# Supplementary Notes on General Physics

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## Chapter 1

## **Essential Mathematics**

## 1.1 Derivatives

The derivative of a continuous function f(x) is usually written as f'(x) or df/dx. From its definition

$$f'(x) \equiv \lim_{\Delta x \to 0} \frac{f(x + \Delta x) - f(x)}{\Delta x},$$
(1.1)

it is clear that f'(x) is the slope of the tangent line of the curve y = f(x) at x, and it represents the rate of change of f(x) at x. For instance, if D(t) is the distance of a particle from the origin at time t, then D'(t) is the instantaneous velocity of the particle at time t. If V(x) is the potential energy of a particle at position x, then -V'(x) is the force experienced by the particle at position x.

The operation of deriving f'(x) from f(x) is called differentiation. From the definition in Eq. (1.1) it is clear that differentiation is a linear operation. Namely, if h(x) = af(x) + bg(x), where a and b are two constants, then h'(x) = af'(x) + bg'(x).

Let us see what is the derivative of a polynomial. Because differentiation is a linear operation, it is sufficient to consider the derivative of  $x^n$ .

$$(x^n)' = \lim_{\Delta x \to 0} \frac{(x + \Delta x)^n - x^n}{\Delta x}$$

$$= \lim_{\Delta x \to 0} (C_1^n x^{n-1} + C_2^n x^{n-2} \Delta x + \dots + C_{n-1}^n x \Delta x^{n-2} + C_n^n \Delta x^{n-1})$$
  
=  $n x^{n-1}$ . (1.2)

If h(x) = f(x)g(x), then

$$h'(x) = \lim_{\Delta x \to 0} \frac{f(x + \Delta x)g(x + \Delta x) - f(x)g(x)}{\Delta x}$$
  

$$= \lim_{\Delta x \to 0} \frac{f(x + \Delta x)g(x + \Delta x) - f(x)g(x + \Delta x)}{\Delta x}$$
  

$$+ \lim_{\Delta x \to 0} \frac{f(x)g(x + \Delta x) - f(x)g(x)}{\Delta x}$$
  

$$= f'(x)g(x) + g'(x)f(x).$$
(1.3)

This is known as the **multiplication rule** of differentiation. Let g(x) = 1/f(x), then h'(x) = 0. By the multiplication rule we have

$$f'(x)g(x) + g'(x)f(x) = 0.$$
 (1.4)

Namely

$$g'(x) = -\frac{f'(x)}{f(x)^2}.$$
(1.5)

From this formula, we obtain  $(x^{-n})' = -nx^{-n-1}$ .

If h(x) is the composition function of f(x) and g(x), namely h(x) = f[g(x)], then

$$h'(x) = \lim_{\Delta x \to 0} \frac{f[g(x + \Delta x)] - f[g(x)]}{\Delta x}$$
  
= 
$$\lim_{\Delta x \to 0} \frac{f[g(x + \Delta x)] - f[g(x)]}{g(x + \Delta x) - g(x)} \times \frac{g(x + \Delta x) - g(x)}{\Delta x}$$
  
= 
$$f'[g(x)]g'(x).$$
 (1.6)

This is known as the **chain rule** of differentiation. As an example, we have  $[f(x)^n]' = nf(x)^{n-1}f'(x)$ . If f(x) and  $f^{-1}(x)$  are inverse functions of each other, namely  $f[f^{-1}(x)] = x$ , we have

$$1 = f'[f^{-1}(x)](f^{-1})'(x),$$

namely,

$$(f^{-1})'(x) = \frac{1}{f'[f^{-1}(x)]}.$$
(1.7)

#### 1.1. DERIVATIVES

Now we are ready to extend the derivative of  $x^k$  from an integer k to a rational number k. Let k = 1/q where q is an integer, then  $(x^{1/q})^q = x$ . Differentiating both sides, by the chain rule we have

$$1 = q(x^{\frac{1}{q}})^{q-1}(x^{\frac{1}{q}})'.$$
 (1.8)

In other words,

$$(x^{\frac{1}{q}})' = \frac{1}{q} x^{\frac{1}{q}-1}.$$
(1.9)

Now let k = p/q, where p and q are integers. By the chain rule we have

$$(x^{\frac{p}{q}})' = \left[ (x^p)^{\frac{1}{q}} \right]' = \frac{1}{q} (x^p)^{\frac{1}{q} - 1} p \, x^{p-1} = \left( \frac{p}{q} \right) x^{\left( \frac{p}{q} \right) - 1}.$$
(1.10)

Finally let us consider the derivative of  $x^r$  when r is a real number. Before doing that, we must note that the definition of  $x^r$  is not as trivial as  $x^{p/q}$ when p and q are integer. The expression  $x^{p/q}$  is defined by the number  $\alpha$  that satisfies  $\alpha^q = x^p$ . But what do we mean by  $x^r$  when r cannot be expressed as p/q? It turns out that one must use a sequence of rational numbers  $k_1 = p_1/q_1, k_2 = p_2/q_2, k_3 = p_3/q_3, \cdots$  that approaches r to define  $x^r$ . In other words

$$x^r \equiv \lim_{k_n \to r} x^{k_n}.$$
 (1.11)

With this definition we have

$$(x^{r})' = \lim_{\Delta x \to 0} \frac{\lim_{k_n \to r} (x + \Delta x)^{k_n} - \lim_{k_n \to r} x^{k_n}}{\Delta x}$$
$$= \lim_{\Delta x \to 0} \lim_{k_n \to r} \frac{(x + \Delta x)^{k_n} - x^{k_n}}{\Delta x}$$
$$= \lim_{k_n \to r} k_n x^{k_n - 1} = r x^{r-1}.$$
(1.12)

Note that we have swapped the order of the two limiting process  $\Delta x \to 0$ and  $k_n \to r$ . This is not always safe because in some special cases they may lead to two different values. However, how to do it rigorously is beyond the scope of this lecture.

Now we turn our attention to transcendental functions. Consider the derivative of  $a^x$ , where a is a real number.

$$(a^x)' = \lim_{\Delta x \to 0} \frac{a^{x + \Delta x} - a^x}{\Delta x} = a^x \lim_{\Delta x \to 0} \frac{a^{\Delta x} - 1}{\Delta x}.$$
 (1.13)

#### CHAPTER 1. ESSENTIAL MATHEMATICS

Assuming the limit in Eq. (1.13) exists, let

$$b = \lim_{\Delta x \to 0} \frac{a^{\Delta x} - 1}{\Delta x}.$$
 (1.14)

We may rewrite the limit as

$$b = \lim_{n \to \infty} \frac{a^{\frac{1}{n}} - 1}{\frac{1}{n}},$$
(1.15)

which means for an arbitrarily small  $\epsilon$  there exists an M such that for any n>M we have

$$b - \epsilon \le \frac{a^{\frac{1}{n}} - 1}{\frac{1}{n}} \le b + \epsilon, \tag{1.16}$$

or equivalently

$$\left(1 + \frac{b - \epsilon}{n}\right)^n \le a \le \left(1 + \frac{b + \epsilon}{n}\right)^n.$$
(1.17)

Note that

$$\left(1 + \frac{b+\epsilon}{n}\right)^n - \left(1 + \frac{b-\epsilon}{n}\right)^n$$
$$= 2\epsilon \left[\frac{1}{n}\sum_{k=0}^{n-1} \left(1 + \frac{b+\epsilon}{n}\right)^k \left(1 + \frac{b-\epsilon}{n}\right)^{n-1-k}\right].$$
(1.18)

Since we can make  $\epsilon$  arbitrarily small by choosing a sufficiently large n, and while doing so the term in the square bracket remains finite, it can be seen from Eqs. (1.17) and (1.18) that

$$a = \lim_{n \to \infty} \left( 1 + \frac{b}{n} \right)^n.$$
(1.19)

Let us consider the special case of b = 1. In this case  $(a^x)' = a^x$  and we have

$$\alpha_n = \sum_{k=0}^n C_k^n \left(\frac{1}{n}\right)^k.$$
(1.20)

Consider another sequence of numbers  $s_n$  defined by

$$s_n = \sum_{k=0}^n \frac{1}{k!}.$$
 (1.21)

#### 1.1. Derivatives

Since

$$C_k^n \left(\frac{1}{n}\right)^k = \frac{n(n-1)(n-2)\dots(n-k+1)}{k!n^k} \le \frac{1}{k!},$$
 (1.22)

we have  $\alpha_n \leq s_n$ . Consider yet another sequence of numbers  $r_m(n)$  (m < n) defined by

$$r_{m}(n) = \sum_{k=0}^{m} C_{k}^{n} \left(\frac{1}{n}\right)^{k}$$
  
=  $1 + 1 + \frac{(n-1)}{2n} + \frac{(n-1)(n-2)}{6n^{2}} \dots$   
+  $\frac{(n-1)(n-2)\dots(n-m+1)}{m!n^{m-1}}.$  (1.23)

Since  $r_m(n)$  contains only the first *m* terms of  $\alpha_n$  and every term in  $\alpha_n$  is positive, we have  $r_m(n) \leq \alpha_n \leq s_n$ . Taking the limit of  $n \to \infty$  we obtain

$$s_m = \lim_{n \to \infty} r_m(n) \le \lim_{n \to \infty} \alpha_n \le \lim_{n \to \infty} s_n.$$
(1.24)

In other words, for any m we have

$$s_m \le a \le \lim_{n \to \infty} s_n. \tag{1.25}$$

Therefore

$$a = \lim_{n \to \infty} s_n = \sum_{k=0}^{\infty} \frac{1}{k!} \approx 2.718282 .$$
 (1.26)

This is a special number which makes  $(a^x)' = a^x$ , therefore it is the natural choice for the base of the exponential function in calculus. It deserves to be represented by a special symbol, hence from now on we use e to represent this number.

$$e = \lim_{n \to \infty} \left( 1 + \frac{1}{n} \right)^n = \sum_{k=0}^{\infty} \frac{1}{k!} \approx 2.718282 .$$
 (1.27)

Now we can go back to Eq. (1.13) and write

$$(e^x)' = e^x. (1.28)$$

Let us define the inverse function of  $e^x$  to be  $\ln x \equiv \log_e x$ . Eq. (1.13) can be written as

$$(a^{x})' = \left[ \left( e^{\ln a} \right)^{x} \right]' = \left( e^{x \ln a} \right)' = (\ln a) e^{x \ln a} = (\ln a) a^{x}.$$
(1.29)



Fig. 1.1: The radius of the arc is 1, and the angle of span is x. The area enclosed in the small triangle is  $\sin x/2$ , in the arc is x/2, and in the large triangle is  $\tan x/2$ .

