Part I

Fundamentals

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An Introduction to Quantum Theory

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Chapter 1

The classical state

In the first quarter of the 20th century it was discovered that the laws of motion formulated by Galileo, Newton, Lagrange, Hamilton, Maxwell, and many others were inadequate to explain a wide range of phenomena involving electrons, atoms, and light. After a great deal of effort, a new theory (together with a new law of motion) emerged in 1924. That theory is known as 'quantum mechanics', and it is now the basic framework for understanding atomic, nuclear, and subnuclear physics, as well as condensed-matter physics. The laws of motion (due to Galileo, Newton, …) which preceded quantum theory are referred to as 'classical mechanics'.

Although classical mechanics is now regarded as only an approximation to quantum mechanics, it is still true that much of the structure of the quantum theory is inherited from the classical theory that it replaced. So we begin with a lightning review of classical mechanics, whose formulation begins (but does not end!) with Newton's law $F = ma$.

1.1 Baseball, $F = ma$, and the principle of least action

Take a baseball and throw it straight up in the air. After a fraction of a second, or perhaps a few seconds, the baseball will return to your hand. Denote the height of the baseball, as a function of time, as $x(t)$. If we make a plot of x as a function of t, then the curve (we will call it a 'trajectory') in the x–t plane will, in a uniform gravitational field assuming air resistance is negligible, have the form of a parabola. There are an infinite number of possible trajectories. Which one of these the baseball actually follows is determined by the momentum of the baseball at the moment it leaves your hand.

However, if we require that the baseball returns to your hand exactly Δt seconds after leaving it, then there is only one trajectory that the ball can follow. For a baseball moving in a uniform gravitational field it is a simple exercise to determine this trajectory exactly, but we would like to develop a method which can be applied

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to a particle moving in *any* potential field $V(x)$. So let us begin with Newton's law $F = ma$, which is actually a second-order differential equation

$$m\frac{\mathrm{d}^2x}{\mathrm{d}t^2} = -\frac{\mathrm{d}V}{\mathrm{d}x} \tag{1.1}$$

It is useful to reexpress this second-order equation as a pair of first-order equations

$$\begin{aligned}\frac{\mathrm{d}x}{\mathrm{d}t} &= \frac{p}{m}\\ \frac{\mathrm{d}p}{\mathrm{d}t} &= -\frac{\mathrm{d}V}{\mathrm{d}x}\end{aligned} \tag{1.2}$$

where m is the mass and p is the momentum of the baseball. We want to find the solution of these equations such that $x(t_0) = X_{in}$ and $x(t_0 + \Delta t) = X_f$, where X_{in} and X_f are, respectively, the (initial) height of your hand when the baseball leaves it, and the (final) height of your hand when you catch the ball.[1]

With the advent of the computer, it is often easier to solve equations of motion numerically, rather than struggle to find an analytic solution which may or may not exist (particularly when the equations are non-linear). Although the object of this section is not really to develop numerical methods for solving problems in baseball, we will, for the moment, proceed as though it were. To make the problem suitable for a computer, divide the time interval Δt into N smaller time intervals of duration $\epsilon = \Delta t/N$, and denote, for $n = 0, 1, \ldots, N$,

$$\begin{aligned}&t_n \equiv t_0 + n\epsilon,\\ &x_n = x(t_n), \qquad p_n = p(t_n),\\ &x_0 = X_{in}, \qquad x_N = X_f\end{aligned}$$

An approximation to a continuous trajectory $x(t)$ is given by the set of points $\{x_n\}$ connected by straight lines, as shown in figure 1.1. We can likewise approximate derivatives by finite differences, i.e.

