2} p_k \delta \dot{q}_k dt &= \int_{t_1}^{t_2} p_k \frac{d}{dt}\left(\delta q_k\right) dt \\
&= p_k \delta q_k \Big|_{t_1}^{t_2} - \int_{t_1}^{t_2} \dot{p}_k \delta q_k dt \\
&= -\int_{t_1}^{t_2} \dot{p}_k \delta q_k dt.
\end{aligned} \tag{5.24}
$$

Using equation (5.24) into equation (5.23)

$$
\int_{t_1}^{t_2} \left[\left(\dot{q}_k - \frac{\partial H}{\partial p_k} \right) \delta p_k - \left(\dot{p}_k + \frac{\partial H}{\partial q_k} \right) \delta q_k \right] dt = 0. \tag{5.25}
$$

Since the δq_k and δp_k are independent variations, we retrieve Hamilton's (or the canonical) equations

$$
\begin{aligned}
\dot{q}_k &= \frac{\partial H}{\partial p_k} \\
\dot{p}_k &= -\frac{\partial H}{\partial q_k}.
\end{aligned} \tag{5.26}
$$

5.3 Canonical Transformations

As we saw in our previous example of the spherical pendulum, there is one case when the solution of Hamilton's equation is trivial. This happens when a given coordinate is cyclic; in that case the corresponding momentum is a constant of motion. For example, consider the case where the Hamiltonian is a constant of motion, and where all coordinates q_j are cyclic. The momenta are then constants

$$
p_j = \alpha_j, \tag{5.27}
$$

and since the Hamiltonian is not be a function of the coordinates or time, we can write

$$
H = H\left(\alpha_j\right), \tag{5.28}
$$

where $j = 1, \ldots, n$ with n the number of degrees of freedom. Applying the canonical equation (5.26) for the coordinates, we find

$$
\dot{q}_j = \frac{\partial H}{\partial \alpha_j} = \omega_j, \tag{5.29}
$$

where the ω_j's can only be a function of the momenta (i.e., the α_j's) and are, therefore, also constant. Equation (5.29) can easily be integrated to yield

$$q_j = \omega_j t + \beta_j, \tag{5.30}$$

where the β_j's are constants of integration that will be determined by the initial conditions.

It may seem that such a simple example can only happen very rarely, since usually not every generalized coordinates of a given set is cyclic. But there is, however, a lot of freedom in the selection of the generalized coordinates. Going back, for example, to the case of the spherical pendulum, we could choose the Cartesian coordinates to solve the problem, but we now know that the spherical coordinates allow us to eliminate one coordinate (i.e., ϕ) from the expression for the Hamiltonian. We can, therefore, surmise that there exists a way to optimize our choice of coordinates for maximizing the number of cyclic variables. There may even exist a choice for which all coordinates are cyclic. We now try to determine the procedure that will allow us to transform form one set of variable to another set that will be more appropriate.

In the Hamiltonian formalism the generalized momenta and coordinates are considered independent, so a general coordinate transformation from the (q_j, p_j) to, say, (Q_j, P_j) sets can be written as

$$\begin{aligned} Q_j &= Q_j(q_k, p_k, t) \\ P_j &= P_j(q_k, p_k, t). \end{aligned} \tag{5.31}$$

Since we are strictly interested in sets of coordinates that are canonical, we require that there exits some function $K(Q_k, P_k, t)$ such that

$$\begin{aligned} \dot{Q}_j &= \frac{\partial K}{\partial P_j} \\ \dot{P}_j &= -\frac{\partial K}{\partial Q_j}. \end{aligned} \tag{5.32}$$

The new function K plays the role of the Hamiltonian. It is important to note that the transformation defined by equations (5.31)-(5.32) must be independent of the problem considered. That is, the pair (Q_j, P_j) must be canonical coordinates in general, for any system considered.

We know from our study of the modified Hamilton's Principle in section 5.2 that the canonical equations resulted from the condition

$$\delta \int_{t_1}^{t_2} \left[p_k \dot{q}_k - H(q_j, p_j, t) \right] dt = 0, \tag{5.33}$$

which we can similarly write for equations (5.32)

$$\delta\int_{t_1}^{t_2}\left[P_k\dot{Q}_k - K\left(Q_j, P_j, t\right)\right]dt = 0. \tag{5.34}$$

Now consider an arbitrary function F (with a continuous second order derivative), which can be dependent on any mixture of q_j, p_j, Q_j, and P_j, and time (e.g., $F = F\left(q_j, P_j, t\right)$, or $F = F\left(Q_j, p_j, t\right)$, or $F = F\left(q_j, Q_j, t\right)$, etc.). Such a function has the following characteristic

$$\begin{aligned}\delta\int_{t_1}^{t_2}\frac{dF}{dt}dt &= \delta\int_{t_1}^{t_2}dF\,dt\\ &= \delta\left(F\Big|_{t_1}^{t_2}\right)\\ &= \delta\left[F\left(t_2\right) - F\left(t_1\right)\right]\\ &= 0.\end{aligned} \tag{5.35}$$

The last step is valid because of the fact the no variations of the generalized coordinates are allowed at the end points of the system's trajectory. The function F is called the *generating function* of the transformation.