From Eqs. (1.7) and (1.28),

$$\ln'(x) = \frac{1}{e^{\ln x}} = \frac{1}{x} . \tag{1.30}$$

To derive the derivative of  $\sin x$  and  $\cos x$ , we note that for small x,  $\sin x \le x \le \tan x$  as shown in Fig. 1.1. Therefore

$$1 \le \lim_{x \to 0} \frac{x}{\sin x} \le \lim_{x \to 0} \frac{1}{\cos x} = 1,$$
(1.31)

hence

$$\lim_{x \to 0} \frac{\sin x}{x} = 1.$$
(1.32)

We will also need the following limit.

$$\lim_{x \to 0} \frac{1 - \cos x}{x} = 0. \tag{1.33}$$

To prove Eq. (1.33), let us note

$$\frac{1 - \cos x}{x} = \frac{1 - \cos^2 x}{x(1 + \cos x)} = \frac{\sin^2 x}{x(1 + \cos x)}.$$
 (1.34)

Since

$$\lim_{x \to 0} \frac{\sin x}{x} = 1,$$
 (1.35)

$$\lim_{x \to 0} \frac{\sin x}{1 + \cos x} = 0, \tag{1.36}$$

we have Eq. (1.33). With Eqs. (1.32) and (1.33), we can derive

$$\sin' x = \lim_{\Delta x \to 0} \frac{\sin x \cos(\Delta x) + \cos x \sin(\Delta x) - \sin x}{\Delta x}$$
  
=  $\cos x.$  (1.37)  
$$\cos' x = \lim_{\Delta x \to 0} \frac{\cos x \cos(\Delta x) - \sin x \sin(\Delta x) - \cos x}{\Delta x}$$
  
=  $-\sin x.$  (1.38)

## 1.2 Integration

Consider a continuous function f(x) defined in [a, b]. Let us divide [a, b]into n intervals  $[x_i, x_{i+1}]$ , where  $i = 1, 2, \dots, n$ ,  $x_1 = a$ ,  $x_{n+1} = b$ , and  $x_{i+1} - x_i = \Delta x = (b-a)/n$ . In each interval we select an arbitrary sample point  $\bar{x}_i \in (x_i, x_{i+1})$ . Integration of a function f(x) from a to b is defined by

$$\int_{a}^{b} f(x) dx \equiv \lim_{\Delta x \to 0} \sum_{i=1}^{n} f(\bar{x}_{i}) \Delta x.$$
(1.39)

It is known as the **Riemann sum** of f(x) over the interval [a, b], which represents the area under the curve y = f(x) between x = a and x = b as shown in Fig. 1.2. To have a well-defined Riemann sum, it is important that the limit in Eq. (1.39) does not depend on the choice of  $\bar{x}_i$ . To prove that, let us first consider the following function defined in [a, b].

$$g(x) = f(x) - \frac{f(b) - f(a)}{b - a}(x - a) - f(a).$$
(1.40)

Since g(a) = g(b) = 0, there is some real number  $c \in [a, b]$  such that g(c) is maximum or minimum, hence g'(c) = 0. Then we have

$$f'(c) = \frac{f(b) - f(a)}{b - a}.$$
(1.41)

For a different choice  $\bar{x}'_i$  in Eq. (1.39), we have

$$\lim_{\Delta x \to 0} \sum_{i=1}^{n} \left[ f(\bar{x}_i) - f(\bar{x}'_i) \right] \Delta x \leq \lim_{\Delta x \to 0} \sum_{i=1}^{n} \left| f(\bar{x}_i) - f(\bar{x}'_i) \right| \Delta x$$
$$= \lim_{\Delta x \to 0} \sum_{i=1}^{n} \left| f'(c_i) \right| (\Delta x)^2$$
$$\leq \lim_{\Delta x \to 0} \sum_{i=1}^{n} M(\Delta x)^2$$
$$= \lim_{\Delta x \to 0} M(b-a)\Delta x = 0, \qquad (1.42)$$

where  $c_i$  is some number in between  $\bar{x}_i$  and  $\bar{x}'_i$ , and M is the maximum value of |f'(x)| in [a, b]. Now consider the integration

$$I(y) = \int_{y_0}^{y} f(x) \, dx, \qquad (1.43)$$

where  $y_0 < y$  is an arbitrary starting point. The derivative of I(y) is

$$I'(y) = \lim_{\Delta y \to 0} \frac{\int_{y_0}^{y + \Delta y} f(x) \, dx - \int_{y_0}^y f(x) \, dx}{\Delta y}$$
$$= \lim_{\Delta y \to 0} \frac{\int_y^{y + \Delta y} f(x) \, dx}{\Delta y} = f(y).$$
(1.44)

This is known as the **fundamental theorem of calculus.** Hence if I'(x) = f(x), we have

$$\int_{a}^{b} f(x) \, dx = \int_{y_0}^{b} f(x) \, dx - \int_{y_0}^{a} f(x) \, dx = I(b) - I(a). \tag{1.45}$$

Note that the condition I'(x) = f(x) does not determine I(x) completely. An arbitrary constant can be added to I(x) without changing I'(x). We must know the value of I(x) for at least one x to determine the constant c. In Eq. (1.43) the definition itself requires that  $I(y_0) = 0$ . Therefore if we redefine I(x) by the equation I'(x) = f(x) instead of Eq. (1.43), we may write

$$I(y) = \int^{y} f(x) \, dx + c, \qquad (1.46)$$

where  $\int^y f(x) dx$  represents any function whose derivative is f(x) and c is to be determined by the value of I(x) at some x.

**Example 1.1.** To demonstrate the usefulness of the fundamental theorem of calculus, let us calculate the volume V of a pyramid shown in Fig. 1.3. We can cut the pyramid into n slices in the direction parallel to the base plane of the pyramid. At a distance  $z_i$  from the tip of the pyramid, the area of the *i*th slice is  $L^2 z_i^2/h^2$ , where L is the side-length of the base and h is the height of the pyramid. The sum of the volume of all the slices can be written as

$$V = \sum_{i}^{n} \frac{L^2 z_i^2}{h^2} \Delta z.$$
 (1.47)

In the limit of  $\Delta z \to 0$ ,

$$V = \int_0^h \frac{L^2}{h^2} z^2 \, dz. \tag{1.48}$$



Fig. 1.2: The area under f(x) between a and b is equal to the Riemann sum of f(x) over the interval [a, b].

Let us define V(y) by

$$V(y) = \int_{y_0}^{y} \frac{L^2}{h^2} z^2 \, dz. \tag{1.49}$$

If we know what V(y) is, then V in Eq. (1.48) is simply equal to V(h) - V(0). According to the fundamental theorem of calculus,  $V'(y) = L^2 y^2/h^2$ . From  $(x^n)' = nx^{n-1}$ , we can easily see  $V(y) = L^2 y^3/(3h^2) + c$ , where c is an arbitrary constant. Since V(0) = 0, we have c = 0. Thus the volume of the pyramid is  $V(h) = hL^2/3$ .

From the view point of analytical calculation, in most cases integration is much more difficult than differentiation. Given f(x), there is no general rules to find an I(x) such that I'(x) = f(x). And what is worse, among the infinite varieties of f(x) there are only finite classes for which analytical expressions of I(x) can be found. In what follows, we shall illustrate three commonly used methods that may help to change an integral into a more familiar form.

The first method is known as integration by substitution. Consider

$$I(y) = \int_{a}^{b} f(x) \, dx.$$
 (1.50)

If we change the integration variable by x = q(s), then

$$I(y) = \int_{g^{-1}(a)}^{g^{-1}(b)} f[g(s)]g'(s) \, ds.$$
(1.51)



Fig. 1.3: A pyramid and a thin slice parallel to the base plane. The volume of the pyramid is equal to the sum of the volume of all the infinitesimally thin slices.

For some substitutions, f[g(s)]g'(s) is easier to integrate than f(x).

Example 1.2. It is not obvious how to integrate

$$I(y) = \int_0^y \frac{1}{x^2 + 1} \, dx. \tag{1.52}$$

By substituting  $x = \tan \theta$  and  $dx = \sec^2 \theta \, d\theta$ , the integration can be reduced to

$$I(y) = \int_0^{\tan^{-1} y} d\theta = \tan^{-1} y.$$
 (1.53)

#### Example 1.3.

$$I = \int_0^1 \sqrt{1 - x^2} \, dx. \tag{1.54}$$

By substituting  $x = \sin \theta$  and  $dx = \cos \theta \, d\theta$ , the integration can be reduced to

$$I = \int_0^{\pi/2} \cos^2 \theta \ d\theta = \int_0^{\pi/2} \frac{1 + \cos(2\theta)}{2} \ d\theta = \frac{\pi}{4}.$$
 (1.55)

Because the equation for a circle of unit radius in the first quadrant is  $y(x) = \sqrt{1 - x^2}$ , Eq. (1.54) represents the area of a circle in the first quadrant, as shown in Fig. 1.4. Hence the area of a full circle of unit radius is  $\pi$ .



Fig. 1.4: The part of a circle in the first quadrant. Its area is equal to the sum of the area of all the infinitesimally thin strips.

**Example 1.4.** Consider the arc length of a parabolic described by  $y = x^2/2$ . The line element is

$$ds = \sqrt{dx^2 + dy^2} = \sqrt{1 + \left(\frac{dy}{dx}\right)^2} \, dx = \sqrt{1 + x^2} \, dx \tag{1.56}$$

Hence the arc length from x = 0 to x = a is

$$s(a) = \int_0^a \sqrt{1 + x^2} \, dx. \tag{1.57}$$

Define

$$\sinh x \equiv \frac{e^x - e^{-x}}{2},$$
$$\cosh x \equiv \frac{e^x + e^{-x}}{2}.$$
(1.58)

We have

$$1 + \sinh^{2} x = \cosh^{2} x$$
$$\frac{d}{dx} \sinh x = \cosh x,$$
$$\frac{d}{dx} \cosh x = \sinh x.$$
(1.59)

Let  $x = \sinh u$ . The integration becomes

$$s(a) = \int_0^{\sinh^{-1} a} \cosh^2 u \, du = \int_0^{\sinh^{-1} a} \frac{\cosh 2u + 1}{2} \, du$$

$$= \left(\frac{\sinh 2u}{4} + \frac{1}{2}u\right)\Big|_{0}^{\sinh^{-1}a}$$
  
=  $\frac{1}{2}\left[a\sqrt{a^{2}+1} + \ln\left(a + \sqrt{a^{2}+1}\right)\right].$  (1.60)

Example 1.5.

$$I(y) = \int_0^y \frac{1}{\cos x} \, dx.$$
 (1.61)

By substituting  $u = \tan(x/2)$ , we have

$$\cos x = \frac{1 - u^2}{1 + u^2},$$
  

$$\sin x = \frac{2u}{1 + u^2},$$
  

$$dx = \frac{2}{1 + u^2} du.$$
(1.62)

This is a well-known substitution to reduce rational expressions of trigonometry functions to rational functions. Hence we have

$$I(y) = \int_{0}^{y} \frac{1}{\cos x} dx = \int_{0}^{\tan(y/2)} \frac{2}{1-u^{2}} du$$
  

$$= \int_{0}^{\tan(y/2)} \left(\frac{1}{1+u} + \frac{1}{1-u}\right) du$$
  

$$= \ln\left(\frac{1+u}{1-u}\right)\Big|_{0}^{\tan(y/2)}$$
  

$$= \ln\left(\frac{1+u^{2}}{1-u^{2}} + \frac{2u}{1-u^{2}}\right)\Big|_{0}^{\tan(y/2)}$$
  

$$= \ln(\sec y + \tan y).$$
(1.63)

The second method is known as **integration by parts.** It is based on the identity [u(x)v(x)]' = u(x)v'(x) + v(x)u'(x) which implies

$$\int_{a}^{b} u(x)v'(x) dx = \int_{a}^{b} [u(x)v(x)]' dx - \int_{a}^{b} v(x)u'(x) dx$$
$$= u(b)v(b) - u(a)v(a) - \int_{a}^{b} v(x)u'(x) dx. \quad (1.64)$$

The technique is useful when v(x)u'(x) is easier to integrate than u(x)v'(x).