$$\begin{aligned}\left(\frac{\mathrm{d}x}{\mathrm{d}t}\right)_{t=t_n} &\to \frac{x(t_{n+1}) - x(t_n)}{\epsilon} = \frac{x_{n+1} - x_n}{\epsilon}\\ \left(\frac{\mathrm{d}p}{\mathrm{d}t}\right)_{t=t_n} &\to \frac{p(t_{n+1}) - p(t_n)}{\epsilon} = \frac{p_{n+1} - p_n}{\epsilon}\\ \left(\frac{\mathrm{d}^2x}{\mathrm{d}t^2}\right)_{t=t_n} &\to \frac{1}{\epsilon}\left\{\left(\frac{\mathrm{d}x}{\mathrm{d}t}\right)_{t=t_n} - \left(\frac{\mathrm{d}x}{\mathrm{d}t}\right)_{t=t_{n-1}}\right\}\\ &\to \frac{1}{\epsilon}\left\{\frac{(x_{n+1} - x_n)}{\epsilon} - \frac{(x_n - x_{n-1})}{\epsilon}\right\}\end{aligned} \tag{1.3}$$

[1] We will allow these positions to be different, in general, since you might move your hand to another position while the ball is in flight.

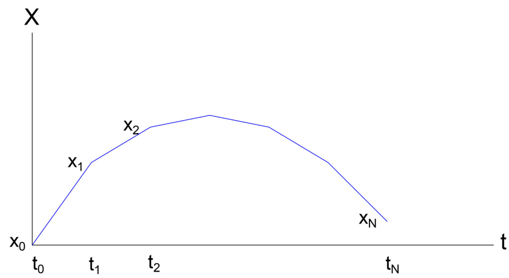

Figure 1.1. A discrete approximation to the continuous path $x(t)$.

and integrals by sums

$$\int_{t_0}^{t_0+\Delta t} \mathrm{d}t\, f(t) \to \sum_{n=0}^{N-1} \epsilon f(t_n) \tag{1.4}$$

where $f(t)$ is any function of time. As we know from elementary calculus, the right-hand side of (1.3) and (1.4) equals the left-hand side in the limit that $\epsilon \to 0$, which is also known as the ***continuum limit***.

We can now approximate the laws of motion, by replacing time derivatives in (1.2) by the corresponding finite differences, and find

$$\begin{aligned} x_{n+1} &= x_n + \left(\frac{p_n}{m}\right)\epsilon \\ p_{n+1} &= p_n - \left(\frac{\mathrm{d}V(x_n)}{\mathrm{d}x_n}\right)\epsilon \end{aligned} \tag{1.5}$$

These are iterative equations. Given position x and momentum p at time $t = t_n$, we can use (1.5) to find the position and momentum at time $t = t_{n+1}$. The finite difference approximation of course introduces a slight error; x_{n+1} and p_{n+1}, computed from x_n and p_n by (1.5) will differ from their exact values by an error of order ϵ^2. This error can be made negligible, in principle, by taking ϵ sufficiently small. It is then possible to use the computer to find an approximation to the trajectory by the 'shooting' method. The method is to make a guess for the initial momentum $p_0 = P_0$, and then use (1.2) to solve for x_1, p_1, x_2, p_2, and so on, until x_N, p_N. If $x_N \approx X_f$, then stop; the set $\{x_n\}$ is the (approximate) trajectory. If not, make a different guess $p_0 = P'_0$, and solve again for $\{x_n, p_n\}$. By trial and error, one can eventually converge on an initial choice for p_0 such that $x_N \approx X_f$. For that choice of initial momentum, the corresponding set of points $\{x_n\}$, connected by straight-line segments, gives the approximate trajectory of the baseball. This process is illustrated in figure 1.2.

Now let us return to the second-order form of Newton's laws, written in equation (1.1). Remarkably, $F = ma$ can be expressed as the condition that a certain function is stationary. Again using (1.3) to replace derivatives by finite differences, the equation $F = ma$ at each time t_n becomes

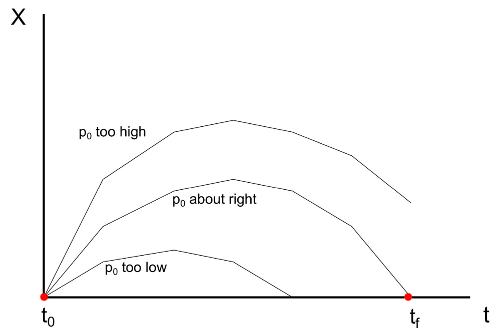

Figure 1.2. The 'shooting method' for finding a trajectory with fixed end points.

