6 Hamiltonian Mechanics

Following our discussion of two applications of Lagrangian mechanics—central forces and coupled oscillations—we return to further developments in the formulation of classical mechanics. We have already explored the advantages of Lagrangian mechanics in solving a variety of problems. However, a limitation of the Lagrangian approach is that the Lagrangian function itself has no direct physical interpretation.

In this chapter, we introduce Hamiltonian mechanics, which is based on a new functional, the *Hamiltonian* (H). The Hamiltonian is a function of a set of n generalized coordinates (q_i) and n generalized momenta (p_i). Interestingly, in many physical systems, the Hamiltonian $H(q_i, p_i; t)$ corresponds to the total energy of the system. The Hamiltonian formulation of mechanics serves as the foundation for the *Hamilton-Jacobi formulation*, an essential alternative approach to classical mechanics.

More importantly, the Hamiltonian framework plays a crucial role in nearly all branches of modern physics, including *quantum mechanics*, *statistical mechanics*, *particle physics*, *astrophysics*, and *accelerator physics*, among others.

6.1 Hamilton's EoM

In Lagrangian mechanics, the Lagrangian functional $L(q_i, \dot{q}_i; t)$ depends on $2n$ independent variables: the n generalized coordinates q_i and the n generalized velocities $\dot{q}_i$. For the n independent generalized coordinates, there are n second-order differential EoMs, requiring $2n$ initial conditions, typically specified at $t = 0$:

$$\{q_1(t=0), \ldots, q_n(t=0), \quad \dot{q}_1(t=0), \ldots, \dot{q}_n(t=0)\}.$$

In the Hamiltonian formalism, there are again $2n$ independent variables, but the system is governed by first-order differential EoMs. Therefore, as in Lagrangian mechanics, we still require $2n$ initial conditions to solve the problem. The choice of the $2n$ variables is as follows:

- The first n variables are the generalized coordinates $q_i = \{q_1, q_2, \ldots, q_n\}$,
- The remaining n variables are the generalized momenta $p_i = \{p_1, p_2, \ldots, p_n\}$, defined by

$$p_i = \frac{\partial L}{\partial \dot{q}_i}.$$

The set of variables (q_i, p_i) is referred to as *canonically conjugate* variables, and they define a $2n$-dimensional *phase space*.

To obtain the EoMs, consider time derivative of the Lagrangian

$$\begin{aligned}
\frac{dL}{dt} &= \sum_i \frac{\partial L}{\partial q_i}\frac{dq_i}{dt} + \sum_i \frac{\partial L}{\partial \dot{q}_i}\frac{d\dot{q}_i}{dt} + \frac{\partial L}{\partial t}, \\
&= \sum_i \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right)\frac{dq_i}{dt} + \sum_i \frac{\partial L}{\partial \dot{q}_i}\frac{d\dot{q}_i}{dt} + \frac{\partial L}{\partial t}, \\
&= \frac{d}{dt}\left(\sum_i \frac{\partial L}{\partial \dot{q}_i}\dot{q}_i\right) + \frac{\partial L}{\partial t},
\end{aligned}$$

So

$$\frac{d}{dt}\left(\sum_i \frac{\partial L}{\partial \dot{q}_i}\dot{q}_i - L\right) = -\frac{\partial L}{\partial t},$$

On the left side of the above equation, the functional within the brackets is called a Hamiltonian of a system

$$\boxed{H \equiv H(q_i, p_i, t) = \sum_i \frac{\partial L}{\partial \dot{q}_i}\dot{q}_i - L = \sum_i \dot{q}_i p_i - L(q_i, \dot{q}_i, t)}. \tag{76}$$

Note that unlike the Lagrangian, the Hamiltonian is a function of the generalized coordinates and generalized momentum. Recall that it is identical to the energy function h we discussed in chapter 2. So we have

$$\frac{dH}{dt} = -\frac{\partial L}{\partial t}\,, \tag{77}$$

If L does not depend explicitly on time then $\frac{\partial L}{\partial t} = 0$ and

$$\frac{dH}{dt} = 0\,, \quad H \text{ is conserved}$$

Since $L \equiv L(q_i, \dot{q}_i, t)$ we can write

$$\begin{aligned} dL &= \frac{\partial L}{dq_i}dq_i + \frac{\partial L}{\partial \dot{q}_i}d\dot{q}_i + \frac{\partial L}{\partial t}dt\,, \\ &= \dot{p}_i dq_i + p_i d\dot{q}_i + \frac{\partial L}{\partial t}dt\,, \text{we used EL EoM and } p_i = \frac{\partial L}{\partial \dot{q}_i} \end{aligned}$$

From the expression $H \equiv H(q_i, p_i, t) = \sum \dot{q}_i p_i - L$ we get

$$\begin{aligned} dH &= p_i d\dot{q}_i + \dot{q}_i dp_i - dL\,, \\ &= p_i d\dot{q}_i + \dot{q}_i dp_i - \left(\dot{p}_i dq_i + p_i d\dot{q}_i + \frac{\partial L}{\partial t}dt\right) \\ &= \dot{q}_i dp_i - \dot{p}_i dq_i - \frac{\partial L}{\partial t} \end{aligned} \tag{78}$$

Since $H \equiv H(q_i, p_i, t)$

$$dH = \frac{\partial H}{\partial q_i}dq_i + \frac{\partial H}{\partial p_i}dp_i + \frac{\partial H}{\partial t}\,, \tag{79}$$

Comparing the last two equation we get

$$\boxed{\begin{aligned} \dot{q}_i &= \frac{\partial H}{\partial p_i} \\ \dot{p}_i &= -\frac{\partial H}{\partial q_i} \\ \frac{\partial H}{\partial t} &= -\frac{\partial L}{\partial t} \end{aligned}} \tag{80}$$

This list of equations is called Hamilton's EoMs.