#### 1.2. INTEGRATION

Example 1.6. Consider

$$I = \int_0^{\pi/2} x \cos x \, dx. \tag{1.65}$$

Let  $v(x) = \sin x$  and u(x) = x, then the integral can be reduced to

$$I = \frac{\pi}{2}\sin\frac{\pi}{2} - \int_0^{\pi/2}\sin x \, dx. \tag{1.66}$$

Example 1.7.

$$I(y) = \int_{1}^{y} \ln x \, dx.$$
 (1.67)

Let v(x) = x and  $u(x) = \ln x$ , then the integral can be reduced to

$$I(y) = y \ln y - \int_{1}^{y} dx = y \ln y - y + 1.$$
 (1.68)

Example 1.8.

$$I(y) = \int_0^y \tan^{-1} x \, dx. \tag{1.69}$$

Let v(x) = x and  $u(x) = \tan^{-1} x$ , then integration by parts leads to

$$I(y) = y \tan^{-1} y - \int_0^y \frac{x}{1+x^2} \, dx.$$
 (1.70)

Substituting  $s = x^2 + 1$  and ds = 2xdx,

$$I(y) = y \tan^{-1} y - \int_{1}^{y^{2}+1} \frac{1}{2s} \, ds = y \tan^{-1} y - \frac{1}{2} \ln(y^{2}+1). \tag{1.71}$$

The third method, known as **integration by partial fractions**, can be used for the integration of rational functions. Consider the integration of a rational function

$$\int f(x) \, dx = \int \frac{p(x)}{q(x)} \, dx, \qquad (1.72)$$

where p(x) and q(x) are polynomials of x. If the order of p(x) is larger than or equal to that of q(x), we may reduce the integration to

$$\int f(x) dx = \int h(x) dx + \int \frac{r(x)}{q(x)} dx, \qquad (1.73)$$

#### CHAPTER 1. ESSENTIAL MATHEMATICS

where h(x) is a polynomial and the order of r(x) is smaller than that of q(x). Since we already know how to integrate h(x), we shall consider only the case in which the order of p(x) is smaller than that of q(x). Let us assume the order of q(x) is n and the n roots of q(x) are  $r_i$  (i = 1, 2, ..., n), then we may express f(x) as

$$\frac{p(x)}{q(x)} = \sum_{i=1}^{n} \frac{a_i}{x - r_i},$$
(1.74)

where  $a_i$  (i = 1, 2, ..., n) are *n* constants. The reason we can always do that is because the order of p(x) is at most n - 1, hence we have

$$p(x) = \sum_{i=0}^{n-1} c_i x^i, \qquad (1.75)$$

where  $c_i$  (i = 0, 2, ..., n - 1) are *n* constants. For any set of  $c_i$  we may solve Eq. (1.74) to find the corresponding set of  $a_i$ . A unique solution exists because the number of  $c_i$  is the same as that of  $a_i$ . Once we have done the decomposition in Eq. (1.74), the integration of f(x) becomes trivial.

Finally, we note that some useful integrals in physics are difficult to evaluate directly, but can be evaluated by introducing another dimension, as shown in the following examples.

Example 1.9. To evaluate

$$I(\alpha) = \int_{-\infty}^{\infty} e^{-\alpha x^2} dx, \qquad (1.76)$$

one may evaluate the following integral first.

$$I^{2}(1) = \int_{-\infty}^{\infty} e^{-x^{2}} dx \int_{-\infty}^{\infty} e^{-y^{2}} dy = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-(x^{2}+y^{2})} dx dy.$$
(1.77)

By changing variables to the polar coordinates, we have

$$I^{2}(1) = \int_{0}^{\infty} \int_{0}^{2\pi} e^{-r^{2}} r dr d\theta = -\pi \left. e^{-r^{2}} \right|_{0}^{\infty} = \pi.$$
(1.78)

Therefore

$$I(1) = \int_{-\infty}^{\infty} e^{-x^2} dx = \sqrt{\pi}.$$
 (1.79)

Changing variable from x to  $\sqrt{\alpha}x$ , we obtain

$$I(\alpha) = \int_{-\infty}^{\infty} e^{-\alpha x^2} dx = \sqrt{\frac{\pi}{\alpha}}.$$
 (1.80)

#### 1.2. INTEGRATION

Example 1.10. To evaluate

$$I_{2n}(\alpha) = \int_{-\infty}^{\infty} x^{2n} e^{-\alpha x^2} dx,$$
 (1.81)

one may differentiate Eq. (1.80) with respect to  $\alpha$  n times.

$$I_{2}(\alpha) = -\frac{d}{d\alpha} \int_{-\infty}^{\infty} e^{-\alpha x^{2}} dx = \frac{1}{2} \alpha^{-\frac{3}{2}} \sqrt{\pi}, \qquad (1.82)$$

$$I_4(\alpha) = \left(-\frac{d}{d\alpha}\right)^2 \int_{-\infty}^{\infty} e^{-\alpha x^2} dx = \frac{1}{2} \frac{3}{2} \alpha^{-\frac{5}{2}} \sqrt{\pi},$$
 (1.83)

$$I_{2n}(\alpha) = \left(-\frac{d}{d\alpha}\right)^n \int_{-\infty}^{\infty} e^{-\alpha x^2} dx = \frac{(2n)!}{n! 2^{2n}} \alpha^{-\frac{2n+1}{2}} \sqrt{\pi}.$$
 (1.84)

Example 1.11.

$$I = \int_0^\infty \frac{\sin x}{x} dx. \tag{1.85}$$

To get rid of the x in the denominator which makes the integration difficult, we may evaluate the following function first.

÷

$$g(y;\epsilon) = \int_{\epsilon}^{\infty} \frac{e^{-xy} \sin x}{x} dx,$$
(1.86)

where  $\epsilon$  is a positive constant much smaller than 1. Differentiate with respect to y, we have

$$g'(y;\epsilon) = -\int_{\epsilon}^{\infty} e^{-xy} \sin x \, dx = -\int_{\epsilon}^{\infty} \frac{e^{-xy+ix} - e^{-xy-ix}}{2i} dx$$
  
=  $\frac{i}{2} \left[ \frac{-e^{\epsilon(i-y)}}{i-y} + \frac{-e^{-\epsilon(i+y)}}{i+y} \right].$  (1.87)

Expanding  $e^{\epsilon(i-y)}$  and  $e^{-\epsilon(i+y)}$  to the second order of  $\epsilon$ , we have

$$g'(y;\epsilon) \approx -\frac{1}{1+y^2} + \frac{\epsilon^2}{2}.$$
 (1.88)

From Eq. (1.53) we have

$$g(y;\epsilon) \approx -\tan^{-1}y + \frac{\epsilon^2}{2}y + c.$$
(1.89)

Because Eq. (1.89) is valid for any  $\epsilon$  as long as it is sufficiently small, for a sufficiently large y we have

$$g(y; 1/y) \approx -\tan^{-1} y + \frac{1}{2y} + c.$$
 (1.90)

Let  $y \to \infty$ , the left-hand side of Eq. (1.90) approaches zero, therefore  $c = \pi/2$ . Now let y be a small number and remember again that Eq. (1.89) is valid for any  $\epsilon$  as long as it is sufficiently small, we have

$$g(y;y) \approx -\tan^{-1}y + \frac{y^3}{2} + \frac{\pi}{2}.$$
 (1.91)

Let  $y \to 0$ , we have

$$\int_0^\infty \frac{\sin x}{x} dx = \frac{\pi}{2}.$$
(1.92)

#### **1.3** Taylor Expansion

Consider a continuous function f(x) in the neighborhood of a fixed point a. If f(x) is a polynomial, we have

$$f(x) = f(a) + \sum_{k=1}^{n} c_k (x-a)^k,$$
(1.93)

where  $c_k$  is the coefficients. Differentiating both sides by m times and substituting in x = a, we have

$$f^{(m)}(a) = c_m m!, (1.94)$$

therefore  $c_m = f^{(m)}(a)/m!$ . If f(x) is a not a polynomial, intuitively we can use a polynomial to approximate it. The more complex f(x) is, the higher-order polynomial is needed. Hence we can write

$$f(x) \approx f(a) + \sum_{k=1}^{n} \frac{f^{(k)}(a)}{k!} (x-a)^{k}.$$
 (1.95)

#### 1.3. TAYLOR EXPANSION

This is known as the **Taylor expansion** of f(x) around a.

In Taylor expansion, in principle n can approach infinity. But in practice at which n should we truncate the series? To answer this question we need to know how good the approximation is. Let us rewrite the Taylor expansion as

$$f(x) = f(a) + \sum_{k=1}^{n} \frac{f^{(k)}(a)}{k!} (x-a)^{k} + R_{n}(x,a), \qquad (1.96)$$

where  $R_n(x, a)$  is the *n*th remainder. Now we shall estimate how large  $|R_n(x, a)|$  can be. In the following Taylor expansion, consider *b* to be fixed and the point of expansion *a* to be variable.

$$f(b) = f(a) + \sum_{k=1}^{n} \frac{f^{(k)}(a)}{k!} (b-a)^{k} + R_{n}(b,a).$$
(1.97)

Differentiating Eq. (1.97) with respect to a, from the multiplication rule it becomes

$$0 = f'(a) + \sum_{k=1}^{n} \left[ \frac{f^{(k+1)}(a)}{k!} (b-a)^k - \frac{f^{(k)}(a)}{(k-1)!} (b-a)^{k-1} \right] + R'_n(b,a).$$
(1.98)

The second term in the bracket for k = i cancels the first term in the bracket for k = i + 1, therefore almost all terms cancel out and we are left with

$$0 = \frac{f^{(n+1)}(a)}{n!}(b-a)^n + R'_n(b,a).$$
(1.99)

Integrating with respect to a, we obtain

$$R_n(b,a) = \int_{y_0}^a -\frac{f^{(n+1)}(x)}{n!} (b-x)^n \, dx + c. \tag{1.100}$$

Because  $R_n(b, b) = 0$ , we have

$$c = \int_{y_0}^{b} \frac{f^{(n+1)}(x)}{n!} (b-x)^n \, dx,$$
(1.101)

hence

$$R_n(b,a) = \int_a^b \frac{f^{(n+1)}(x)}{n!} (b-x)^n \, dx.$$
(1.102)

We can find the upper bound of  $|R_n(b, a)|$  by

$$|R_n(b,a)| \le \int_a^b \frac{|f^{(n+1)}(x)|}{n!} |(b-x)^n| \, dx \le M \frac{|(b-a)^{n+1}|}{(n+1)!}, \qquad (1.103)$$

where M is assumed to be the common upper bound of  $|f^{(n+1)}(x)|$  in [a, b] for all n. Because  $(n+1)! \gg |(b-a)^{n+1}|$  for sufficiently large n,  $\lim_{n\to\infty} |R_n(b, a)| = 0$  if M exists.