Equations (5.33)-(5.35) imply that

$$\lambda\left[p_k\dot{q}_k - H\left(q_j, p_j, t\right)\right] = P_k\dot{Q}_k - K\left(Q_j, P_j, t\right) + \frac{dF}{dt}, \tag{5.36}$$

where λ is some constant. But since it will always be possible to scale the new variables Q_j and P_j, it is sufficient to only consider the case when $\lambda = 1$. We, therefore, rewrite equation (5.36) as

$$p_k\dot{q}_k - H\left(q_j, p_j, t\right) = P_k\dot{Q}_k - K\left(Q_j, P_j, t\right) + \frac{dF}{dt}. \tag{5.37}$$

Let's consider the case where

$$F = F\left(q_j, Q_j, t\right). \tag{5.38}$$

Equation (5.37) then takes the form

$$
\begin{aligned}
p_k \dot{q}_k - H &= P_k \dot{Q}_k - K + \frac{dF}{dt} \\
&= P_k \dot{Q}_k - K + \frac{\partial F}{\partial t} + \frac{\partial F}{\partial q_k}\dot{q}_k + \frac{\partial F}{\partial Q_k}\dot{Q}_k .
\end{aligned}
\tag{5.39}
$$

This equation will be satisfied if

$$
\begin{aligned}
p_j &= \frac{\partial F}{\partial q_j} \\
P_j &= -\frac{\partial F}{\partial Q_j} \\
K &= H + \frac{\partial F}{\partial t}.
\end{aligned}
\tag{5.40}
$$

The first of equations (5.40) represent a system of n equations that define the p_j as functions of the q_k, Q_k, and t. If these equations can be inverted, we then have established relations for the Q_j in terms of the q_k, p_k, and t, which can then be inserted in the second of equations (5.40) to find the P_j as functions of q_k, p_k, and t. Finally, the last of equations (5.40) is used to connect K with the old Hamiltonian H (where everything is expressed as functions of the Q_k, and P_k).

Example

Let's consider the problem of the simple harmonic oscillator. The Hamiltonian for this problem can be written as

$$
\begin{aligned}
H &= T + U \\
&= \frac{p^2}{2m} + \frac{kq^2}{2} \\
&= \frac{1}{2m}\left(p^2 + m^2\omega^2 q^2\right),
\end{aligned}
\tag{5.41}
$$

with $k = m\omega^2$. The form of the Hamiltonian (a sum of squares) suggests that the following transformation

$$
\begin{aligned}
p &= f(P)\cos(Q) \\
q &= \frac{f(P)}{m\omega}\sin(Q)
\end{aligned}
\tag{5.42}
$$

will render the Q cyclic. Indeed, we find that

$$
\begin{aligned}
H &= \frac{f^2(P)}{2m}\left(\cos^2(Q)+\sin^2(Q)\right) \\
&= \frac{f^2(P)}{2m},
\end{aligned} \tag{5.43}
$$

and Q is indeed cyclic. We must now find the form of the function $f(P)$ that makes the transformation canonical. Consider the generating function

$$
F = \frac{m\omega q^2}{2}\cot(Q). \tag{5.44}
$$

Using equations (5.40) we get

$$
\begin{aligned}
p &= \frac{\partial F}{\partial q} = m\omega q \cot(Q) \\
P &= -\frac{\partial F}{\partial Q} = \frac{m\omega q^2}{2\sin^2(Q)},
\end{aligned} \tag{5.45}
$$

and we can solve for q, and p using these two equations

$$
\begin{aligned}
q &= \sqrt{\frac{2P}{m\omega}}\sin(Q) \\
p &= \sqrt{2Pm\omega}\cos(Q).
\end{aligned} \tag{5.46}
$$

We can now identify $f(P)$ with the help of equations (5.42)

$$
f(P) = \sqrt{2m\omega P}. \tag{5.47}
$$

It follows that

$$
K = H = \omega P, \tag{5.48}
$$

and once again, Q is indeed cyclic. Identifying the Hamiltonian with the energy E, which is a constant, we find that the generalized momentum P is also a constant

$$
P = \frac{E}{\omega}. \tag{5.49}
$$

The equations of motion for Q is given by

$$\dot{Q} = \frac{\partial K}{\partial P} = \omega, \tag{5.50}$$

which yields

$$Q = \omega t + \alpha, \tag{5.51}$$

where α is an integration constant determined by the initial conditions. Finally, we have from equation (5.46)

$$\begin{aligned} q &= \sqrt{\frac{2E}{m\omega^2}} \sin(\omega t + \alpha) \\ p &= \sqrt{2mE} \cos(\omega t + \alpha). \end{aligned} \tag{5.52}$$

Although the solution of such a simple problem does not require the use of canonical transformations, this example shows how the Hamiltonian can be brought into of form where all generalized coordinated are cyclic.

5.4 The Poisson Bracket

5.4.1 The Poisson Bracket and Canonical Transformations

The Poisson bracket of two functions u and v with respect to the canonical variables q_j and p_j is defined as

$$\{u, v\}_{q,p} = \frac{\partial u}{\partial q_j} \frac{\partial v}{\partial p_j} - \frac{\partial u}{\partial p_j} \frac{\partial v}{\partial q_j}, \tag{5.53}$$

where a summation on the repeated index is implied. Suppose that we choose the functions u and v from the set of generalized coordinates and momenta, we then get the following relations

$$\{q_j, q_k\}_{q,p} = \{p_j, p_k\}_{q,p} = 0, \tag{5.54}$$

and

$$\{q_j, p_k\}_{q,p} = -\{p_j, q_k\}_{q,p} = \delta_{jk}, \tag{5.55}$$

where δ_{jk} is the Kronecker delta tensor. Alternatively, we could choose to express u and v as functions of a set Q_j and P_j, which are canonical transformations of the original generalized coordinates q_k and p_k, and calculate the Poisson bracket in this coordinate system. To simplify calculations, we will limit our analysis to so-called *restricted canonical transformations* where time is not involved in the coordinate transformations. That is,

$$\begin{aligned} Q_j &= Q_j\left(q_k, p_k\right) \\ P_j &= P_j\left(q_k, p_k\right), \end{aligned} \tag{5.56}$$

or, alternatively

$$\begin{aligned} q_j &= q_j\left(Q_k, P_k\right) \\ p_j &= p_j\left(Q_k, P_k\right). \end{aligned} \tag{5.57}$$