$$ma_n \equiv \frac{m}{\epsilon}\left\{\frac{x_{n+1}-x_n}{\epsilon} - \frac{x_n - x_{n-1}}{\epsilon}\right\} = -\frac{\mathrm{d}V(x_n)}{\mathrm{d}x_n} \tag{1.6}$$

The equations have to be solved for $n = 1, 2, \ldots, N-1$, with $x_0 = X_{in}$ and $x_N = X_f$ kept fixed. Now notice that equation (1.6) can be written as a total derivative

$$\frac{\mathrm{d}}{\mathrm{d}x_n}\left\{\frac{1}{2}m\frac{(x_{n+1}-x_n)^2}{\epsilon} + \frac{1}{2}m\frac{(x_n - x_{n-1})^2}{\epsilon} - \epsilon V(x_n)\right\} = 0 \tag{1.7}$$

so that $F = ma$ at some time t_n can be interpreted as a condition that the function in brackets $\{\ldots\}$ should be stationary with respect to variations in the position x_n. But what about all other times? We now introduce a very important expression, crucial in both classical and quantum physics, which is known as the ***action*** of the trajectory. The action is a function which depends on all the points $\{x_n\}$, $n = 0, 1, \ldots, N$ of the trajectory, and in this case it is

$$S[\{x_i\}] \equiv \sum_{n=0}^{N-1}\left[\frac{1}{2}m\frac{(x_{n+1}-x_n)^2}{\epsilon} - \epsilon V(x_n)\right] \tag{1.8}$$

Then Newton's law $F = ma$ can be restated as the condition that the action functional $S[\{x_i\}]$ is stationary with respect to variation of any of the x_i (except for the endpoints x_0 and x_N, which are held fixed). In other words

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}x_k}S[\{x_i\}] &= \frac{\mathrm{d}}{\mathrm{d}x_k}\sum_{n=0}^{N-1}\left[\frac{1}{2}m\frac{(x_{n+1}-x_n)^2}{\epsilon} - \epsilon V(x_n)\right]\\ &= \frac{\mathrm{d}}{\mathrm{d}x_k}\left\{\frac{1}{2}m\frac{(x_{k+1}-x_k)^2}{\epsilon} + \frac{1}{2}m\frac{(x_k - x_{k-1})^2}{\epsilon} - \epsilon V(x_k)\right\}\\ &= \epsilon\{-ma(t_k) + F(t_k)\}\\ &= 0 \qquad \text{for } k = 1, 2, \ldots, N-1\end{aligned} \tag{1.9}$$

This set of conditions is known as the ***principle of least action***. It is the principle that the action S is stationary at any trajectory $\{x_n\}$ satisfying the equations of motion $F = ma$, equation (1.6), at every time $\{t_n\}$.

1.2 Euler–Lagrange and Hamilton's equations

In brief, the Euler–Lagrange equations are the second-order form of the equations of motion (1.1), while Hamilton's equations are the first-order form (1.2). In either form, the equations of motion can be regarded as a consequence of the principle of least action. We will now re-write those equations in a very general way, which can be applied to any mechanical system, including those which are much more complicated than a baseball.

We begin by writing

$$S[\{x_i\}] = \sum_{n=0}^{N-1} \epsilon L[x_n, \dot{x}_n] \tag{1.10}$$

where

$$L[x_n, \dot{x}_n] = \frac{1}{2}m\dot{x}_n^2 - V(x_n) \tag{1.11}$$

and where

$$\dot{x}_n \equiv \frac{x_{n+1} - x_n}{\epsilon} \tag{1.12}$$

$L[x_n, \dot{x}_n]$ is known as the ***Lagrangian*** function. Then the principle of least action requires that, for each k, $1 \leqslant k \leqslant N-1$,

$$\begin{aligned} 0 = \frac{\mathrm{d}}{\mathrm{d}x_k} S[\{x_i\}] &= \sum_{n=0}^{N-1} \epsilon \frac{\mathrm{d}}{\mathrm{d}x_k} L[x_n, \dot{x}_n] \\ &= \epsilon \frac{\partial}{\partial x_k} L[x_k, \dot{x}_k] + \sum_{n=0}^{N-1} \epsilon \frac{\partial L[x_n, \dot{x}_n]}{\partial \dot{x}_n} \frac{d\dot{x}_n}{dx_k} \end{aligned} \tag{1.13}$$