As an example, let us find the Taylor expansion of  $e^x$  around zero. Because  $de^x/dx = e^x$ ,

$$e^x = \sum_{k=0}^{\infty} \frac{x^k}{k!}.$$
 (1.104)

Let x = 1, we have

$$e = \sum_{k=0}^{\infty} \frac{1}{k!} \approx 2.718282 . \qquad (1.105)$$

Similarly, the Taylor expansions for  $\cos x$  and  $\sin x$  around zero are

$$\cos x = \sum_{k=0}^{\infty} \frac{(-1)^k}{(2k)!} x^{2k},$$
  

$$\sin x = \sum_{k=0}^{\infty} \frac{(-1)^k}{(2k+1)!} x^{2k+1}.$$
(1.106)

Comparing Eq. (1.104) with Eq. (1.106), we have the Euler formula

$$e^{ix} = \cos x + i\sin x. \tag{1.107}$$

An important application of Taylor expansion is numerical calculation. For example, a simple method for calculating the numerical value of  $\pi$  is using Taylor expansion in Eq. (1.52).

$$\frac{\pi}{4} = \int_{0}^{1} \frac{1}{x^{2} + 1} dx$$

$$= \int_{0}^{1} (1 - x^{2} + x^{4} - x^{6} + \cdots) dx$$

$$= 1 - \frac{1}{3} + \frac{1}{5} - \frac{1}{7} + \cdots$$

$$= \sum_{n=0}^{\infty} \left( \frac{1}{4n + 1} - \frac{1}{4n + 3} \right).$$
(1.108)

For large n, this sequence is essentially  $1/(8n^2)$ , hence it converges rather slowly. Noting that  $\tan(\pi/8) = \sqrt{2} - 1$ , it is better to use

$$\frac{\pi}{8} = \int_0^{\sqrt{2}-1} \frac{1}{x^2+1} \, dx$$

#### 1.3. TAYLOR EXPANSION

$$= \int_{0}^{\sqrt{2}-1} (1 - x^{2} + x^{4} - x^{6} + \cdots) dx$$
  
=  $(\sqrt{2}-1) - \frac{(\sqrt{2}-1)^{3}}{3} + \frac{(\sqrt{2}-1)^{5}}{5} - \frac{(\sqrt{2}-1)^{7}}{7} + \cdots$  (1.109)

This series converges much faster because  $\sqrt{2} - 1$  is significantly smaller than 1.

In order to extend the exponential function to the complex domain, we may use Eq. (1.104) as the definition of  $e^z$  when z is a complex number. For any two complex numbers y and z,

$$e^{y}e^{z} = \left(\sum_{k=0}^{\infty} \frac{y^{k}}{k!}\right) \left(\sum_{m=0}^{\infty} \frac{z^{m}}{m!}\right)$$

$$= \sum_{k=0}^{\infty} \sum_{m=0}^{\infty} \frac{y^{k}z^{m}}{k!m!}$$

$$= \sum_{k=0}^{\infty} \sum_{n=k}^{\infty} \frac{y^{k}z^{n-k}}{k!(n-k)!} \frac{n!}{n!}$$

$$= \sum_{n=0}^{\infty} \sum_{k=0}^{n} \frac{y^{k}z^{n-k}}{k!(n-k)!} \frac{n!}{n!}$$

$$= \sum_{n=0}^{\infty} \frac{(y+z)^{n}}{n!}$$

$$= e^{(y+z)}.$$
(1.110)

This allows us to define, for z = x + iy,  $e^z = e^x e^{iy} = e^x(\cos y + i \sin y)$ , and consequently  $\ln z = \ln(|z|e^{i\theta}) = \ln |z| + i \arg z$ . Moreover,  $u^z$  can be defined as  $e^{z \ln u}$ . For any three complex numbers u, y and z,

$$(u^{z})^{y} = e^{y\ln(u^{z})} = e^{y\ln(e^{z\ln u})}.$$
(1.111)

If  $-\pi < \text{Im}(z \ln u) \le \pi$ , we may write

$$\ln(e^{z\ln u}) = z\ln u,\tag{1.112}$$

otherwise

$$\ln(e^{z\ln u}) = z\ln u - 2n\pi i, \tag{1.113}$$

where n is an integer that ensures  $-\pi < \text{Im}(z \ln u - 2n\pi i) \le \pi$ . Eqs. (1.111)–(1.113) show that under the restriction  $-\pi < \text{Im}(z \ln u) \le \pi$  we have

$$(u^{z})^{y} = e^{y\ln(u^{z})} = e^{y\ln(e^{z\ln u})} = e^{yz\ln u} = u^{yz}.$$
(1.114)

Under proper restrictions, Eqs. (1.110) and (1.114) extend the characteristics of the real exponential function to the complex domain.

## **1.4 Ordinary Differential Equations**

An equation that contains differential operators in it is called a differential equation. The order of the differential equation is marked by the highest order of the differential operator in the equation. In physics it often occurs that the rate of change of some variable is a function of the variable itself. In such cases the equation describing that variable is a differential equation. For example, the deceleration of a free-falling particle in air is a function of its speed, and we need to find out from the differential equation dv/dt = f(v) how v change with t. A common form of first-order differential equation is the following, and it can be solved by the method of **separation of variables**.

$$\frac{dx}{dt} = f(x)g(t) \Longrightarrow \int \frac{dx}{f(x)} = \int g(t)dt.$$
(1.115)

Example 1.12. Consider

$$\frac{dx}{dt} = \frac{x(1-x)}{t}.$$
 (1.116)

Separation of variables leads to

$$\int \frac{dx}{x(1-x)} = \int \frac{dt}{t}.$$
(1.117)

The solution is

$$\ln\left(\frac{x}{1-x}\right) = \ln t + c_1, \qquad (1.118)$$

where  $c_1$  is a constant. Solving x in terms of t, we obtain

$$x = \frac{t}{t + c_2}.$$
 (1.119)

The constant  $c_2 = e^{-c_1}$  can be determined by the initial value of the equation. For example, if we know at t = 1, x = 1/2, then  $c_2 = 1$  in the above equation.

Another form of first-order differential equation often encountered in physics is the **linear equation**.

$$\frac{dx}{dt} + f(t)x = g(t). \tag{1.120}$$

#### 1.4. Ordinary Differential Equations

Let us solve first for the special case g(t) = 0. Separation of variable yields

$$\ln x = -\int_{t_0}^t f(s) \, ds + c_0, \tag{1.121}$$

or

$$x(t) = c \exp\left[-\int_{t_0}^t f(s) \, ds\right],$$
 (1.122)

where  $c = x(t_0)$ . We can now modify this solution to suit for the case  $g(t) \neq 0$ . The method is known as **variation of parameters.** In Eq. (1.122), c is a parameter that does not depend on t. If we force it to change with t, then this dependence will generate new terms in Eq. (1.120) to cancel g(t). Let

$$x(t) = c(t)h(t),$$
 (1.123)

where c is now a function of t and

$$h(t) = \exp\left[-\int_{t_0}^t f(s) \, ds\right].$$
 (1.124)

Substitute x(t) = c(t)h(t) into Eq. (1.120), we have

$$\frac{dc(t)}{dt}h(t) = g(t), \qquad (1.125)$$

hence

$$\frac{dc(t)}{dt} = \frac{g(t)}{h(t)},\tag{1.126}$$

or

$$c(t) = \int_{t_0}^t \frac{g(u)}{h(u)} \, du + x(t_0). \tag{1.127}$$

Eqs. (1.123) and (1.126) can be written as

$$\frac{d}{dt} \left[ \frac{x(t)}{h(t)} \right] = \frac{g(t)}{h(t)}.$$
(1.128)

The function 1/h(t) is called the **integration factor**. Because

$$\frac{d}{dt}\left[\frac{1}{h(t)}\right] = -\frac{1}{h^2(t)}\frac{dh(t)}{dt} = \frac{f(t)}{h(t)},\tag{1.129}$$

by multiplying both sides of Eq. (1.120) with the integration factor 1/h(t), it is reduced to Eq. (1.128). The solution is

$$x(t) = h(t) \int_{t_0}^t \frac{g(u)}{h(u)} du + x(t_0)h(t).$$
(1.130)

**Example 1.13.** Consider the equation

$$\frac{dx}{dt} + tx = t^3. \tag{1.131}$$

The integration factor 1/h(t) is obviously  $e^{t^2/2}$ . Multiplying both sides by 1/h(t), the equation becomes

$$\frac{d}{dt}\left(e^{t^2/2}x\right) = e^{t^2/2}t^3.$$
(1.132)

The solution is

$$e^{t^2/2}x = \int_{t_0}^t e^{s^2/2}s^3 \, ds + c_0. \tag{1.133}$$

Using integration by parts by setting  $u = s^2$  and  $dv = se^{s^2/2} ds$ , one obtains

$$\int_{t_0}^t e^{s^2/2} s^3 \, ds = t^2 e^{t^2/2} - 2e^{t^2/2} + c. \tag{1.134}$$

Therefore

$$e^{t^2/2}x(t) = t^2 e^{t^2/2} - 2e^{t^2/2} + c, \qquad (1.135)$$

or equivalently

$$x = t^2 - 2 + ce^{-t^2/2}. (1.136)$$

There is no general method to solve high-order differential equations except when the equation is linear and has constant coefficients,

$$\frac{d^n x}{dt^n} + a_1 \frac{d^{n-1} x}{dt^{n-1}} + a_2 \frac{d^{n-2} x}{dt^{n-2}} + \dots + a_n x = f(t), \qquad (1.137)$$

where  $a_1, a_2, \dots, a_n$  are arbitrary constants. If  $x_1$  and  $x_2$  are two solutions of Eq. (1.137), then their difference  $x_1 - x_2$  satisfies the homogeneous equation

$$\frac{d^n x}{dt^n} + a_1 \frac{d^{n-1} x}{dt^{n-1}} + a_2 \frac{d^{n-2} x}{dt^{n-2}} + \dots + a_n x = 0.$$
(1.138)

#### 1.4. Ordinary Differential Equations

Therefore we only need to find one particular solution  $x_p$  of Eq. (1.137) in addition to the solutions  $x_h$  of the homogeneous Eq. (1.138). All the solutions of Eq. (1.137) can be written as  $x = x_p + x_h$ . The solution  $x_h$  has the form

$$x_h = c e^{\lambda t}, \tag{1.139}$$

where  $\lambda$  satisfies

$$\lambda^{n} + a_1 \lambda^{n-1} + a_2 \lambda^{n-2} + \dots + a_n = 0.$$
 (1.140)

Eq. (1.140) has n roots, therefore the general solution for  $x_h$  is

$$x_h = \sum_{i=1}^n c_i e^{\lambda_i t},$$
 (1.141)

where the coefficients  $c_i$  are determined by specifying the initial conditions

$$x(0), \left. \frac{dx}{dt} \right|_{x=0}, \dots \left. \frac{d^{(n-1)}x}{dt^{(n-1)}} \right|_{x=0}.$$

If there are *m* roots of the same  $\lambda$  in Eq. (1.140), the *m* linearly independent solutions corresponding to this  $\lambda$  are  $t^m e^{\lambda t}$  (m = 0, 1, ..., m - 1). This can be seen from the following equation:

$$\left(\frac{d}{dt} - \lambda\right)ct^k e^{\lambda t} = ckt^{k-1}e^{\lambda t}.$$
(1.142)

There is no general method to find  $x_p$ . For simple cases  $x_p$  can be derived by guessing from f(t). In what follows we give six examples of such guess work.