Example: A particle moving in a straight line under a potential $U(x)$. The Lagrangian is

$$L(x, \dot{x}) = T - U = \frac{1}{2}m\dot{x}^2 - U(x)\,.$$

To set up the Hamiltonian we find the generalized momentum

$$p = \frac{\partial L}{\partial \dot{x}} = m\dot{x}\,.$$

So the Hamiltonian of the system is

$$H = p\dot{x} - L = \frac{p^2}{m} - \left(\frac{p^2}{2m} - U(x)\right) = \frac{p^2}{2m} + U(x)\,.$$

Here, the first term is the kinetic energy and the second term is the potential energy. So Hamiltonian is the total energy functional. The two Hamilton's EoMs are

$$\dot{x} = \frac{\partial H}{\partial p} = \frac{p}{m}\,, \quad \dot{p} = -\frac{\partial H}{\partial x} = -\frac{dU}{dx} = F(x)\,.$$

So the first equation is the Newton's definition of momentum. The second equation gives the Newton's second law of motion.

Example: A mass m is constrained to move on a frictionless surface of a vertical cone $\rho = cz$ under uniform gravitational field. To obtain the Hamiltonian for the system, we write the Lagrangain

$$\begin{aligned} L &= \frac{1}{2}m\left[\dot{\rho}^2 + (\rho\dot{\phi})^2 + \dot{z}^2\right] - mgz\,, \\ &= \frac{1}{2}m\left[(c^2+1)\dot{z}^2 + (cz\dot{\phi})^2\right] - mgz\,. \end{aligned}$$

The generalized potential

$$p_z = \frac{\partial L}{\partial \dot{z}} = m(c^2+1)\dot{z}\,, \qquad p_\phi = \frac{\partial L}{\partial \dot{\phi}} = mc^2z^2\dot{\phi}\,.$$

Hence the Hamiltonian is

$$H = \frac{1}{2m}\left[\frac{p_z^2}{(c^2+1)} + \frac{p_\phi^2}{c^2z^2}\right] + mgz\,.$$

At first glance, it may seem that there is no distinct advantage to using the Hamiltonian formulation over the Lagrangian formulation. However, in advanced modern theories such as quantum mechanics, statistical mechanics, and particle physics, the Hamiltonian formalism offers significant benefits. In this context, we will explore the elegance of the Hamiltonian formalism in a special scenario involving ignorable coordinates.

Consider a system with two generalized coordinates, q_1 and q_2, and their corresponding conjugate momenta, p_1 and p_2. The Hamiltonian in this case is given by:

$$H = H(q_1, q_2, p_1, p_2)$$

If q_2 is ignorable (i.e., it does not explicitly appear in the Lagrangian), then its conjugate momentum p_2 is conserved and becomes a constant, say k. Thus, the Hamiltonian simplifies to:

$$H = H(q_1, p_1, k)$$

This shows that the Hamiltonian now depends only on the two variables, q_1 and p_1. Now, let's examine the same system from the Lagrangian perspective. The generalized velocities are $\dot{q}_1$ and $\dot{q}_2$. Even though q_2 is ignorable, the Lagrangian still depends on the generalized velocity corresponding to q_2, and is expressed as:

$$L = L(q_1, \dot{q}_1, \dot{q}_2)$$

Therefore, unlike the Hamiltonian, the Lagrangian depends on three variables, q_1, $\dot{q}_1$, and $\dot{q}_2$, highlighting the efficiency of the Hamiltonian formalism when dealing with ignorable coordinates.

6.2 Time dependence of H

The total time derivative of Hamiltonian $H(q_i, \dot{q}_i, t)$ is given by

$$\frac{dH}{dt} = \sum_i \left(\frac{\partial H}{\partial q_i}\dot{q}_i + \frac{\partial H}{\partial p_i}\dot{p}_i\right) + \frac{\partial H}{\partial t} = \frac{\partial H}{\partial t}\,.$$

where the terms within the square bracket vanishes due to Hamilton's EoM (80). The physical significance of the results is that unless the Hamiltonian has explicit time dependence, it is constant in time. This is the energy conservation that we obtained at the end of chapter 2.