In order to carry our calculation more effectively, we will introduce a new notation. Let's construct a column vector $\boldsymbol{\eta}$, which for a system with n degrees of freedom is written as

$$\eta_j = q_j, \qquad \eta_{j+n} = p_j, \qquad j = 1, \ldots, n. \tag{5.58}$$

Similarly, another column vector involving the derivatives of the Hamiltonian relative to the component of $\boldsymbol{\eta}$ is given by

$$\left(\frac{\partial H}{\partial \boldsymbol{\eta}}\right)_j = \frac{\partial H}{\partial q_j}, \qquad \left(\frac{\partial H}{\partial \boldsymbol{\eta}}\right)_{j+n} = \frac{\partial H}{\partial p_j}, \qquad j = 1, \ldots, n. \tag{5.59}$$

Finally, we define a $2n \times 2n$ matrix $\mathbf{J}$ as

$$\mathbf{J} = \begin{bmatrix} \mathbf{0} & \mathbf{1} \\ -\mathbf{1} & \mathbf{0} \end{bmatrix}, \tag{5.60}$$

where the matrices $\mathbf{0}$ and $\mathbf{1}$ are the $n \times n$ zero and unit matrices, respectively. Using equations (5.59) and (5.60), we can write the canonical equations as

$$\dot{\boldsymbol{\eta}} = \mathbf{J}\frac{\partial H}{\partial \boldsymbol{\eta}}. \tag{5.61}$$

It can be easily verified that equation (5.53) for the Poisson bracket can also be rewritten as

$$\{u, v\}_\eta = \left(\frac{\partial u}{\partial \boldsymbol{\eta}}\right)^T \mathbf{J}\frac{\partial v}{\partial \boldsymbol{\eta}}, \tag{5.62}$$

where $\left(\partial u / \partial \boldsymbol{\eta}\right)^T$ is the transpose of $\partial u / \partial \boldsymbol{\eta}$ and, therefore, a row vector. We can also compactly write the results of equations (5.54) and (5.55) as

$$\{\boldsymbol{\eta},\boldsymbol{\eta}\}_{\eta} = \mathbf{J}. \tag{5.63}$$

Equations (5.63) are called the *fundamental Poisson brackets*.

Just as we did for the generalized coordinates q_k and p_k with equation (5.58), we introduce a new column vector $\vec{\varsigma}$ such that

$$\varsigma_j = Q_j, \qquad \varsigma_{j+n} = P_j, \qquad j = 1, \ldots, n. \tag{5.64}$$

Relations similar to equations (5.59), (5.61) and (5.62) exist for $\boldsymbol{\zeta}$ just as they do for $\boldsymbol{\eta}$. We now introduce the Jacobian matrix $\mathbf{M}$ relating the time derivatives between the two systems

$$\dot{\boldsymbol{\zeta}} = \mathbf{M}\dot{\boldsymbol{\eta}}, \tag{5.65}$$

where

$$M_{jk} = \frac{\partial \varsigma_j}{\partial \eta_k}. \tag{5.66}$$

Transformation of derivatives of the Hamiltonian can also be expressed as a function of the Jacobian matrix

$$\frac{\partial H}{\partial \eta_j} = \frac{\partial H}{\partial \varsigma_k}\frac{\partial \varsigma_k}{\partial \eta_j} = M_{kj}\frac{\partial H}{\partial \varsigma_k}, \tag{5.67}$$

or

$$\frac{\partial H}{\partial \boldsymbol{\eta}} = \mathbf{M}^T \frac{\partial H}{\partial \boldsymbol{\zeta}}. \tag{5.68}$$

Using equations (5.65), (5.61), and (5.68) we can write

$$\begin{aligned}\dot{\boldsymbol{\zeta}} &= \mathbf{M}\dot{\boldsymbol{\eta}} \\ &= \mathbf{MJ}\frac{\partial H}{\partial \boldsymbol{\eta}} \\ &= \mathbf{MJM}^T \frac{\partial H}{\partial \boldsymbol{\zeta}} \equiv \mathbf{J}\frac{\partial H}{\partial \boldsymbol{\zeta}}.\end{aligned} \tag{5.69}$$

This last result implies that

$$\mathbf{MJM}^T = \mathbf{J}. \tag{5.70}$$

We are now in a position to obtain a few important results. First, from equations (5.62), (5.66), and (5.70) we have

$$\begin{aligned} \{\boldsymbol{\zeta},\boldsymbol{\zeta}\}_\eta &= \left(\frac{\partial \boldsymbol{\zeta}}{\partial \boldsymbol{\eta}}\right)^T \mathbf{J}\frac{\partial \boldsymbol{\zeta}}{\partial \boldsymbol{\eta}} \\ &= \mathbf{M}^T\mathbf{JM} \\ &= \mathbf{J}. \end{aligned} \tag{5.71}$$

But me must also have a similar result for the fundamental Poisson bracket in the ς_j system, that is

$$\{\boldsymbol{\zeta},\boldsymbol{\zeta}\}_\varsigma = \mathbf{J}. \tag{5.72}$$

We have, therefore, the result that the *fundamental Poisson brackets are invariant under canonical transformations*. We will now show that this result also extends to any arbitrary functions u and v. We first note that

$$\frac{\partial u}{\partial \boldsymbol{\eta}} = \mathbf{M}^T \frac{\partial u}{\partial \boldsymbol{\zeta}}. \tag{5.73}$$

Inserting this equation in (5.62) we have

$$\begin{aligned} \{u,v\}_\eta &= \left(\frac{\partial u}{\partial \boldsymbol{\eta}}\right)^T \mathbf{J}\frac{\partial v}{\partial \boldsymbol{\eta}} \\ &= \left(\mathbf{M}^T\frac{\partial u}{\partial \boldsymbol{\zeta}}\right)^T \mathbf{J}\left(\mathbf{M}^T\frac{\partial v}{\partial \boldsymbol{\zeta}}\right) \\ &= \left(\frac{\partial u}{\partial \boldsymbol{\zeta}}\right)^T \mathbf{MJM}^T\frac{\partial v}{\partial \boldsymbol{\zeta}} \\ &= \left(\frac{\partial u}{\partial \boldsymbol{\zeta}}\right)^T \mathbf{J}\frac{\partial v}{\partial \boldsymbol{\zeta}}, \end{aligned} \tag{5.74}$$

and therefore

$$\{u,v\}_\eta = \{u,v\}_\varsigma \equiv \{u,v\}. \tag{5.75}$$

We thus find that *all Poisson brackets are invariant to canonical transformations*. This is the reason why we dropped any index in the last expression in equation (5.75). Just as the main characteristic of canonical transformations is that the leave the form of Hamilton's equations invariant, the canonical invariance of the Poisson brackets implies that equations expressed in term of Poisson brackets are also invariant in form to canonical transformations. It is important to note that, although we have limited our analysis to restricted canonical transformations, the results obtained here can be shown to be equally valid for coordinate transformations that explicitly involve time.