#### Example 1.14.

$$\frac{d^2x}{dt^2} + 3\frac{dx}{dt} + 2x = t^2.$$
(1.143)

First we solve the homogeneous equation

$$\frac{d^2x}{dt^2} + 3\frac{dx}{dt} + 2x = 0. (1.144)$$

Substituting Eq. (1.138) into Eq. (1.144), we have

$$\lambda^2 + 3\lambda + 2 = 0. \tag{1.145}$$

The solutions are  $\lambda = -1$  and  $\lambda = -2$ , therefore

$$x_h = c_1 e^{-t} + c_2 e^{-2t}. (1.146)$$

For the particular solution, we guess

$$x_p = at^2 + bt + c. (1.147)$$

Substituting this into Eq. (1.143), we have

$$2at^{2} + (6a + 2b)t + (2a + 3b + 2c) = t^{2}.$$
 (1.148)

Comparing the coefficients of both sides, we have

$$2a = 1, \ 6a + 2b = 0, \ 2a + 3b + 2c = 0.$$
 (1.149)

That is

$$a = \frac{1}{2}, \ b = -\frac{3}{2}, \ c = \frac{7}{4}.$$
 (1.150)

Therefore the particular solution is

$$x_p = \frac{1}{2}t^2 - \frac{3}{2}t + \frac{7}{4},$$
(1.151)

and the general solution is

$$x = x_p + x_h = \frac{1}{2}t^2 - \frac{3}{2}t + \frac{7}{4} + c_1e^{-t} + c_2e^{-2t}.$$
 (1.152)

#### Example 1.15.

$$\frac{d^2x}{dt^2} - 4\frac{dx}{dt} - 5x = 3e^t.$$
(1.153)

First we solve the homogeneous equation

$$\frac{d^2x}{dt^2} - 4\frac{dx}{dt} - 5x = 0. (1.154)$$

Since the roots of

$$\lambda^2 - 4\lambda - 5 = 0 \tag{1.155}$$

are  $\lambda = -1$  and  $\lambda = 5$ , we have

$$x_h = c_1 e^{-t} + c_2 e^{5t}. (1.156)$$

For the particular solution, we guess

$$x_p = ae^t. (1.157)$$

Substituting this into Eq. (1.153), we have

$$(a - 4a - 5a)e^t = 3e^t. (1.158)$$

Comparing the coefficients of both sides, we have

$$a = -\frac{3}{8}.$$
 (1.159)

Therefore the particular solution is

$$x_p = -\frac{3}{8}e^t,$$
 (1.160)

and the general solution is

$$x = x_p + x_h = -\frac{3}{8}e^t + c_1e^{-t} + c_2e^{5t}.$$
 (1.161)

#### Example 1.16.

$$\frac{d^2x}{dt^2} - 4\frac{dx}{dt} + 3x = \sin t.$$
(1.162)

First we solve the homogeneous equation

$$\frac{d^2x}{dt^2} - 4\frac{dx}{dt} + 3x = 0. (1.163)$$

Since the roots of

$$\lambda^2 - 4\lambda + 3 = 0 \tag{1.164}$$

are  $\lambda = 1$  and  $\lambda = 3$ , we have

$$x_h = c_1 e^t + c_2 e^{3t}. (1.165)$$

For the particular solution, we guess

$$x_p = a\sin t + b\cos t. \tag{1.166}$$

Substituting this into Eq. (1.162), we have

$$(2a+4b)\sin t + (-4a+2b)\cos t = \sin t. \tag{1.167}$$

Comparing the coefficients of both sides, we have

$$2a + 4b = 1, \ -4a + 2b = 0. \tag{1.168}$$

That is

$$a = \frac{1}{10}, \ b = \frac{1}{5}.$$
 (1.169)

Therefore the particular solution is

$$x_p = \frac{1}{10}\sin t + \frac{1}{5}\cos t, \qquad (1.170)$$

and the general solution is

$$x = x_p + x_h = \frac{1}{10}\sin t + \frac{1}{5}\cos t + c_1e^t + c_2e^{3t}.$$
 (1.171)

## Example 1.17.

$$\frac{d^2x}{dt^2} - 4\frac{dx}{dt} + 3x = e^t.$$
(1.172)

First we solve the homogeneous equation

$$\frac{d^2x}{dt^2} - 4\frac{dx}{dt} + 3x = 0. (1.173)$$

As stated in Eq. (1.165), it is

$$x_h = c_1 e^t + c_2 e^{3t}. (1.174)$$

For the particular solution, we cannot guess  $x_p = ae^t$ , because it is the solution of the homogeneous equation. We guess instead

$$x_p = ate^t. \tag{1.175}$$

Substituting this into Eq. (1.172), we have

$$-2ae^t = e^t. (1.176)$$

Therefore

$$a = -\frac{1}{2}.$$
 (1.177)
### 1.4. Ordinary Differential Equations

The particular solution is then

$$x_p = -\frac{1}{2}te^t, \qquad (1.178)$$

and the general solution is

$$x = x_p + x_h = -\frac{1}{2}te^t + c_1e^t + c_2e^{3t}.$$
(1.179)

Note that the particular solution for

$$\left(\frac{d}{dt} - \lambda_1\right) \left(\frac{d}{dt} - \lambda_2\right) x = ae^{\lambda_2 t}$$
(1.180)

is  $x_p = bte^{\lambda_2 t}$ , because

$$\left(\frac{d}{dt} - \lambda_1\right) \left(\frac{d}{dt} - \lambda_2\right) bt e^{\lambda_2 t} = \left(\frac{d}{dt} - \lambda_1\right) b e^{\lambda_2 t} = b(\lambda_2 - \lambda_1) e^{\lambda_2 t}, \quad (1.181)$$

and b can be chosen to be  $a/(\lambda_2 - \lambda_1)$ .

## Example 1.18.

$$\frac{d^2x}{dt^2} - 4\frac{dx}{dt} + 4x = e^t.$$
(1.182)

First we solve the homogeneous equation

$$\frac{d^2x}{dt^2} - 4\frac{dx}{dt} + 4x = 0. (1.183)$$

Since  $\lambda = 2$  is the multiple root of

$$\lambda^2 - 4\lambda + 4 = 0, \tag{1.184}$$

the second solution for  $x_h$  is  $te^{2t}$ , namely

$$x_h = c_1 e^{2t} + c_2 t e^{2t}. (1.185)$$

For the particular solution, we guess

$$x_p = ae^t. (1.186)$$

Substituting this into Eq. (1.182), we have

$$ae^t = e^t. (1.187)$$

Therefore

$$a = 1.$$
 (1.188)

The particular solution is then

$$x_p = e^t, (1.189)$$

and the general solution is

$$x = x_p + x_h = e^t + c_1 e^{2t} + c_2 t e^{2t}.$$
 (1.190)

Note that the second solution for the homogeneous equation

$$\left(\frac{d}{dt} - \lambda\right)^2 x = 0 \tag{1.191}$$

is  $x_h = cte^{\lambda t}$ , because

$$\left(\frac{d}{dt} - \lambda\right)^2 cte^{\lambda t} = \left(\frac{d}{dt} - \lambda\right)ce^{\lambda t} = 0.$$
(1.192)

Example 1.19.

$$\frac{d^2x}{dt^2} - 4\frac{dx}{dt} + 4x = e^{2t}.$$
(1.193)

First we solve the homogeneous equation

$$\frac{d^2x}{dt^2} - 4\frac{dx}{dt} + 4x = 0. (1.194)$$

As stated in Eq. (1.165), it is

$$x_h = c_1 e^{2t} + c_2 t e^{2t}. (1.195)$$

For the particular solution, we cannot guess  $x_p = ae^{2t}$  or  $x_p = ate^{2t}$ , because they are the solutions of the homogeneous equation. Instead we guess

$$x_p = at^2 e^{2t}.$$
 (1.196)

Substituting this into Eq. (1.193), we have

$$2ae^{2t} = e^{2t}. (1.197)$$

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Therefore

$$a = \frac{1}{2}.$$
 (1.198)

The particular solution is then

$$x_p = \frac{1}{2}t^2 e^{2t},\tag{1.199}$$

and the general solution is

$$x = x_p + x_h = \frac{1}{2}t^2e^{2t} + c_1e^{2t} + c_2te^{2t}.$$
 (1.200)

Note that the particular solution for

$$\left(\frac{d}{dt} - \lambda\right)^2 x = ae^{\lambda t} \tag{1.201}$$

is  $x_p = bt^2 e^{\lambda t}$ , because

$$\left(\frac{d}{dt} - \lambda\right)^2 bt^2 e^{\lambda t} = \left(\frac{d}{dt} - \lambda\right) 2bt e^{\lambda t} = 2be^{\lambda t}, \qquad (1.202)$$

and b can be chosen to be a/2.

In general an n-th order differential equation can be written as

$$\frac{d^n x}{dt^n} = f\left(\frac{d^{n-1}x}{dt^{n-1}}\dots\frac{dx}{dt}, x\right).$$
(1.203)

The solution x(t) must contain n undetermined parameters to accommodate various possible initial conditions. These parameters are determined by the n equations

$$\begin{array}{rcl}
x(t_0) &=& x_0 \\
\dot{x}(t_0) &=& \dot{x}_0 \\
\ddot{x}(t_0) &=& \ddot{x}_0 \\
\vdots & & & (1.204)
\end{array}$$

that specify the initial state  $(x, \dot{x}, \ddot{x}, ...)$  of the system at  $t = t_0$  to be  $(x_0, \dot{x}_0, \ddot{x}_0, ...)$ . If two solutions  $x_1(t)$  and  $x_2(t)$  satisfy the same initial condition, namely

$$\begin{aligned}
x_1(t_0) &= x_2(t_0) \\
\dot{x}_1(t_0) &= \dot{x}_2(t_0) \\
\ddot{x}_1(t_0) &= \ddot{x}_2(t_0) \\
\vdots \\
\end{aligned}$$
(1.205)

then Eq. (1.203) and its derivatives guarantee that

$$\left. \frac{d^m x_1}{dt^m} \right|_{t=t_0} = \left. \frac{d^m x_2}{dt^m} \right|_{t=t_0} \tag{1.206}$$

for all m. This means  $x_1(t)$  and  $x_2(t)$  have the same Taylor expansion at  $t = t_0$ , hence  $x_1(t) = x_2(t)$ . In other words, the solution is uniquely determined by the initial condition.

## 1.5 Fourier Transform

In physics we often deal with periodic functions in space and time. Period functions can be expanded into a series of sine and cosine functions of shorter and shorter periods. Such a series is known as the **Fourier series**. Let us assume for the time being that any periodic function can be constructed with a linear combination of sine and cosine functions. Namely

$$f(x) = a_0 + \sum_{k=1}^{\infty} (a_k \cos kx + b_k \sin kx).$$
(1.207)

Multiplying both sides by  $\cos nx$  and  $\sin nx$  respectively and integrating from  $-\pi$  to  $\pi$ , and using the following relations

$$\int_{-\pi}^{\pi} \cos nx \, dx = \int_{-\pi}^{\pi} \sin nx \, dx = 0,$$
  
$$\int_{-\pi}^{\pi} \cos kx \sin nx \, dx = \int_{-\pi}^{\pi} \frac{1}{2} [\sin(k+n)x - \sin(k-n)x] \, dx = 0,$$
  
$$\int_{-\pi}^{\pi} \cos kx \cos nx \, dx = \int_{-\pi}^{\pi} \frac{1}{2} [\cos(k+n)x + \cos(k-n)x] \, dx = \pi \delta_{kn},$$
  
$$\int_{-\pi}^{\pi} \sin kx \sin nx \, dx = \int_{-\pi}^{\pi} \frac{1}{2} [\cos(k-n)x - \cos(k+n)x] \, dx = \pi \delta_{kn},$$
  
(1.208)

where  $\delta_{kn} = 1$  when k = n and  $\delta_{kn} = 0$  when  $k \neq n$ , we have

$$a_{0} = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(x) dx,$$
  

$$a_{k} = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \cos kx dx,$$
  

$$b_{k} = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \sin kx dx.$$
 (1.209)

### 1.5. FOURIER TRANSFORM

If we imaging  $\cos kx$  and  $\sin kx$  to be vectors of (uncountable) infinite dimensions, Eq. (1.208) means these vectors are orthogonal to each others, and their lengths are  $\sqrt{\pi}$ . Then  $a_k, b_k$  are proportional to the projection of f(x) on these vectors.