and, since

$$\frac{\mathrm{d}\dot{x}_n}{\mathrm{d}x_k} = \begin{cases} \frac{1}{\epsilon} & n = k-1 \\ -\frac{1}{\epsilon} & n = k \\ 0 & \text{otherwise} \end{cases} \tag{1.14}$$

this becomes

$$\frac{\partial}{\partial x_k} L[x_k, \dot{x}_k] - \frac{1}{\epsilon}\left\{ \frac{\partial}{\partial \dot{x}_k} L[x_k, \dot{x}_k] - \frac{\partial}{\partial \dot{x}_{k-1}} L[x_{k-1}, \dot{x}_{k-1}] \right\} = 0 \tag{1.15}$$

Recalling that $x_n = x(t_n)$, this last equation can be written

$$\left(\frac{\partial L[x, \dot{x}]}{\partial x}\right)_{t=t_n} - \frac{1}{\epsilon}\left\{ \left(\frac{\partial L[x, \dot{x}]}{\partial \dot{x}}\right)_{t=t_n} - \left(\frac{\partial L[x, \dot{x}]}{\partial \dot{x}}\right)_{t=t_n-\epsilon} \right\} = 0 \tag{1.16}$$

This is the Euler–Lagrange equation for the baseball. It becomes simpler when we take the $\epsilon \to 0$ limit (the 'continuum' limit). In that limit, we have

$$\begin{aligned} \dot{x}_n &= \frac{x_{n+1} - x_n}{\epsilon} \to \dot{x}(t) = \frac{\mathrm{d}x}{\mathrm{d}t} \\ S &= \sum_{n=1}^{N-1} \epsilon L[x_n, \dot{x}_n] \to S = \int_{t_0}^{t_0+\Delta t} \mathrm{d}t \; L[x(t), \dot{x}(t)] \end{aligned} \tag{1.17}$$

where the Lagrangian function for the baseball is

$$L[x(t), \dot{x}(t)] = \frac{1}{2}m\dot{x}^2(t) - V[x(t)] \tag{1.18}$$

and the Euler–Lagrange equation, in the continuum limit, becomes

$$\frac{\partial L}{\partial x(t)} - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{x}(t)} = 0 \tag{1.19}$$

In taking partial derivatives of L with respect to x and $\dot{x}$, it is important to understand that we have to pretend that x and $\dot{x}$ are independent variables which have nothing to do with one another, despite the fact that $\dot{x}$ is really the time derivative of x. That is just the meaning of the partial derivative notation.

For the Lagrangian of the baseball, equation (1.18), the relevant partial derivatives are

$$\begin{aligned} \frac{\partial L}{\partial x(t)} &= -\frac{\mathrm{d}V[x(t)]}{\mathrm{d}x(t)} \\ \frac{\partial L}{\partial \dot{x}(t)} &= m\dot{x}(t) \end{aligned} \tag{1.20}$$

which, when substituted into equation (1.19) give

$$m\frac{\partial^2 x}{\partial t^2} + \frac{\mathrm{d}V}{\mathrm{d}x} = 0 \tag{1.21}$$

This is simply Newton's law $F = ma$, in the second-order form of equation (1.1).

We now want to rewrite the Euler–Lagrange equation in first-order form. Of course, we already know the answer, which is equation (1.2), but let us 'forget' this answer for a moment, in order to introduce a very general method. The reason the Euler–Lagrange equation is second-order in the time derivatives is that $\partial L/\partial \dot{x}$ is first-order in the time derivative. So let us define the ***momentum*** corresponding to the coordinate x to be

$$p \equiv \frac{\partial L}{\partial \dot{x}} \tag{1.22}$$

This gives p as a function of x and $\dot{x}$, but, alternatively, we can solve for $\dot{x}$ as a function of x and p, i.e.

$$\dot{x} = \dot{x}(x, p) \tag{1.23}$$

Next, we introduce the ***Hamiltonian*** function

$$H[p, x] = p\dot{x}(x, p) - L[x, \dot{x}(x, p)] \tag{1.24}$$

Since $\dot{x}$ is a function of x and p, H is also a function of x and p.