The algebraic properties of the Poisson bracket are therefore of considerable importance. Here are some important relations

$$\begin{aligned}
&\{u,u\}=0\\
&\{u,v\}=-\{v,u\}\\
&\{au+bv,w\}=a\{u,w\}+b\{v,w\}\\
&\{uv,w\}=u\{v,w\}+\{u,w\}v\\
&\{u,vw\}=v\{u,w\}+\{u,v\}w\\
&\{u,\{v,w\}\}+\{v,\{w,u\}\}+\{w,\{u,v\}\}=0.
\end{aligned} \tag{5.76}$$

The last of equations (5.76) is called *Jacobi's identity*.

It is important to note that although we restricted our analysis to canonical transformations where time was not involved, it can be shown that the results obtained apply equally well to the more general case.

5.4.2 **The Equations of Motion**

Practically the entire Hamiltonian formalism can be restated in terms of Poisson brackets. Because of their invariance to canonical transformations, the relations expressed with Poisson brackets will be independent of whichever set of generalized coordinates and momenta are used. Let's consider, for example the total time derivative of a function u

$$\begin{aligned}
\frac{du}{dt}&=\frac{\partial u}{\partial q_j}\dot{q}_j+\frac{\partial u}{\partial p_j}\dot{p}_j+\frac{\partial u}{\partial t}\\
&=\frac{\partial u}{\partial q_j}\frac{\partial H}{\partial p_j}-\frac{\partial u}{\partial p_j}\frac{\partial H}{\partial q_j}+\frac{\partial u}{\partial t},
\end{aligned} \tag{5.77}$$

or

$$\boxed{\frac{du}{dt}=\{u,H\}+\frac{\partial u}{\partial t}} \tag{5.78}$$

Equation (5.78) is indeed independent of the system of coordinates. Special cases for equation (5.78) are that of Hamilton's equations of motion

$$\dot{q}_j = \{q_j, H\}$$
$$\dot{p}_j = \{p_j, H\}. \tag{5.79}$$

Equations (5.79) can be combined into a single vector equation using the notation defined earlier

$$\dot{\boldsymbol{\eta}} = \{\boldsymbol{\eta}, H\}. \tag{5.80}$$

We can also verify that

$$\frac{dH}{dt} = \{H, H\} + \frac{\partial H}{\partial t} = \frac{\partial H}{\partial t}. \tag{5.81}$$

Finally, if a function u is a constant of motion, that is $\dot{u} = 0$, then

$$\{H, u\} = \frac{\partial u}{\partial t}, \tag{5.82}$$

and for function that are independent of time, we find that

$$\{H, u\} = 0. \tag{5.83}$$

5.4.3 **The Transition to Quantum Mechanics**

In quantum mechanics, simple functions, such as u and v, must be replaced by corresponding operators $\hat{u}$ and $\hat{v}$, so we write

$$u \to \hat{u}$$
$$v \to \hat{v}. \tag{5.84}$$

For example, if we have a quantum system that we represent by the "ket" $|\Psi\rangle$ on which we want to measure the position x of a certain particle that is part of the system, the action of the measurement of x is represented by $\hat{x}|\Psi\rangle$. In cases where $|\Psi\rangle$ is an eigenvector of the operator $\hat{x}$ (it is often useful to think of the operators and the kets as matrices and vectors, respectively), we can write

$$\hat{x}|\Psi\rangle = x|\Psi\rangle. \tag{5.85}$$

In other words, $\hat{x}$ can be thought of some measuring apparatus for x, and $|\Psi\rangle$ the physical system on which the measurement is made. Quantum mechanics also requires that for any quantity that can be measured experimentally, a so-called *observable*, corresponds a linear and hermitian operator. A hermitian operator is defined such that

$$\hat{u}^{\dagger} = \hat{u}, \tag{5.86}$$

where the $\dagger$ sign denotes the "adjoint" operation. For example, when a matrix is used to represent the operator $\hat{u}$ we get

$$\hat{u}_{jk}^{\dagger} = \hat{u}_{kj}^{*}, \tag{5.87}$$

and when the operator is hermitian we have

$$\hat{u}_{jk}^{\dagger} = \hat{u}_{kj}^{*} = \hat{u}_{jk}. \tag{5.88}$$

Hermitian operators also have the property that their eigenvalues are real. This is to be expected if they are to adequately represent experimentally measurable quantities.

There are at least two other important facts that characterize measurements in quantum mechanics:

1. The quantization of certain physical quantities is an experimental reality incompatible with classical mechanics.
2. The sequence with which successive measurements are made has consequences that will affect their results.