Let us define the partial sum  $S_n(x)$  by

$$S_n(x) = \sum_{k=0}^n (a_k \cos kx + b_k \sin kx).$$
(1.210)

We wish to show that  $\lim_{n\to\infty} S_n(x)$  converges to f(x). Before doing that, let us show first that  $a_k \to 0$ ,  $b_k \to 0$  as  $k \to \infty$ . This is of course a necessary condition for the convergence of Eq. (1.207). Consider the following integral

$$\int_{-\pi}^{\pi} \left[ f(x) - S_n(x) \right]^2 dx = \int_{-\pi}^{\pi} \left[ f^2(x) - 2f(x)S_n(x) + S_n^2(x) \right] dx$$
$$= \int_{-\pi}^{\pi} f^2(x) dx - 2\pi \sum_{k=0}^n (a_k^2 + b_k^2) + \pi \sum_{k=0}^n (a_k^2 + b_k^2).$$
(1.211)

Since the left-hand side cannot be negative, we have

$$\sum_{k=0}^{n} (a_k^2 + b_k^2) \le \frac{1}{\pi} \int_{-\pi}^{\pi} f^2(x) \, dx.$$
(1.212)

This implies  $a_k \to 0$ ,  $b_k \to 0$  as  $k \to \infty$  if  $\int_{-\pi}^{\pi} f^2(x) dx$  is finite. Namely

$$\lim_{k \to \infty} \int_{-\pi}^{\pi} f(x) \cos kx \, dx = \lim_{k \to \infty} \int_{-\pi}^{\pi} f(x) \sin kx \, dx = 0.$$
(1.213)

Using Eq. (1.209), we can rewrite  $S_n(x)$  as

$$S_n(x) = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(t) dt + \frac{1}{\pi} \int_{-\pi}^{\pi} f(t) \sum_{k=1}^n (\cos kt \cos kx + \sin kt \sin kx) dt$$
  
=  $\frac{1}{2\pi} \int_{-\pi}^{\pi} f(t) dt + \frac{1}{\pi} \int_{-\pi}^{\pi} f(t) \sum_{k=1}^n \cos k(t-x) dt.$  (1.214)

Changing variable to  $\tau = t - x$ , we have

$$S_n(x) = \frac{1}{2\pi} \int_{-\pi-x}^{\pi-x} f(\tau+x) d\tau + \frac{1}{\pi} \int_{-\pi-x}^{\pi-x} f(\tau+x) \sum_{k=1}^n \cos k\tau \, d\tau. \quad (1.215)$$

Since  $f(\tau+x)$  and  $\cos k\tau$  are periodic functions with period  $2\pi$ , it is equivalent to

$$S_n(x) = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(\tau + x) \, d\tau + \frac{1}{\pi} \int_{-\pi}^{\pi} f(\tau + x) \sum_{k=1}^n \cos k\tau \, d\tau. \quad (1.216)$$

Using the formula

$$\sin \frac{\tau}{2} \sum_{k=1}^{n} \cos k\tau = \frac{1}{2} \sum_{k=1}^{n} \left[ \sin \left( k + \frac{1}{2} \right) \tau - \sin \left( k - \frac{1}{2} \right) \tau \right]$$
$$= \frac{1}{2} \left[ \sin \left( n + \frac{1}{2} \right) \tau - \sin \frac{\tau}{2} \right], \qquad (1.217)$$

namely

$$\sum_{k=1}^{n} \cos k\tau = \frac{\sin\left(n + \frac{1}{2}\right)\tau}{2\sin\frac{\tau}{2}} - \frac{1}{2},$$
(1.218)

we have

$$S_n(x) = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x+\tau) \frac{\sin\left(n+\frac{1}{2}\right)\tau}{2\sin\frac{\tau}{2}} d\tau$$
$$= \frac{1}{\pi} \int_{-\pi}^{\pi} \left[\frac{f(x+\tau)+f(x-\tau)}{2}\right] \frac{\sin\left(n+\frac{1}{2}\right)\tau}{2\sin\frac{\tau}{2}} d\tau. \quad (1.219)$$

By integrating Eq. (1.218), we have

$$\int_{-\pi}^{\pi} \frac{\sin\left(n + \frac{1}{2}\right)\tau}{2\sin\frac{\tau}{2}} d\tau = \pi.$$
 (1.220)

As we shall see, the application of Fourier series is not limited to continuous functions. Therefore let us define

$$f(x^{+}) \equiv \lim_{\epsilon \to 0} f(x + |\epsilon|),$$
  

$$f(x^{-}) \equiv \lim_{\epsilon \to 0} f(x - |\epsilon|).$$
(1.221)

Using Eq. (1.220) in Eq. (1.219), we obtain

$$S_n(x) - \frac{f(x^+) + f(x^-)}{2} = \frac{1}{\pi} \int_{-\pi}^{\pi} g(\tau) \sin\left(n + \frac{1}{2}\right) \tau \, d\tau$$
$$= \frac{1}{\pi} \int_{-\pi}^{\pi} g(\tau) \left(\sin n\tau \cos\frac{\tau}{2} + \cos n\tau \sin\frac{\tau}{2}\right) \, d\tau, \qquad (1.222)$$

where

$$g(\tau) = \frac{f(x+\tau) + f(x-\tau) - f(x^+) - f(x^-)}{4\sin\frac{\tau}{2}}.$$
 (1.223)

#### 1.5. FOURIER TRANSFORM

Note that  $g(\tau)$  is finite as  $\tau \to 0$  even though it has a factor of  $\sin(\tau/2)$  in the denominator. This can be seen by expanding both the numerator and the denominator in Taylor series.

$$\lim_{\tau \to 0} |g(\tau)| = \left| \frac{f'(x^+)\tau - f'(x^-)\tau}{2\tau} \right| = \left| \frac{f'(x^+) - f'(x^-)}{2} \right|.$$
(1.224)

Therefore one can safely argue that by Eq. (1.213), the right-hand side of Eq. (1.222) approached zero as  $n \to \infty$ . In other words,

$$\lim_{n \to \infty} S_n(x) = \frac{f(x^+) + f(x^-)}{2}.$$
 (1.225)

Using the Euler formula, Eq. (1.207) can be written as

$$f(x) = a_0 + \sum_{k=1}^{\infty} \left( \frac{a_k - ib_k}{2} e^{ikx} + \frac{a_k + ib_k}{2} e^{-ikx} \right).$$
(1.226)

If we define  $c_0 \equiv a_0$ ,  $c_k \equiv (a_k - ib_k)/2$ , and  $c_{-k} \equiv (a_k + ib_k)/2$ , Eq. (1.226) becomes

$$f(x) = \sum_{m=-\infty}^{\infty} c_m e^{imx}, \qquad (1.227)$$

where we have changed the dummy index from k to m. From Eq. (1.209), the coefficients  $c_m$  can be written as

$$c_m = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(x) e^{-imx} \, dx.$$
 (1.228)

In Eq. (1.207) f(x) has a fixed period  $2\pi$ . If we replace x by  $2\pi y/T$ , the expansion can be used on functions of period T.

$$g(y) = \sum_{m=-\infty}^{\infty} c_m e^{i\left(\frac{2\pi m}{T}\right)y}, \qquad (1.229)$$

$$c_m = \frac{1}{2\pi} \frac{2\pi}{T} \int_{-\frac{T}{2}}^{\frac{T}{2}} g(y) e^{-i\left(\frac{2\pi m}{T}\right)y} \, dy.$$
(1.230)

If we define a real variable  $k \equiv 2\pi m/T$  and a function  $u(k) \equiv c_m T/\sqrt{2\pi}$ , such that the mapping  $k \to u(k)$  corresponds to  $2\pi m/T \to c_m T/\sqrt{2\pi}$ , Eqs. (1.229) and (1.230) can be written as

$$g(y) = \frac{1}{\sqrt{2\pi}} \sum_{m=-\infty}^{\infty} u(k) e^{iky} \left(\frac{2\pi}{T}\right) = \frac{1}{\sqrt{2\pi}} \sum_{m=-\infty}^{\infty} u(k) e^{iky} \Delta k, (1.231)$$

$$u(k) = \frac{1}{\sqrt{2\pi}} \int_{-\frac{T}{2}}^{\frac{1}{2}} g(y) e^{-iky} \, dy, \qquad (1.232)$$

where  $\Delta k = 2\pi (m+1)/T - 2\pi m/T = 2\pi/T$ . If we let  $T \to \infty$ , then  $\Delta k \to 0$ . Eq. (1.231) becomes the Riemann sum of  $u(k)e^{iky}/\sqrt{2\pi}$  with respect to k. Therefore we can write

$$g(y) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} u(k) e^{iky} \, dk, \qquad (1.233)$$

$$u(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} g(y) e^{-iky} \, dy.$$
 (1.234)

In Eq. (1.234) u(k) is the Fourier transform of g(y), and in Eq. (1.233) g(y) is the inverse Fourier transform of u(k).

Eq. (1.233) and Eq. (1.234) can be combined to yield an identity:

$$u(k) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} u(k') e^{ik'y} dk' e^{-iky} dy$$
  
=  $\frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} u(k') e^{i(k'-k)y} dy dk'.$  (1.235)

A short-hand notation for the "generalized function"  $\delta(k'-k)$  has been invented, which is well defined only as part of the integrand, such that

$$u(k) = \int_{-\infty}^{\infty} u(k')\delta(k'-k)\,dk'.$$
(1.236)

Comparing with Eq. (1.235), we have

$$\delta(k'-k) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i(k'-k)y} \, dy.$$
 (1.237)

The integral on the right-hand side does not converge by itself, therefore it is not well defined as a stand-alone expression. It can only be used in an integral.