The reason for introducing the Hamiltonian is that its first derivatives with respect to x and p have a remarkable property; namely, on a trajectory satisfying the Euler–Lagrange equations, the x and p derivatives of H are proportional to the *time* derivatives of p and x. To see this, first differentiate the Hamiltonian with respect to p,

$$\begin{aligned}\frac{\partial H}{\partial p} &= \dot{x} + p\frac{\partial \dot{x}(x, p)}{\partial p} - \frac{\partial L}{\partial \dot{x}}\frac{\partial \dot{x}(p, x)}{\partial p} \\ &= \dot{x}\end{aligned} \tag{1.25}$$

where we have applied (1.22). Next, differentiating H with respect to x,

$$\begin{aligned}\frac{\partial H}{\partial x} &= p\frac{\partial \dot{x}(x, p)}{\partial x} - \frac{\partial L}{\partial x} - \frac{\partial L}{\partial \dot{x}}\frac{\partial \dot{x}(p, x)}{\partial x} \\ &= -\frac{\partial L}{\partial x}\end{aligned} \tag{1.26}$$

Using the Euler–Lagrange equation (1.19) (and this is where the equations of motion enter), we find

$$\begin{aligned}\frac{\partial H}{\partial x} &= -\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{x}} \\ &= -\frac{\mathrm{d}p}{\mathrm{d}t}\end{aligned} \tag{1.27}$$

Thus, with the help of the Hamiltonian function, we have rewritten the single second-order Euler–Lagrange equation (1.19) as a pair of first-order differential equations

$$\begin{aligned}\frac{\mathrm{d}x}{\mathrm{d}t} &= \frac{\partial H}{\partial p} \\ \frac{\mathrm{d}p}{\mathrm{d}t} &= -\frac{\partial H}{\partial x}\end{aligned} \tag{1.28}$$

which are known as ***Hamilton's equations***.

For a baseball, the Lagrangian is given by equation (1.18), and therefore the momentum is

$$p = \frac{\partial L}{\partial \dot{x}} = m\dot{x} \tag{1.29}$$

This is inverted to give

$$\dot{x} = \dot{x}(p, x) = \frac{p}{m} \tag{1.30}$$

and the Hamiltonian is

$$\begin{aligned} H &= p\dot{x}(x, p) - L[x, \dot{x}(x, p)] \\ &= p\frac{p}{m} - \left[\frac{1}{2}m\left(\frac{p}{m}\right)^2 - V(x)\right] \\ &= \frac{p^2}{2m} + V(x) \end{aligned} \tag{1.31}$$

Note that the Hamiltonian for the baseball is simply the kinetic energy plus the potential energy; i.e. the Hamiltonian is an expression for the total energy of the baseball. Substituting H into Hamilton's equations, one finds

$$\begin{aligned} \frac{\mathrm{d}x}{\mathrm{d}t} &= \frac{\partial}{\partial p}\left[\frac{p^2}{2m} + V(x)\right] = \frac{p}{m} \\ \frac{\mathrm{d}p}{\mathrm{d}t} &= -\frac{\partial}{\partial x}\left[\frac{p^2}{2m} + V(x)\right] = -\frac{\mathrm{d}V}{\mathrm{d}x} \end{aligned} \tag{1.32}$$

which is simply the first-order form of Newton's law (1.2).

1.3 Classical mechanics in a nutshell

All the machinery of the least action principle, the Lagrangian function, and Hamilton's equations, is overkill in the case of a baseball. In that case, we knew the equation of motion from the beginning. But for more involved dynamical systems, involving, say, wheels, springs, levers, and pendulums, all coupled together in some complicated way, the equations of motion are often far from obvious, and what is needed is some systematic way to derive them.