Although both statements are extremely important, we will now concentrate on the last and write its mathematical equivalent. For example, let's assume that we want to measure two quantities u and v on the system $|\Psi\rangle$ using their corresponding operators $\hat{u}$ and $\hat{v}$. We could do this in two different ways. That is, we can first measure u and then v, or proceed in the opposite sequence. If we denote by $|1\rangle$ and $|2\rangle$ the state of the system after the two sets of measurements, we can write

$$\begin{aligned} |1\rangle &= \hat{v}\left(\hat{u}|\Psi\rangle\right) \\ |2\rangle &= \hat{u}\left(\hat{v}|\Psi\rangle\right). \end{aligned} \tag{5.89}$$

According to statement 2 above, in quantum mechanics we have the (extremely) non-classical result that, in general,

$$|1\rangle \neq |2\rangle. \tag{5.90}$$

We can express the difference in the results obtained between the two sets of measurements as

$$\begin{aligned} |2\rangle - |1\rangle &= \left(\hat{u}\hat{v} - \hat{v}\hat{u}\right)|\Psi\rangle \\ &= \left[\hat{u},\hat{v}\right]|\Psi\rangle, \end{aligned} \tag{5.91}$$

where the quantity

$$\left[\hat{u},\hat{v}\right]=\hat{u}\hat{v}-\hat{v}\hat{u} \tag{5.92}$$

is called the *commutator* of $\hat{u}$ and $\hat{v}$. The reason for the importance of the sequence with which measurements are made in quantum mechanics lays in the fact that quantum, or microscopic, systems can be affected by the action of measurement itself. That is, a system can be changed by a measurement. Of course, this behavior is alien to classical mechanics, i.e., it does not matter what order we use to make a series of measurements on a macroscopic system.

Starting from equation (5.92) we can calculate the following properties for the commutators of different operators

$$\begin{aligned}
&\left[\hat{u},\hat{u}\right]=0\\
&\left[\hat{u},\hat{v}\right]=-\left[\hat{v},\hat{u}\right]\\
&\left[a\hat{u}+b\hat{v},\hat{w}\right]=a\left[\hat{u},\hat{w}\right]+b\left[\hat{v},\hat{w}\right]\\
&\left[\hat{u}\hat{v},\hat{w}\right]=\hat{u}\left[\hat{v},\hat{w}\right]+\left[\hat{u},\hat{w}\right]\hat{v}\\
&\left[\hat{u},\hat{v}\hat{w}\right]=\hat{v}\left[\hat{u},\hat{w}\right]+\left[\hat{u},\hat{v}\right]\hat{w}\\
&\left[\hat{u},\left[\hat{v},\hat{w}\right]\right]+\left[\hat{v},\left[\hat{w},\hat{u}\right]\right]+\left[\hat{w},\left[\hat{u},\hat{v}\right]\right]=0.
\end{aligned} \tag{5.93}$$

Comparison with equations (5.76) will show that the commutator in quantum mechanics behave just like the Poisson bracket in classical mechanics. It is, therefore, tempting to try to make the transition from classical to quantum mechanics using the Poisson bracket as our tool. That is, we will attempt to find a relationship between the Poisson bracket and the commutator. To do so, let's start by evaluating the bracket $\left\{u_1u_2,v_1v_2\right\}$. This can be done in two different ways using the fourth and fifth of equations (5.76). That is

$$\begin{aligned}
\left\{u_1u_2,v_1v_2\right\}&=u_1\left\{u_2,v_1v_2\right\}+\left\{u_1,v_1v_2\right\}u_2\\
&=u_1\left(v_1\left\{u_2,v_2\right\}+\left\{u_2,v_1\right\}v_2\right)+\left(v_1\left\{u_1,v_2\right\}+\left\{u_1,v_1\right\}v_2\right)u_2\\
&=u_1v_1\left\{u_2,v_2\right\}+u_1\left\{u_2,v_1\right\}v_2+v_1\left\{u_1,v_2\right\}u_2+\left\{u_1,v_1\right\}v_2u_2,
\end{aligned} \tag{5.94}$$

or

$$\begin{aligned}
\left\{u_1u_2,v_1v_2\right\}&=v_1\left\{u_1u_2,v_2\right\}+\left\{u_1u_2,v_1\right\}v_2\\
&=v_1\left(u_1\left\{u_2,v_2\right\}+\left\{u_1,v_2\right\}u_2\right)+\left(u_1\left\{u_2,v_1\right\}+\left\{u_1,v_1\right\}u_2\right)v_2\\
&=v_1u_1\left\{u_2,v_2\right\}+v_1\left\{u_1,v_2\right\}u_2+u_1\left\{u_2,v_1\right\}v_2+\left\{u_1,v_1\right\}u_2v_2.
\end{aligned} \tag{5.95}$$

Equating the last of equations (5.94) and (5.95) we get

$$u_1 v_1 \{u_2, v_2\} + \{u_1, v_1\} v_2 u_2 = v_1 u_1 \{u_2, v_2\} + \{u_1, v_1\} u_2 v_2, \tag{5.96}$$

or again

$$(u_1 v_1 - v_1 u_1)\{u_2, v_2\} = \{u_1, v_1\}(u_2 v_2 - v_2 u_2). \tag{5.97}$$

But since the functions u_1 and v_1 can be chosen to be completely independent from the u_2 and v_2 functions, we must have

$$\begin{aligned} (u_1 v_1 - v_1 u_1) &= g\{u_1, v_1\} \\ (u_2 v_2 - v_2 u_2) &= g\{u_2, v_2\}, \end{aligned} \tag{5.98}$$

where g is some universal constant.

Now, when making a transition from the classical to the quantum world we must come to a domain intermediate to the two, where both descriptions are valid. Therefore, because of the resemblance of the terms on the left side of equations (5.98) to commutators, we take the step of identifying these terms as such, and make the following correspondence

$$[\hat{u}, \hat{v}] \leftrightarrow g\{u, v\}, \tag{5.99}$$

for any classical functions u and v and their corresponding hermitian operators $\hat{u}$ and $\hat{v}$. We now have in equation (5.99) a relation that is both quantum and classical mechanical.