Eq. (1.237) can be used to prove an important theorem in Fourier transform: Let h(x) be the convolution of f(x) and g(x), namely,

$$h(u) = \int_{-\infty}^{\infty} f(x)g(u-x) \, dx,$$
 (1.238)

and  $\tilde{h}(k)$ ,  $\tilde{f}(k)$ , and  $\tilde{g}(k)$  be the Fourier transform of h(x), f(x), and g(x) respectively. Then

$$\tilde{h}(k) = \sqrt{2\pi} \tilde{f}(k)\tilde{g}(k).$$
(1.239)

### 1.5. FOURIER TRANSFORM

This is known as the **convolution theorem of Fourier transform**. To prove the theorem, let us express f(x) and g(u-x) in terms of their Fourier transforms.

$$h(u) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{\tilde{f}(k')e^{ik'x}}{\sqrt{2\pi}} \frac{\tilde{g}(k)e^{ik(u-x)}}{\sqrt{2\pi}} dk'dkdx$$
  

$$= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \tilde{f}(k')\tilde{g}(k)e^{iku} \left[\int_{-\infty}^{\infty} \frac{e^{i(k'-k)x}}{2\pi} dx\right] dk'dk$$
  

$$= \int_{-\infty}^{\infty} \tilde{g}(k)e^{iku} \left[\int_{-\infty}^{\infty} \tilde{f}(k')\delta(k'-k)dk'\right] dk$$
  

$$= \int_{-\infty}^{\infty} \tilde{f}(k)\tilde{g}(k)e^{iku}dk.$$
(1.240)

Comparing with Eq. (1.233), we have

$$\tilde{h}(k) = \sqrt{2\pi}\tilde{f}(k)\tilde{g}(k).$$
(1.241)

An important relation that is often used in physics is the Fourier transform of the Gaussian function. Let us first evaluate the following integrals.

$$I_0 = \int_{-\infty}^{\infty} e^{-x^2} \, dx. \tag{1.242}$$

We may write

$$I_0^2 = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-(x^2 + y^2)} \, dx \, dy = \int_0^{\infty} \int_0^{2\pi} e^{-r^2} r \, d\phi \, dr = \pi.$$
(1.243)

Hence  $I_0 = \sqrt{\pi}$ . Next we evaluate

$$I_2 = \int_0^\infty x^2 e^{-x^2} dx.$$
 (1.244)

Set u = x and  $dv = xe^{-x^2}dx$ , one obtains from integration by parts

$$\int_0^\infty x^2 e^{-x^2} dx = -\frac{x}{2} e^{-x^2} \Big|_0^\infty + \frac{1}{2} \int_0^\infty e^{-x^2} dx \qquad (1.245)$$

$$= \frac{1}{2} \int_0^\infty e^{-x^2} dx = \frac{1}{2} \frac{\sqrt{\pi}}{2}.$$
 (1.246)

Similarly set  $u = x^3$  and  $dv = xe^{-x^2}dx$ , one obtains from integration by parts

$$\int_0^\infty x^4 e^{-x^2} dx = \frac{3}{2} \int_0^\infty x^2 e^{-x^2} dx = \frac{3}{2} \frac{1}{2} \frac{\sqrt{\pi}}{2}$$

$$\int_0^\infty x^{2n} e^{-x^2} dx = \frac{2n-1}{2} \cdots \frac{3}{2} \frac{1}{2} \frac{\sqrt{\pi}}{2} = \frac{(2n)!}{n! 2^{2n}} \frac{\sqrt{\pi}}{2}.$$
 (1.247)

This is the same formula we have derived in Eq. (1.84) using a different method. To evaluate

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$$\int_{-\infty}^{\infty} e^{-x^2} e^{-ikx} \, dx = 2 \int_{0}^{\infty} e^{-x^2} \cos(kx) dx, \qquad (1.248)$$

we expand  $\cos(kx)$  into its Taylor series and use the integrals evaluated above.

$$2\int_0^\infty e^{-x^2}\cos(kx)dx = 2\sum_{n=0}^\infty \frac{(-1)^n k^{2n}}{(2n)!} \int_0^\infty x^{2n} e^{-x^2}dx \quad (1.249)$$

$$= 2\sum_{n=0}^{\infty} \frac{(-1)^n k^{2n}}{n! 2^{2n}} \frac{\sqrt{\pi}}{2}$$
(1.250)

$$= \sqrt{\pi}e^{-k^2/4}.$$
 (1.251)

We see that the Fourier transform of the Gaussian function is the Gaussian function itself. The fact can be written in a more symmetric form:

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-x^2/2} e^{-ikx} \, dx = e^{-k^2/2}.$$
(1.252)

Another relation in that is often used in elementary physics is the Fourier transform of the following function

$$g(x) = \begin{cases} e^{-\alpha x} \sin \beta x & \text{when } x \ge 0\\ 0 & \text{when } x < 0. \end{cases}$$
(1.253)

A simple integration yields

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} g(x) e^{-ikx} dx = \frac{1}{\sqrt{2\pi}} \frac{1}{2i} \int_{0}^{\infty} e^{(-\alpha + i\beta - ik)x} - e^{(-\alpha - i\beta - ik)x} dx$$
$$= \frac{1}{\sqrt{2\pi}} \left(\frac{-1}{2}\right) \left[\frac{1}{k - (\beta + i\alpha)} - \frac{1}{k - (\beta - i\alpha)}\right]$$
$$= \frac{1}{\sqrt{2\pi}} \left[\frac{\beta}{(\alpha^{2} + \beta^{2}) + 2ik\alpha - k^{2}}\right]. \quad (1.254)$$

### **1.6** Volume Elements

Consider the volume V spanned by n vectors in an n-dimensional space. We shall prove that V is simply the determinant of the matrix made of these nvectors. Let us write these n vectors as  $a_{ij}$ , where  $i = 1 \dots n$  is the index for the vectors and  $j = 1 \dots n$  is the index for the components of each vector. One can imagine that  $V = D_n A(S_n)$ , where  $A(S_n)$  is the area of the hyperplane  $S_n$  spanned by the n-1 vectors  $a_{ij}$   $(i = 1 \dots n-1)$  and  $D_n$  is the projection of  $a_{nj}$  along the normal vector of the hyperplane. If we add a vector  $c_n a_{1j}$  to  $a_{nj}$ , where  $c_n$  is a constant, to make a new vector  $b_{nj} = a_{nj} + c_n a_{1j}$ , then it is clear that the volume spanned by  $b_{nj}$  and  $a_{ij}$   $(i = 1 \dots n - 1)$  is still V, because adding a vector on the hyperplane to  $a_{nj}$  does not change the projection  $D_n$ . For a reason that will become apparent in a moment, we choose  $c_n$  is such a way that it makes  $b_{n1}$  zero. Namely,  $c_n = -a_{n1}/a_{11}$ . Next, we consider another hyperplane  $S_{n-1}$  spanned by the n-1 vectors  $a_{ij}$   $(i = 1 \dots n-2)$ and  $b_{nj}$ . Let  $D_{n-1}$  be the projection of  $a_{(n-1)j}$  along the normal vector of this new hyperplane. Again we have  $V = D_{n-1}A(S_{n-1})$ , where  $A(S_{n-1})$  is the area of the new hyperplane. We can add  $c_{n-1}a_{1j}$  to  $a_{(n-1)j}$  to make a new vector  $b_{(n-1)j}$ , in such a way that  $b_{(n-1)1} = 0$ . Repeating this process to all  $a_{ij}$  except for i = 1, we find that V is equal to the volume spanned by  $a_{1j}$ and  $b_{ij}$  (i = 2...n). Since  $b_{i1} = 0$ ,  $b_{ij}$  (i = 2...n) spans a hyperplane  $S_1$  in an (n-1)-dimensional space. As before, we have  $V = D_1 A(S_1)$ , where  $D_1$ is simply  $a_{11}$ .

For a 2-dimensional surface spanned by two vectors  $(a_{11}, a_{12})$  and  $(a_{21}, a_{22})$ it is clear that the area is det $[a_{ij}]$ . Assume for the (n-1)-dimensional space the volume is also det $[a_{ij}]$ . We have  $A(S_1) = det[b_{ij}]$ . For the *n*-dimensional space we have already known that  $V = D_1A(S_1) = a_{11}det[b_{ij}]$ , and that can be written as

$$V = \det \begin{bmatrix} a_{11} & a_{12} & a_{13} & \dots & a_{1n} \\ 0 & b_{22} & b_{23} & \dots & b_{2n} \\ 0 & b_{32} & b_{33} & \dots & b_{3n} \\ \vdots & \vdots & \vdots & \ddots & \\ 0 & b_{n2} & b_{n3} & & b_{nn} \end{bmatrix}.$$
 (1.255)

Because the transformation from  $a_{ij}$  to  $b_{ij}$  (i = 2...n) does not change the

determinant, we have

$$\det [a_{ij}] = \det \begin{bmatrix} a_{11} & a_{12} & a_{13} & \dots & a_{1n} \\ 0 & b_{22} & b_{23} & \dots & b_{2n} \\ 0 & b_{32} & b_{33} & \dots & b_{3n} \\ \vdots & \vdots & \vdots & \ddots & \\ 0 & b_{n2} & b_{n3} & & b_{nn} \end{bmatrix},$$
(1.256)

therefore

$$V = \det\left[a_{ij}\right]. \tag{1.257}$$

One may wonder what does it mean if det  $[a_{ij}] < 0$ ? In fact, a volume element in *n*-dimensional space is just a surface element in n+1-dimensional space. A surface element can be treated as a vector pointing to the normal direction of the surface with a length equal to the area of the surface element. In this point of view, a "volume" element can indeed have a negative value depending on its "orientation". This will become clear when we discuss vector analysis in Section 1.9.

# 1.7 Change of Variables

Consider the integration of a function

$$S = \int f(p,q,r) \, dp \, dq \, dr. \tag{1.258}$$

If we change variables to (u, v, w) by

$$p = p(u, v, w), q = q(u, v, w), r = r(u, v, w),$$
(1.259)

how should we write S in terms of (u, v, w)? Eq. (1.259) implies

$$dp = \left(\frac{\partial p}{\partial u}\right) du + \left(\frac{\partial p}{\partial v}\right) dv + \left(\frac{\partial p}{\partial w}\right) dw,$$
  

$$dq = \left(\frac{\partial q}{\partial u}\right) du + \left(\frac{\partial q}{\partial v}\right) dv + \left(\frac{\partial q}{\partial w}\right) dw,$$
  

$$dr = \left(\frac{\partial r}{\partial u}\right) du + \left(\frac{\partial r}{\partial v}\right) dv + \left(\frac{\partial r}{\partial w}\right) dw.$$
(1.260)

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### 1.7. CHANGE OF VARIABLES

In the matrix notation, we have

$$\begin{bmatrix} dp \\ dq \\ dr \end{bmatrix} = \begin{bmatrix} \frac{\partial p}{\partial u} & \frac{\partial p}{\partial v} & \frac{\partial p}{\partial w} \\ \frac{\partial q}{\partial u} & \frac{\partial q}{\partial v} & \frac{\partial q}{\partial w} \\ \frac{\partial r}{\partial u} & \frac{\partial r}{\partial v} & \frac{\partial r}{\partial w} \end{bmatrix} \begin{bmatrix} du \\ dv \\ dw \end{bmatrix}.$$
 (1.261)

Let us denote the matrix in Eq. (1.261)  $\mathbf{M}$ , which is known as the **Jacobian** matrix. We have

$$\begin{bmatrix} dp \\ dq \\ dr \end{bmatrix} = \mathbf{M} \begin{bmatrix} du \\ dv \\ dw \end{bmatrix}, \qquad (1.262)$$

or

$$\begin{bmatrix} du \\ dv \\ dw \end{bmatrix} = \mathbf{M}^{-1} \begin{bmatrix} dp \\ dq \\ dr \end{bmatrix}.$$
(1.263)