For any mechanical system, the ***generalized coordinates*** $\{q^i\}$ are a set of variables needed to describe the configuration of the system at a given time. These could be a set of Cartesian coordinates of a number of different particles, or the angular displacement of a pendulum, or the displacement of a spring from equilibrium, or all of the above. The dynamics of the system, in terms of these coordinates, is given by a Lagrangian function L, which depends on the generalized coordinates $\{q^i\}$ and their first time derivatives $\{\dot{q}^i\}$. Normally, in non-relativistic mechanics, we first specify

1. **The Lagrangian**

$$L\left[\left\{q^i, \dot{q}^i\right\}\right] = \text{Kinetic Energy} - \text{Potential Energy} \tag{1.33}$$

One then defines

2. **The action**

$$S = \int \mathrm{d}t\ L\left[\left\{q^i, \dot{q}^i\right\}\right] \tag{1.34}$$

From the least action principle, following a method similar to the one we used for the baseball, we derive

3. **The Euler–Lagrange equations**

$$\frac{\partial L}{\partial q^i} - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{q}^i} = 0 \tag{1.35}$$

These are the second-order equations of motion. To go to the first-order form, first define

4. **The generalized momenta**

$$p_i \equiv \frac{\partial L}{\partial \dot{q}^i} \tag{1.36}$$

which can be inverted to give the time derivatives $\dot{q}^i$ of the generalized coordinates in terms of the generalized coordinates and momenta

$$\dot{q}^i = \dot{q}^i\left[\left\{q^n, p_n\right\}\right] \tag{1.37}$$

Viewing $\dot{q}$ as a function of p and q, one then defines

5. **The Hamiltonian**

$$H\left[\left\{q^i, p_i\right\}\right] \equiv \sum_n p_n \dot{q}^n - L\left[\left\{q^i, \dot{q}^i\right\}\right] \tag{1.38}$$

Usually the Hamiltonian has the form

$$H[p, q] = \text{Kinetic Energy} + \text{Potential Energy} \tag{1.39}$$

Finally, the equations of motion in first-order form are given by

6. **Hamilton's equations**

$$\begin{aligned} \dot{q}^i &= \frac{\partial H}{\partial p_i} \\ \dot{p}_i &= -\frac{\partial H}{\partial q^i} \end{aligned} \tag{1.40}$$

If the potential energy does not depend explicitly on time, then Hamilton's equations imply that H is time-independent,

$$\begin{aligned} \frac{\mathrm{d}H}{\mathrm{d}t} &= \sum_i \left\{\frac{\partial H}{\partial q^i}\frac{\partial q^i}{\partial t} + \frac{\partial H}{\partial p_i}\frac{\partial p_i}{\partial t}\right\} \\ &= \sum_i \left\{-\frac{\partial p_i}{\partial t}\frac{\partial q^i}{\partial t} + \frac{\partial q^i}{\partial t}\frac{\partial p_i}{\partial t}\right\} \\ &= 0 \end{aligned} \tag{1.41}$$

as we would expect if H is the total energy of the system.

Example: the plane pendulum
Our pendulum is a mass m at the end of a weightless rigid rod of length l, which pivots in a plane around the point P. The 'generalized coordinate', which specifies the position of the pendulum at any given time, is the angle θ between the rod and the vertical axis.

1. The Lagrangian

$$L = \frac{1}{2}ml^2\dot{\theta}^2 - (V_0 - mgl\cos(\theta)) \tag{1.42}$$

   where V_0 is the gravitational potential at the height of point P, which the pendulum reaches at $\theta = \pi/2$. Since V_0 is arbitrary, we will just set it to $V_0 = 0$.
2. The action

$$S = \int_{t_0}^{t_1} \mathrm{d}t \left[\frac{1}{2}ml^2\dot{\theta}^2 + mgl\cos(\theta)\right] \tag{1.43}$$

