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 do not assist materially in a complete solution of a system's equations of motion, but they are a great help in discussing and finding the integrals of motion. They also provide the most direct transition between theoretical mechanics and quantum mechanics (in Heisenberg's picture). Here, we shall content ourselves with the definition and some of the relevant properties of the Poisson brackets.

Given a dynamic system with a set of coordinates q_j and a set of conjugate momenta p_j, the Poisson bracket of any two dynamic variables $F(q, p, t)$ and $G(q, p, t)$, written as $[F, G]$, is defined by

$$[F,\ G] = \sum_j \left(\frac{\partial F}{\partial q_j}\frac{\partial G}{\partial p_j} - \frac{\partial F}{\partial p_j}\frac{\partial G}{\partial q_j} \right). \tag{5.42}$$

5.5.1 Fundamental Properties of Poisson Brackets

The following properties follow immediately from definition 5.42:

1. $[F, F] = 0$ (5.43a)
2. $[F, G] = -[G, F]$ (antisymmetry) (5.43b)
3. $[F, aG + bX] = [F, G] + [F, X]$ (linearity, for constants a and b) (5.43c)
4. $[F, GX] = [F, G]X + G[F, X]$ (5.43d)
5. $[F, [G, X]] + [G, [X, F]] + [X, [F, G]] = 0$. (Jacobi's identity) (5.43e)

where F, G, and X are functions of canonical variables and time. The Jacobi's identity (5.43e) states that the sum of the cyclic permutation of the double Poisson bracket of three functions is zero. Some of the applications of this equation are discussed later.

Any pair of functions for which the Poisson bracket vanishes, $[F,$ G$] = 0$, are said to commute with each other.

5.5.2 Fundamental Poisson Brackets

An important Poisson bracket is that between a generalized coordinate and its conjugate momentum:

$$[q_j,\ p_\mathrm{k}] = \sum_i \left(\frac{\partial q_j}{\partial q_i}\frac{\partial p_k}{\partial p_i} - \frac{\partial q_j}{\partial p_i}\frac{\partial p_k}{\partial q_i} \right).$$

The second term on the right-hand side vanishes, and we are left with the first term only. Now $\partial q_j/\partial q_i$ is zero unless $i = j$, in which case it is equal to unity. A similar argument holds for $\partial p_j/\partial p_i$; hence, we obtain the result

$$[q_j,\ p_k] = \delta_{jk}. \tag{5.44a}$$

Similarly,

$$[q_j, q_k] = 0 \quad [p_j, p_k] = 0. \tag{5.44b}$$

These are known as the fundamental Poisson brackets.

5.5.3 Poisson Brackets and Integrals of Motion

As mentioned earlier, the Poisson brackets do not assist materially in the complete solution of a system's equations of motion but are of great help in finding the integrals of motion. Let us take a close look at this. To this end, let us put G equal to the Hamiltonian H of the system. Then Equation 5.42 becomes, with the help of Hamilton's equations,

$$[F,\ H] = \sum_i \left(\frac{\partial F}{\partial q_i}\frac{\partial H}{\partial p_i} - \frac{\partial H}{\partial q_i}\frac{\partial F}{\partial p_i} \right) = \sum_i \left(\frac{\partial F}{\partial q_i}\dot{q}_i + \dot{p}_i \frac{\partial F}{\partial p_i} \right) = \frac{\mathrm{d}F}{\mathrm{d}t} - \frac{\partial F}{\partial t}$$

from which we have

$$\frac{\mathrm{d}F}{\mathrm{d}t} = [F,\ H] + \frac{\partial F}{\partial t}. \tag{5.45}$$

This result gives us an easy way to find the integrals of motion. From Equation 5.45, we see that the condition for the quantity F to be an integral of the motion becomes

$$\partial F/\partial t + [F, H] = 0. \tag{5.46}$$

If the integral of motion F does not explicitly depend on time, then Equation 5.46 reduces to

$$[F, H] = 0. \tag{5.47}$$

That is, when the integral of motion F does not contain t explicitly, its Poisson bracket with the Hamiltonian of the system vanishes.

Another important property of Poisson brackets is that, if F and G are two integrals of motion, then the Poisson bracket of F and G, $[F, G]$, is also an integral of motion; that is,

$$[F, G] = \text{constant} \tag{5.48}$$

during the motion. This is known as Poisson's theorem.