6.3 Phase space

For a mechanical system with n degrees of freedom (dof), the Hamiltonian can be expressed in terms of $2n$ coordinates: the generalized coordinates $q_i \equiv \{q_1, q_2, \ldots, q_n\}$ and the canonical momenta $p_i \equiv \{p_1, p_2, \ldots, p_n\}$. The pair (q_i, p_i) forms a $2n$-dimensional coordinate system, referred to as the *phase space*. At any given time, a point in phase space is uniquely defined by a set of $2n$ coordinates, which fully describe the state of the system. As the system evolves over time, it traces a path, known as the *trajectory*, through this phase space. The crucial insight here is that if the initial positions and momenta of the system are known, the entire system's evolution can be determined using Hamilton's equations of motion (EoMs).

To illustrate the construction of phase space, let's consider a one-dimensional simple harmonic oscillator with coordinate x and momentum p. The Hamiltonian for the system is given by:

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 = A,$$

where A is a constant related to the system's energy.

Let's assume that the oscillation starts with the position $x = A$ and zero momentum, so the total energy of the system is:

$$E = \frac{1}{2}m\omega^2 A^2.$$

Since the total energy is conserved, we can write the energy equation as:

$$\frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 = \frac{1}{2}m\omega^2 A^2.$$

Dividing through by $\frac{1}{2}m\omega^2 A^2$ gives:

$$\frac{x^2}{A^2} + \frac{p^2}{(m\omega A)^2} = 1.$$

This equation describes an ellipse in the x-p phase space, as shown in Figure 10. The oscillator begins at $x = A$, where $p = 0$. As the oscillator moves, the restoring force drives it toward $x = 0$, increasing its momentum. When $x = 0$, the momentum reaches its maximum value of $p = -m\omega A$. The oscillator then overshoots and moves to $x = -A$, at which point the momentum is again zero. This cycle repeats indefinitely.

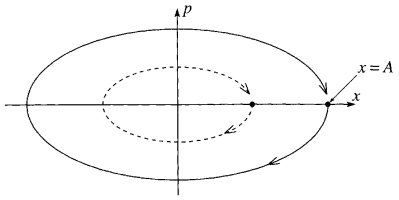

Figure 10: Phase space of a one-dimensional harmonic oscillator. The outer ellipse represents the trajectory for an oscillator starting at $x = A$, and the inner ellipse corresponds to an oscillator with initial condition $x = A/2$.

Two key points about the phase space trajectories are noteworthy:

1. The direction of time is indicated by the arrows, showing the evolution of the system in phase space.
2. Phase space trajectories never cross each other. This non-intersection occurs because each point in phase space uniquely determines the system's state, and Hamilton's equations govern the evolution of the system in a deterministic manner. Given a specific point, the system's future trajectory is uniquely determined, and it can only evolve in one direction.

6.4 Phase space density and Liouville's Theorem

In the previous example, we considered a single particle. Now, let's extend the scenario to four identical particles, each allowed to move solely under the influence of gravity. At $t = 0$, the initial conditions of the system are as follows:

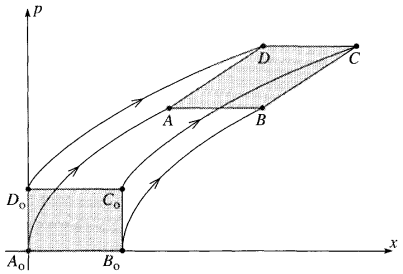

Figure 11: Phase space of four identical falling bodies.

The four initial conditions are:

- A_0: $x = 0, p = 0$ — released from rest at $x = 0$
- B_0: $x = X, p = 0$ — released from rest at $x = X$
- C_0: $x = X, p = P$ — released from X with initial momentum P
- D_0: $x = 0, p = P$ — released from rest with momentum P

The four initial points A_0, B_0, C_0, D_0 form a square in phase space, as shown in Figure 12. After some time t, the positions of the particles in phase space evolve to points A, B, C, D, respectively. These new points form a parallelogram, denoted $ABCD$.

In motion under gravity, two bodies released with the same initial velocities at the same time will maintain the same vertical distance from one another throughout the motion. Similarly, bodies released with different initial velocities will maintain the same velocity difference. As a result, the area of the parallelogram remains constant over time, which can be understood intuitively even though we will not explicitly prove it here.

Several important lessons can be drawn from this example:

1. **Deformation of Phase Space**: The four sides of the square in phase space deform into the four sides of the parallelogram as time progresses. Therefore, any point that started inside the square will end up inside the parallelogram. This illustrates how the initial distribution of particles transforms under the system's dynamics.

2. **Phase Space and Fluid-like Behavior**: If we imagine many particles (falling bodies), the initial square could be filled with numerous points, each representing a different particle. As the system evolves, the points within the square remain confined to the square's boundaries, but the shape of the square deforms over time into the parallelogram. This behavior is akin to the flow of a fluid, where the local density of points remains constant, even though the overall shape changes.

3. **Liouville's Theorem**: This scenario exemplifies the statement of *Liouville's theorem*, which asserts that in a canonical system (i.e., a system governed by Hamilton's equations of motion), the local density of points in phase space remains constant over time. Thus, the evolution of the system preserves the volume in phase space, meaning that the density of falling bodies within any region of phase space will not change as time progresses.