Applying the adjoint operation on both sides of equation (5.99) we get

$$\begin{aligned} [\hat{u}, \hat{v}]^\dagger &= (\hat{u}\hat{v} - \hat{v}\hat{u})^\dagger \\ &= (\hat{u}\hat{v})^\dagger - (\hat{v}\hat{u})^\dagger \\ &= \hat{v}^\dagger \hat{u}^\dagger - \hat{u}^\dagger \hat{v}^\dagger \\ &= \hat{v}\hat{u} - \hat{u}\hat{v} \\ &= -[\hat{u}, \hat{v}], \end{aligned} \tag{5.100}$$

and

$$\begin{aligned} (g\{u, v\})^\dagger &= (g\{u, v\})^* \\ &= g^*\{u, v\}^* \\ &= g^*\{u, v\} \end{aligned} \tag{5.101}$$

since the Poisson bracket is real when u and v are real. Inserting equations (5.100) and (5.101) into equation (5.99) we have

$$-[\hat{u},\hat{v}] \leftrightarrow g^*\{u,v\}. \tag{5.102}$$

The combination of equations (5.99) and (5.102) implies that the constant g must be a complex quantity. We therefore further define g as

$$g = i\hbar, \tag{5.103}$$

with $\hbar$ some new real universal constant, commonly called *Planck's constant*. We finally have from equation (5.99)

$$\{u,v\} \leftrightarrow \frac{1}{i\hbar}[\hat{u},\hat{v}]. \tag{5.104}$$

We are now in a position where we can use the classical equation for the time evolution of function v, given by equation (5.78), to obtain its quantum mechanical equivalent by making the substitution suggested in equation (5.104). That is,

$$\boxed{\frac{d\hat{u}}{dt} = \frac{1}{i\hbar}\left[\hat{u},\hat{H}\right] + \frac{\partial \hat{u}}{\partial t}} \tag{5.105}$$

with $\hat{H}$ the quantum mechanical Hamiltonian operator. Equation (5.105) is famously known for representing Heisenberg's "picture" of quantum mechanics. It is often called *Heisenberg's equation*.

The Schrödinger and Heisenberg pictures

In the Schrödinger picture of quantum mechanics the operators are often (but not always) independent of time, while the evolution of the system is contained in the ket representing it. For example, the time dependent Schrödinger equation is written as

$$i\hbar\frac{\partial}{\partial t}\left|\Psi_S(t)\right\rangle = H(t)\left|\Psi_S(t)\right\rangle, \tag{5.106}$$

where the subscript S specifies that we are dealing with the Schrödinger representation. On the other hand, in the Heisenberg picture the kets are constant in time and the evolution of the system is contained in the operators (as specified by equation (5.105)). We can certainly choose the representation of the Schrödinger ket at time t_0 for the Heisenberg ket, since t_0 is constant. That is,

$$\left|\Psi_H\right\rangle = \left|\Psi_S(t_0)\right\rangle. \tag{5.107}$$

Let's consider the operator $U(t,t_0)$ that allows the passage of the Schrödinger ket from time t_0 to time t such that

$$\left|\Psi_S(t)\right\rangle = U(t,t_0)\left|\Psi_S(t_0)\right\rangle. \tag{5.108}$$

It can also be shown that $U(t,t_0)$ is unitary, that is

$$U^\dagger(t,t_0) = U^{-1}(t,t_0), \tag{5.109}$$

or alternatively

$$U^\dagger(t,t_0)U(t,t_0) = \mathbf{1} \tag{5.110}$$

with $\mathbf{1}$ the unit operator. Inserting equation (5.108) into equation (5.106) we find that

$$i\hbar\frac{\partial}{\partial t}U(t,t_0) = H_S(t)U(t,t_0). \tag{5.111}$$

Now, given an observable operator, it is clear that the evolution of its mean value must be the same irrespective of which picture is used, and we must have

$$\left\langle\hat{u}(t)\right\rangle = \left\langle\Psi_H\left|\hat{u}_H(t)\right|\Psi_H\right\rangle = \left\langle\Psi_S(t)\left|\hat{u}_S(t)\right|\Psi_S(t)\right\rangle, \tag{5.112}$$

and therefore upon insertion of equation (5.108) into this last equation, we have

$$\begin{aligned}\left\langle\Psi_H\left|\hat{u}_H(t)\right|\Psi_H\right\rangle &= \left\langle\Psi_S(t)\left|\hat{u}_S(t)\right|\Psi_S(t)\right\rangle \\ &= \left\langle\Psi_S(t)\left|U^\dagger(t,t_0)\hat{u}_S(t)U(t,t_0)\right|\Psi_S(t)\right\rangle.\end{aligned} \tag{5.113}$$

It follows that the representation of operator $\hat{u}_H$, i.e., using Heisenberg's picture, is related to $\hat{u}_S$, the same operator in Schrödinger's representation, by the following relation

$$\hat{u}_H(t) = U^\dagger(t,t_0)\hat{u}_S(t)U(t,t_0). \tag{5.114}$$

If we now calculate the time derivative of the last equation we get

$$\begin{aligned}\frac{d\hat{u}_H}{dt} &= \left(\frac{\partial}{\partial t}U^\dagger(t,t_0)\right)\hat{u}_S U(t,t_0) + U^\dagger(t,t_0)\frac{\partial\hat{u}_S}{\partial t}U(t,t_0) \\ &\quad + U^\dagger(t,t_0)\hat{u}_S\frac{\partial U(t,t_0)}{\partial t} \\ &= -\frac{1}{i\hbar}U^\dagger(t,t_0)H_S(t)\hat{u}_S U(t,t_0) + U^\dagger(t,t_0)\frac{\partial\hat{u}_S}{\partial t}U(t,t_0) \\ &\quad + \frac{1}{i\hbar}U^\dagger(t,t_0)\hat{u}_S H_S(t)U(t,t_0),\end{aligned} \tag{5.115}$$

where we used equation (5.111) to obtain the last equation. If we now insert $U(t,t_0)U^\dagger(t,t_0)=\mathbf{1}$ between $H_S(t)$ and $\hat{u}_S$ in the first and third term on the right-hand side of the last of equations (5.115) we have

$$\begin{aligned}\frac{d\hat{u}_H}{dt} = &-\frac{1}{i\hbar}U^\dagger(t,t_0)H_S(t)U(t,t_0)U^\dagger(t,t_0)\hat{u}_S U(t,t_0)+U^\dagger(t,t_0)\frac{\partial \hat{u}_S}{\partial t}U(t,t_0)\\ &+\frac{1}{i\hbar}U^\dagger(t,t_0)\hat{u}_S U(t,t_0)U^\dagger(t,t_0)H_S(t)U(t,t_0),\end{aligned} \tag{5.116}$$

and finally upon using equation (5.114) (and a similar one for the Hamiltonian) we have

$$\begin{aligned}\frac{d\hat{u}_H}{dt} = &-\frac{1}{i\hbar}H_H(t)\hat{u}_H + U^\dagger(t,t_0)\frac{\partial \hat{u}_S}{\partial t}U(t,t_0)\\ &+\frac{1}{i\hbar}\hat{u}_H H_H(t),\end{aligned} \tag{5.117}$$

or

$$\boxed{\frac{d\hat{u}_H}{dt} = \frac{1}{i\hbar}\left[\hat{u}_H, H_H\right] + \left(\frac{\partial \hat{u}_S}{\partial t}\right)_H} \tag{5.118}$$