The proof of the Poisson theorem starts by noting that, because F and G are integrals of motion, we have

$$\frac{\mathrm{d}F}{\mathrm{d}t} = \frac{\partial F}{\partial t} + [F,\ H] = 0,$$

and

$$\frac{\mathrm{d}G}{\mathrm{d}t} = \frac{\partial G}{\partial t} + [G,\ H] = 0$$

or

$$\frac{\partial F}{\partial t} = -[F,\ H]$$

and

$$\frac{\partial G}{\partial t} = -[G,\ H]. \tag{5.49}$$

Now, from Equation 5.45, we have

$$\frac{\mathrm{d}[F,G]}{\mathrm{d}t} = \big[[F,G],H\big] + \frac{\partial [F,G]}{\partial t}$$
$$= \big[[F,G],H\big] + \left[\frac{\partial F}{\partial t}, G\right] + \left[F, \frac{\partial G}{\partial t}\right]$$

which, with the aid of Equation 5.49, becomes

$$\frac{\mathrm{d}[F,G]}{\mathrm{d}t} = \big[[F,G],H\big] - \big[[F,\ H],G\big] - \big[F,\ [G,\ H]\big]$$
$$= \big[[F,G],H\big] + \big[[H,\ F],G\big] + \big[[G,\ H],F\big] = 0.$$

In the last step, Jacobi's identity was used. Hence, we have

$$[F,\ G] = \text{constant}.$$

Example 5.5

A particle of mass m is moving in a central potential V that does not depend on velocity. Find the integrals of motion.

Solution:

The kinetic energy of the particle, in spherical coordinates, is

$$T = \frac{1}{2} m\left(\dot{r}^2 + r^2\dot{\theta}^2 + r^2 \sin^2\theta\ \dot{\phi}^2\right)$$

and its Lagrangian function is $L = T - V$. Because V does not depend on V, hence,

$$p_j = \partial L/\partial \dot{q}_j = \partial T/\partial \dot{q}_j$$

from which we obtain

$$p_r = m\dot{r}, \quad p_\theta = mr^2\dot{\theta}, \quad p_\phi = mr^2 \sin^2\theta\dot{\phi}.$$

The Hamiltonian H is

$$H = \sum_j p_j \dot{q}_j - L = \frac{1}{2m}\left(p_r^2 + \frac{p_\theta^2}{r^2} + \frac{p_\phi^2}{r^2} \sin^2\theta\right) + V.$$

Because V is central, it depends on r only, so

$$[p_\theta,\ H] = 0,$$

that is, p_θ is an integral of the motion. The following Poisson bracket also vanishes:

$$\left[p_\theta^2 + \frac{p_\phi^2}{\sin^2\theta},\ H\right] = \left[p_\theta^2 + \frac{p_\phi^2}{\sin^2\theta},\ \frac{p_r^2}{2m}\right] + \left[p_\theta^2 + \frac{p_\phi^2}{\sin^2\theta},\ \frac{1}{2mr^2}\left(p_\theta^2 + \frac{p_\phi^2}{\sin^2\theta}\right)\right]$$

$$= 0 + \frac{1}{2mr^2}\left[p_\theta^2 + \frac{p_\phi^2}{\sin^2\theta},\ p_\theta^2 + \frac{p_\phi^2}{\sin^2\theta}\right] = 0$$

which shows that the quantity $p_\theta^2 + p_\phi^2/\sin^2\theta$ is also an integral of the motion.

5.5.4 Equations of Motion in Poisson Bracket Form

If we set $G = H$ and $F = q$ in the defining Equation 5.37, we have

$$\left[q_j,\ H\right] = \sum_k \left(\frac{\partial q_j}{\partial q_k}\frac{\partial H}{\partial p_k} - \frac{\partial q_j}{\partial p_k}\frac{\partial H}{\partial q_k}\right) = \frac{\partial H}{\partial p_j} = \dot{q}_j \tag{5.50a}$$

because $\partial q_j/\partial q_k = \delta_{jk}$ and $\partial q_j/\partial p_k = 0$ for all k. Similarly, we have

$$\left[p_j, H\right] = \dot{p}_j. \tag{5.50b}$$

These are the equations of motion in Poisson bracket form. We can also obtain them from Equation 5.40 with F replaced by the canonical variables q_j and p_j, respectively. As an example, consider a charged particle moving in an electromagnetic field. The Hamiltonian of the particle has been shown to be

$$\frac{1}{2}m(p_i - eA_i)(p_i - eA_i) + e\phi$$

where we have used the result

$$p_i = mv - eA_i.$$

Now, it is easy to verify that

$$\left[x_j, H\right] = \frac{1}{m}(p_j - eA_j) = \dot{x}_j.$$

Similarly, we have

$$\left[p_j,\ H\right] = \dot{p}_j$$

in accordance with Equation 5.50.

5.5.5 Canonical Invariance of Poisson Brackets

Like Hamilton's equations of motion, Poisson brackets are canonical invariants. This means that if (q, p) and (Q, P) are two canonically conjugating sets, then

$$[F, G]_{q,p} = [F, G]_{Q,P} \tag{5.51}$$

for any pair of functions F and G, where the q, p and the Q, P are related by a canonical transformation, such as Equation 5.21. The proof is straightforward, but it is tedious. We shall not pursue it here.

It is easy to show that the fundamental Poisson brackets are canonical invariants. Suppose we make the canonical transformation from a set of variables (q, p) to a new set of (Q, P). Now, any canonical transformation preserves the form of Hamilton's equations so that Equations 5.45 to 5.51 still hold for the new variables as do Equations 5.44a and 5.44b.

The Poisson-bracket description of mechanics is preserved by a canonical transformation. Equivalently, a canonical transformation can be defined as one that preserves the Poisson-bracket description of mechanics. So the fundamental Poisson brackets provide a convenient way to decide whether a given transformation of the form Equation 5.21 is canonical. In fact, they are sufficient conditions for a canonical transformation.