3. The Euler–Lagrange equations
   We have

$$\begin{aligned}\frac{\partial L}{\partial \theta} &= - mgl\sin\theta \\ \frac{\partial L}{\partial \dot{\theta}} &= ml^2\dot{\theta}\end{aligned} \tag{1.44}$$

   and therefore

$$ml^2\ddot{\theta} + mgl\sin\theta = 0 \tag{1.45}$$

   is the Euler–Lagrange form of the equations of motion.
4. The generalized momentum

$$p = \frac{\partial L}{\partial \dot{\theta}} = ml^2\dot{\theta} \tag{1.46}$$

5. The Hamiltonian
   Insert

$$\dot{\theta} = \frac{p}{ml^2} \tag{1.47}$$

   into

$$H = p\dot{\theta} - \left[\frac{1}{2}ml^2\dot{\theta}^2 + mgl\cos(\theta)\right] \tag{1.48}$$

to obtain

$$H = \frac{1}{2}\frac{p^2}{ml^2} - mgl\cos(\theta) \tag{1.49}$$

6. Hamilton's equations

$$\begin{aligned} \dot{\theta} &= \frac{\partial H}{\partial p} = \frac{p}{ml^2} \\ \dot{p} &= -\frac{\partial H}{\partial \theta} = -mgl\sin\theta \end{aligned} \tag{1.50}$$

which are easily seen to be equivalent to the Euler–Lagrange equations.

1.4 The classical state

Prediction is rather important in physics, since the only reliable test of a scientific theory is the ability, given the state of affairs at present, to predict the future.

Stated rather abstractly, the process of prediction works as follows. By a slight disturbance known as a ***measurement***, an object is assigned a mathematical representation which we will call its ***physical state***. The laws of motion are mathematical rules by which, given a physical state at a particular time, one can deduce the physical state of the object at some later time. The later physical state is the prediction, which can be checked by a subsequent measurement of the object.

From the discussion so far, it is easy to see that what is meant in classical physics by the 'physical state' of a system is simply its set of generalized coordinates *and* the generalized momenta $\{q^a, p_a\}$. These are supposed to be obtained, at some time t_0, by the measurement process. Given the physical state at some time t, the state at $t + \epsilon$ is obtained by the rule

$$\begin{aligned} q^a(t+\epsilon) &= q^a(t) + \epsilon\left(\frac{\partial H}{\partial p_a}\right)_t \\ p_a(t+\epsilon) &= p_a(t) - \epsilon\left(\frac{\partial H}{\partial q^a}\right)_t \end{aligned} \tag{1.51}$$

In this way, the physical state at any later time can be obtained (in principle) to an arbitrary degree of accuracy, by making the time-step ϵ sufficiently small (or else, if possible, by solving the equations of motion exactly). Note that the coordinates $\{q^a\}$ alone are *not* enough to specify the physical state, because they are not sufficient to predict the future. Information about the momenta $\{p_a\}$ is also required.

The space of all possible $\{q^a, p_a\}$ is known as ***phase space***. For a single particle moving in three dimensions, there are three components of position and three components of momentum, so the 'physical state' is specified by six numbers (x, y, z, p_x, p_y, p_z), which can be viewed as a point in six-dimensional phase space. Likewise, the physical state of a system of N particles consists of three coordinates for each particle ($3N$ coordinates in all), and three components of momentum for each particle ($3N$ momentum components in all), so the state is given by a set of $6N$ numbers, which can be viewed as a single point in $6N$-dimensional space.

As we will see in the next chapters, classical mechanics fails to predict correctly the behavior of both light and matter at the atomic level, and is replaced by quantum mechanics. But classical and quantum mechanics have a lot in common: they both assign physical states to objects, and these physical states evolve according to differential equations which are first order in the time derivatives. The difference lies mainly in the contrast between a physical state as understood by classical mechanics, the 'classical state', and its quantum counterpart, the 'quantum state'. This difference will be explored in the next few chapters.

Problems

1. Two point-like particles moving in three dimensions have masses m_1 and m_2 respectively, and interact via a potential $V(\mathbf{x}_1 - \mathbf{x}_2)$. Find Hamilton's equations of motion for the particles.
2. Suppose, instead of a rigid rod, the mass of the plane pendulum is connected to point P by a weightless spring. The potential energy of the spring is $\frac{1}{2}k(L - L_0)^2$, where L is the length of the spring, and L_0 is its length when not displaced by an external force. Choosing L and θ as the generalized coordinates, find Hamilton's equations.