Comparison of equation (5.118) with equation (5.105) shows that the two pictures of quantum mechanics are equivalent if we set

$$\frac{\partial \hat{u}_H}{\partial t} \equiv \left(\frac{\partial \hat{u}_S}{\partial t}\right)_H = U^\dagger(t,t_0)\frac{\partial \hat{u}_S}{\partial t}U(t,t_0). \tag{5.119}$$

The Schrödinger and Heisenberg are equivalent representations of quantum mechanics.

5.5 The Hamilton-Jacobi Theory

Referring back to section 5.3 on canonical transformations, where

$$\begin{aligned}Q_j &= Q_j(q_k, p_k, t)\\ P_j &= P_j(q_k, p_k, t), \qquad j,k = 1, \ldots, n,\end{aligned} \tag{5.120}$$

we consider the case where the generating function F is now a function the old coordinates and the new momenta q_j, and P_j, respectively. We write

$$F = S(q_j, P_j, t) - Q_k P_k. \tag{5.121}$$

Similarly as what was done for our analysis when $F = F\left(q_j, Q_j, t\right)$, we can write for the Lagrangian

$$
\begin{aligned}
p_k \dot{q}_k - H &= P_k \dot{Q}_k - K + \frac{dF}{dt} \\
&= P_k \dot{Q}_k - K + \frac{\partial F}{\partial t} + \frac{\partial F}{\partial q_k} \dot{q}_k + \frac{\partial F}{\partial Q_k} \dot{Q}_k + \frac{\partial F}{\partial P_k} \dot{P}_k \\
&= P_k \dot{Q}_k - K + \frac{\partial S}{\partial t} + \frac{\partial S}{\partial q_k} \dot{q}_k - P_k \dot{Q}_k + \frac{\partial S}{\partial P_k} \dot{P}_k - Q_k \dot{P}_k \\
&= -Q_k \dot{P}_k - K + \frac{\partial S}{\partial t} + \frac{\partial S}{\partial q_k} \dot{q}_k + \frac{\partial S}{\partial P_k} \dot{P}_k.
\end{aligned} \tag{5.122}
$$

Equation (5.122) will be satisfied if

$$
\begin{aligned}
p_j &= \frac{\partial S}{\partial q_j} \\
Q_j &= \frac{\partial S}{\partial P_j} \\
K &= H + \frac{\partial S}{\partial t}.
\end{aligned} \tag{5.123}
$$

We now seek a transformation that ensures that both the new coordinates and momenta are constant in time. From the canonical equations we then have

$$
\begin{aligned}
\dot{Q}_j &= \frac{\partial K}{\partial P_j} = 0 \\
\dot{P}_j &= -\frac{\partial K}{\partial Q_j} = 0.
\end{aligned} \tag{5.124}
$$

Equations (5.124) will be satisfied if we simply force the transformed Hamiltonian K to be identically zero, or alternatively

$$
H\left(q_j, p_j, t\right) + \frac{\partial S}{\partial t} = 0. \tag{5.125}
$$

We can use the first of equations (5.123) to replace the old momenta p_j in equation (5.125)

$$H\left(q_j, \frac{\partial S}{\partial q_j}, t\right) + \frac{\partial S}{\partial t} = 0, \tag{5.126}$$

with $j, k = 1, \ldots, n$. Equation (5.126), know as the *Hamilton-Jacobi equation*, constitutes a partial differential equation in $(n+1)$ variables, q_j, and t, for the generating function S. The solution S is commonly called *Hamilton's principal function*.

The integration of equation (5.126) only provides the dependence on the old coordinates q_j and time; it does not appear to give information on how the new momenta P_j are contained in S. We do know, however, from equations (5.124) that they are constants. Mathematically, once equation (5.126) is solved it will yield $(n+1)$ constants of integration $\alpha_1, \ldots, \alpha_{n+1}$. But one of the constants of integration, however, is irrelevant to the solution since S itself does not appear in equation (5.126); only its partial derivatives to q_j and t are involved. Therefore, if S is a solution, so is $S + \alpha$, where α is anyone of the $(n+1)$ constants. We can then write for the solution

$$S = S\left(q_j, \alpha_j, t\right), \qquad j = 1, \ldots, n, \tag{5.127}$$

and we choose to identify the new momenta to the n (non-additive) constants, that is

$$P_j = \alpha_j. \tag{5.128}$$

An interesting corollary is that the new coordinates and momenta can now be expressed as functions of the initial conditions for the old coordinates and momenta, i.e., $q_j(t_0)$ and $p_j(t_0)$. This is because we have in the first two equations of (5.123)

$$\begin{aligned} p_j &= \frac{\partial S\left(q_k, \alpha_k, t\right)}{\partial q_j} \\ Q_j &= \frac{\partial S\left(q_k, \alpha_k, t\right)}{\partial \alpha_j} = \beta_j, \end{aligned} \tag{5.129}$$

relations that can be evaluated at time t_0. The first equation allows us to connect the constants α_k (which are, in fact, the new momenta) with the initial conditions when $t = t_0$ is set in equation (5.129), and the second equation completes the connection by defining the new coordinates in terms of the same initial conditions (through, in part, the α_k's). The new coordinates Q_j are also identified with a new set of constants β_j (see equation (5.124).