Example 5.6

Show that, using the Poisson brackets, the following transformation

$$Q = \sqrt{e^{-2q} - p^2}, \quad p = \cos^{-1}(pe^q)$$

is canonical.

Solution:

It is obvious that

$$[Q, Q] = 0, \text{ and } [P, P] = 0.$$

The Poisson bracket for $[Q, P]$ is

$$[Q, P] = \frac{\partial Q}{\partial q}\frac{\partial P}{\partial p} - \frac{\partial Q}{\partial p}\frac{\partial P}{\partial q}.$$

Now,

$$\frac{\partial Q}{\partial q} = \frac{-e^{-2q}}{\sqrt{e^{-2q} - p^2}}, \quad \frac{\partial Q}{\partial p} = \frac{-p}{\sqrt{e^{-2q} - p^2}}$$

$$\frac{\partial P}{\partial q} = \frac{-p}{\sqrt{e^{-2q} - p^2}}, \quad \frac{\partial P}{\partial p} = \frac{-1}{\sqrt{e^{-2q} - p^2}}.$$

Substituting these into the expression for the Poisson bracket for $[Q, P]$, we find

$$[Q, P] = 1.$$

Thus, the transformation is canonical.

5.6 POISSON BRACKETS AND QUANTUM MECHANICS

Hamiltonian dynamics has close connections with quantum mechanics. We now briefly discuss such connections. There are two formulations of quantum mechanics. One is by Heisenberg who worked with matrices, and one is by Schrödinger who developed a differential equation. Later, Dirac unified the two seemingly different systems.

We start with Heisenberg's approach. He relied on the fact that operators represent observable dynamic quantities in quantum mechanics and that operators can be represented by matrices. Operators and matrices, in general, do not commute. This non-commutability of two operators is vital to Heisenberg's work. The commutator of two operators $\underset{\sim}{A}$ and $\underset{\sim}{B}$ that represent the dynamic variables A and B is defined as

$$\left[\underset{\sim}{A},\underset{\sim}{B}\right]=\underset{\sim}{A}\underset{\sim}{B}-\underset{\sim}{B}\underset{\sim}{A}.$$

From this definition, we can see that the commutator of two operators possesses the same properties of the Poisson brackets as indicated by Equation 5.38. Dirac was the first physicist who realized this and was inspired enough to postulate that the commutator was the quantum mechanical Poisson bracket and made the connection

$$\left[A,B\right]_{P.B.}\rightarrow\frac{1}{i\hbar}\left[\underset{\sim}{A},\underset{\sim}{B}\right]$$

where $i=\sqrt{-1}$ is necessary to ensure that observed quantities are real and the $\hbar$ ($h/2\pi$, h is the Planck constant) keeps things dimensionally correct. Accordingly, once a theoretical Poisson-bracket equation of a system is written, the quantum equation may be written down directly. Thus, from Equation 5.44, we have

$$[q_k,p_j]=i\hbar\delta_{jk},\quad [p_j,p_k]=[q_j,q_k]=0.$$

Similarly, from Equation 5.45, we can write down the quantum equation for the operator $\underset{\sim}{O}$ as

$$\frac{\mathrm{d}\underset{\sim}{O}}{\mathrm{d}t}=\frac{\partial\underset{\sim}{O}}{\partial t}+\frac{1}{i\hbar}\left[\underset{\sim}{O},\underset{\sim}{\mathrm{H}}\right].$$

This is Heisenberg's operator equation of motion. In Heisenberg's approach (known as the Heisenberg picture of quantum mechanics), all of the time dependence is put into the operators while the state vectors of a system are time independent.

In contrast to Heisenberg picture, an observable (such as position, energy, or momentum, etc. that can be measured are called observables) is represented in the Schrödinger picture by a constant operator that does not contain the time explicitly; the time dependence enters the state vector (called the wave function or the state function) through a partial differential equation, known as the Schrödinger wave equation. Schrödinger noted that geometrical optics required extension to include wave optical effects, such as diffraction, and he argued that perhaps in analogy, mechanics could also be extended. This leads to his partial differential wave equation, which is closely connected with the Hamilton–Jacobi equation. Unfortunately, it is beyond our scope to reproduce his detailed treatment. The Schrödinger picture of quantum mechanics is known as wave mechanics.

In 1948, Feynman proposed an alternative formulation, using a Lagrangian operator and the action S. Given a system at the initial state A, theoretically, only one path is important to reach state B, the path for which the action S is least. Quantum mechanically, various paths are possible, and all we can say is that there is a certain probability we shall get to state B. Feynman suggested that all possible paths must be considered, and they can be considered from the point of view of the action, and he postulated that the probability amplitude associated with a particular path was related to the action by the expression $\exp(iS/\hbar)$. The quantum mechanical amplitude is then obtained by summing over all paths. Feynman's path integral formulation was finally laid out in clear textbook fashion in 1966 (Feynman and Hibbs 1966).