The problem can finally be solved by, first inverting the second of equations (5.129) to get

$$q_j = q_j\left(\alpha_k, \beta_k, t\right), \tag{5.130}$$

and using the first of equations (5.129) to replace q_j in the relation for p_j to get

$$p_j = p_j\left(\alpha_k, \beta_k, t\right). \tag{5.131}$$

To get a better understanding of the physical significance of Hamilton's principal function, let's calculate it total time derivative

$$\begin{aligned} \frac{dS}{dt} &= \frac{\partial S}{\partial q_j}\dot{q}_j + \frac{\partial S}{\partial \alpha_j}\dot{\alpha}_j + \frac{\partial S}{\partial t} \\ &= \frac{\partial S}{\partial q_j}\dot{q}_j + \frac{\partial S}{\partial t}, \end{aligned} \tag{5.132}$$

since the new momenta $P_j = \alpha_j$ are constants. But from the first of equations (5.123) and the fact that we set $K = 0$, we can rewrite equation (5.132) as

$$\frac{dS}{dt} = p_j\dot{q}_j - H = L. \tag{5.133}$$

Alternatively, we have

$$S = \int L\,dt + cste, \tag{5.134}$$

where the integral is now indefinite. We know that by applying Hamilton's Principle to the definite integral form of the action, we could solve a problem through Lagrange's equations of motion. We now further find that the indefinite form of the same action integral furnishes a different way to solve the same problem through the formalism presented in this section.

A simplification arises when the Hamiltonian is not a function of time. We can then write

$$H\left(q_j, p_j\right) = a, \tag{5.135}$$

where a is a constant. From equation (5.126) we can write

$$S\left(q_j, \alpha_j, t\right) = W\left(q_j, \alpha_j\right) - at, \tag{5.136}$$

and

$$H = H\left(q_j, \frac{\partial W}{\partial q_j}\right). \tag{5.137}$$

The function $W\left(q_j, \alpha_j\right)$ is called *Hamilton's characteristic function*. Its physical significance is understood from its total time derivative

$$\frac{dW}{dt} = \frac{\partial W}{\partial q_j}\dot{q}_j + \frac{\partial W}{\partial \alpha_j}\dot{\alpha}_j = \frac{\partial W}{\partial q_j}\dot{q}_j. \tag{5.138}$$

But since

$$p_j = \frac{\partial S}{\partial q_j} = \frac{\partial W}{\partial q_j}, \tag{5.139}$$

we find

$$\frac{dW}{dt} = p_j\dot{q}_j. \tag{5.140}$$

Equation (5.140) can be integrated to give

$$W = \int p_j\dot{q}_j dt = \int p_j dq_j, \tag{5.141}$$

a quantity usually called the *abbreviated action*.

Example

We go back to the one-dimensional harmonic oscillator problem. The Hamiltonian for this problem is

$$H = \frac{1}{2m}\left(p^2 + m^2\omega^2 q^2\right) \equiv E, \tag{5.142}$$

with

$$\omega = \sqrt{\frac{k}{m}}. \tag{5.143}$$

We now write the Hamlton-Jacobi equation for Hamilton's principal function S by setting $p = \partial S/\partial q$ in the Hamiltonian

$$\frac{1}{2m}\left[\left(\frac{\partial S}{\partial q}\right)^2 + m^2\omega^2 q^2\right] + \frac{\partial S}{\partial t} = 0. \tag{5.144}$$

Since the Hamiltonian is not a function of time, we can use equation (5.136) for S and write

$$\frac{1}{2m}\left[\left(\frac{\partial W}{\partial q}\right)^2 + m^2\omega^2 q^2\right] = \alpha. \tag{5.145}$$

It is clear that, in this case, the constant of integration α is to be identified with the total energy E.

Equation (5.145) can be integrated to

$$W = \sqrt{2mE}\int dq\sqrt{1 - \frac{m\omega^2 q^2}{2E}}, \tag{5.146}$$

and

$$S = \sqrt{2mE}\int dq\sqrt{1 - \frac{m\omega^2 q^2}{2E}} - Et. \tag{5.147}$$

Although we could solve equation (5.147) for S, we are mostly interested in its partial derivatives such as

$$\begin{aligned}\beta' = \frac{\partial S}{\partial \alpha} = \frac{\partial S}{\partial E} &= \sqrt{\frac{m}{2E}}\int \frac{dq}{\sqrt{1 - \frac{m\omega^2 q^2}{2E}}} - t \\ &= \frac{1}{\omega}\arcsin\left(q\sqrt{\frac{m\omega^2}{2E}}\right) - t.\end{aligned} \tag{5.148}$$

Equation (5.148) is easily inverted to give

$$q = \sqrt{\frac{2E}{m\omega^2}}\sin\left(\omega t + \beta\right), \tag{5.149}$$

where

$$\beta = \omega\beta'. \tag{5.150}$$

The momentum can be evaluated with

$$
\begin{aligned}
p = \frac{\partial S}{\partial q} = \frac{\partial W}{\partial q} &= \sqrt{2mE - m^2\omega^2 q^2} \\
&= \sqrt{2mE\left[1 - \sin^2(\omega t + \beta)\right]} \\
&= \sqrt{2mE}\cos(\omega t + \beta).
\end{aligned}
\tag{5.151}
$$

Finally, we can connect the constants E (or α) and β to the initial conditions q_0 and p_0 at $t = 0$. Therefore, setting $t = 0$ in equations (5.149) and (5.151), and rearranging them we have

$$
2mE = p_0^{\ 2} + m^2\omega^2 q_0^{\ 2}. \tag{5.152}
$$

Using the same equations, we can also easily find that

$$
\tan(\beta) = m\omega\frac{q_0}{p_0}. \tag{5.153}
$$

Thus, Hamilton's principal function is the generator of a canonical transformation to a new coordinate that measures the phase angle of the oscillation and to a new momentum identified as the energy.