This leads to

$$dp \, dq \, dr = \det(\mathbf{M}) \, du \, dv \, dw. \tag{1.264}$$

or

$$du\,dv\,dw = \det(\mathbf{M}^{-1})\,dp\,dq\,dr,\tag{1.265}$$

Hence we have

$$S = \int f(u, v, w) \det(\mathbf{M}) \, du dv dw.$$
 (1.266)

Consider the differentiation of a function

$$df = \left(\frac{\partial f}{\partial p}\right)dp + \left(\frac{\partial f}{\partial q}\right)dq + \left(\frac{\partial f}{\partial r}\right)dr.$$
 (1.267)

Using Eq. (1.261), we have

$$df = \left(\frac{\partial f}{\partial p}\frac{\partial p}{\partial u} + \frac{\partial f}{\partial q}\frac{\partial q}{\partial u} + \frac{\partial f}{\partial r}\frac{\partial r}{\partial u}\right)du + \left(\frac{\partial f}{\partial p}\frac{\partial p}{\partial v} + \frac{\partial f}{\partial q}\frac{\partial q}{\partial v} + \frac{\partial f}{\partial r}\frac{\partial r}{\partial v}\right)dv + \left(\frac{\partial f}{\partial p}\frac{\partial p}{\partial w} + \frac{\partial f}{\partial q}\frac{\partial q}{\partial w} + \frac{\partial f}{\partial r}\frac{\partial r}{\partial w}\right)dw.$$
(1.268)

But we also have

$$df = \left(\frac{\partial f}{\partial u}\right) du + \left(\frac{\partial f}{\partial v}\right) dv + \left(\frac{\partial f}{\partial w}\right) dw.$$
(1.269)

Comparing the coefficients of du, dv, and dw, and using the matrix notation, we have

$$\begin{bmatrix} \frac{\partial f}{\partial u}\\ \frac{\partial f}{\partial v}\\ \frac{\partial f}{\partial w} \end{bmatrix} = \mathbf{M}^{\mathrm{T}} \begin{bmatrix} \frac{\partial f}{\partial p}\\ \frac{\partial f}{\partial q}\\ \frac{\partial f}{\partial r} \end{bmatrix}, \qquad (1.270)$$

where  $\mathbf{M}^{\mathrm{T}}$  is the transpose of  $\mathbf{M}$ . This is the formula for the transformation of differential operators under the change of variables.

# 1.8 Diagonalizing a Matrix

Consider a transformation  $\mathbf{T}$  that maps a vector to another vector in an n-dimensional vector space. If  $\mathbf{T}$  satisfies

$$\mathbf{T}(a\mathbf{v}_1 + b\mathbf{v}_2) = a\mathbf{T}(\mathbf{v}_1) + b\mathbf{T}(\mathbf{v}_2)$$
(1.271)

for any two vectors  $\mathbf{v}_1$  and  $\mathbf{v}_2$ , where *a* and *b* are two arbitrary constants, we call **T** a linear transformation. Let us expand an arbitrary vector **v** in terms of a set of basis vectors  $\mathbf{e}_i$   $(i = 1 \dots n)$ . We have

$$\mathbf{v} = a_j \mathbf{e}_j, \tag{1.272}$$

where repeated indices are summed over from 1 to n to simplify the notation. Similarly let us expand  $\mathbf{T}(\mathbf{v})$ . We have

$$\mathbf{T}(\mathbf{v}) = b_i \mathbf{e}_i = a_j \mathbf{T}(\mathbf{e}_j). \tag{1.273}$$

Expanding  $\mathbf{T}(\mathbf{e}_j)$  also in terms of the basis vectors and using  $M_{kj}$  to represent the coefficients, we have

$$\mathbf{T}(\mathbf{e}_j) = M_{kj} \mathbf{e}_k. \tag{1.274}$$

Putting back to Eq. (1.273), we have

$$\mathbf{T}(\mathbf{v}) = b_i \mathbf{e}_i = a_j M_{kj} \mathbf{e}_k. \tag{1.275}$$

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#### 1.8. DIAGONALIZING A MATRIX

Taking the inner product with  $\mathbf{e}_l$  and noting that  $\mathbf{e}_l \cdot \mathbf{e}_i = \delta_{il}$ , we have

$$b_i \mathbf{e}_l \cdot \mathbf{e}_i = b_l = a_j M_{kj} \mathbf{e}_l \cdot \mathbf{e}_k = a_j M_{lj}. \tag{1.276}$$

Replacing l by i, we have

$$b_i = M_{ij}a_j. \tag{1.277}$$

Eq. (1.277) shows that any linear transformation  $\mathbf{T}$  can be represented by a matrix  $M_{ij}$ . For any vector represented by  $a_j$ , the transformation is simply the matrix product  $b_i = M_{ij}a_j$ .

Since we can choose the basis vectors freely, it is natural to ask what basis vectors will simplify the form of  $M_{ij}$ ? To answer this question, let us consider how  $M_{ij}$  changes under a change of basis vectors. Because any one of the new basis vectors  $\mathbf{e}'_i$  can be expressed as a linear combination of the old basis vectors  $\mathbf{e}_k$ , the two bases are related by a the following equation,

$$\mathbf{e}_i' = S_{ki} \mathbf{e}_k, \tag{1.278}$$

where  $S_{ki}$  is a matrix and its column vectors are the coefficients of the linear combinations. If a vector **u** is represented by  $u_l \mathbf{e}_l$  in the old basis, it will be represented by  $u'_i \mathbf{e}'_i$  in the new basis according to

$$u_j' \mathbf{e}_j' = u_j' S_{kj} \mathbf{e}_k = u_l \mathbf{e}_l. \tag{1.279}$$

Taking the inner product with  $\mathbf{e}_i$  and noting that  $\mathbf{e}_i \cdot \mathbf{e}_k = \delta_{ik}$ ,  $\mathbf{e}_i \cdot \mathbf{e}_l = \delta_{il}$ , we have

$$u_i = S_{ij} u'_j. \tag{1.280}$$

With the new basis vectors, Eq. (1.274) can be written as

$$\mathbf{\Gamma}(\mathbf{e}'_i) = M'_{ij}\mathbf{e}'_i,\tag{1.281}$$

where  $M'_{ij}$  is another matrix representing **T** in the new basis. From Eq. (1.278) we have

$$\mathbf{T}(\mathbf{e}'_{j}) = \mathbf{T}(S_{kj}\mathbf{e}_{k}) = S_{kj}\mathbf{T}(\mathbf{e}_{k}) = S_{kj}M_{lk}\mathbf{e}_{l}$$
$$= M'_{ij}S_{mi}\mathbf{e}_{m}.$$
(1.282)

Taking the inner product with  $\mathbf{e}_n$  and noting that  $\mathbf{e}_n \cdot \mathbf{e}_l = \delta_{nl}$ ,  $\mathbf{e}_n \cdot \mathbf{e}_m = \delta_{nm}$ we have

$$S_{ni}M'_{ij} = M_{nk}S_{kj}.$$
 (1.283)

In the matrix notation we have

$$\mathbf{SM}' = \mathbf{MS},\tag{1.284}$$

or

$$\mathbf{M}' = \mathbf{S}^{-1}\mathbf{M}\mathbf{S}.\tag{1.285}$$

The transformation from  $\mathbf{M}$  to  $\mathbf{M}'$  as a result of changing bases is called the **similarity transformation**.

The simplest form of  $\mathbf{M}'$  one can imagine is the diagonal form  $M'_{ij} = \delta_{ij}\lambda^{(i)}$ . In this form we have

$$\mathbf{T}(\mathbf{e}'_j) = M'_{ij}\mathbf{e}'_i = \lambda^{(j)}\mathbf{e}'_j, \qquad (1.286)$$

which means the transformation does not mix up vector components. Each component  $\mathbf{e}'_j$  is only multiplied by a constant  $\lambda^{(j)}$  after transformation. Namely, for any  $\mathbf{v} = a'_j \mathbf{e}'_j$ ,  $\mathbf{T}(\mathbf{v}) = \lambda^{(j)} a'_j \mathbf{e}'_j$ . But how do we find the basis vectors  $\mathbf{e}'_j$  that simplify  $\mathbf{T}$  to such an extent? We note that Eq. (1.286) can be written as

$$[\mathbf{M}' - \lambda^{(j)}\mathbf{I}](\mathbf{e}'_{j}) = 0, \qquad (1.287)$$

where  $\mathbf{I}$  is the identity matrix. Substituting into Eq. (1.285), we have

$$\mathbf{S}^{-1}[\mathbf{M} - \lambda^{(j)}\mathbf{I}]\mathbf{S}(\mathbf{e}'_{j}) = 0.$$
(1.288)

Because det  $\mathbf{S} \neq 0$ , this implies det $[\mathbf{M} - \lambda^{(j)}\mathbf{I}] = 0$  for j = 1...n. We can find  $\lambda^{(j)}$  by solving the algebraic equation

$$\det(\mathbf{M} - \lambda \mathbf{I}) = 0 \tag{1.289}$$

which is called the **characteristic equation** of **M**. Since the equation is an *n*th-order algebraic equation, it has *n* roots corresponding to  $\lambda^{(j)}$ , j = (1...n). The value  $\lambda^{(j)}$  is called the *j*th **eigenvalue** of **T**. Since det[ $\mathbf{M} - \lambda^{(j)}\mathbf{I}$ ] = 0, the matrix  $\mathbf{M} - \lambda^{(j)}\mathbf{I}$  must map at least one vector  $\mathbf{u}_j$  to the null vector. The vectors that are mapped by  $\mathbf{M} - \lambda^{(j)}\mathbf{I}$  to the null vector are called the **eigenvectors** of **T** corresponding to the eigenvalue  $\lambda^{(j)}$ .

A linear transformation **T** is **Hermitian** if  $M_{ij} = M_{ji}^*$ . In the matrix notation we write  $\mathbf{M}^{\dagger} = \mathbf{M}$ , where  $\mathbf{M}^{\dagger}$  defined by

$$\mathbf{M}^{\dagger} \equiv \left(\mathbf{M}^{\mathrm{T}}\right)^{*} \tag{1.290}$$

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is called the Hermitian conjugate of **M**. For any two complex vectors  $\mathbf{w} = w_i \mathbf{e}_i$  and  $\mathbf{v} = v_j \mathbf{e}_j$ , the inner product is defined by

$$\mathbf{w} \cdot \mathbf{v} \equiv w_i^* v_i. \tag{1.291}$$

This is an extension of the definition of inner product for real vectors, which ensures  $\mathbf{v} \cdot \mathbf{v} \geq 0$  for any complex vector  $\mathbf{v}$ . Consider the following inner products.

$$\mathbf{w} \cdot \mathbf{T}(\mathbf{v}) = (w_i \mathbf{e}_i) \cdot \mathbf{T}(v_j \mathbf{e}_j) = w_i^* v_j M_{kj} \mathbf{e}_i \cdot \mathbf{e}_k = w_i^* v_j M_{ij},$$
  
$$\mathbf{T}(\mathbf{w}) \cdot \mathbf{v} = \mathbf{T}(w_i \mathbf{e}_i) \cdot (v_j \mathbf{e}_j) = v_j w_i^* M_{ki}^* \mathbf{e}_j \cdot \mathbf{e}_k = v_j w_i^* M_{ji}^*.$$
(1.292)

If **T** is Hermitian, we have  $\mathbf{w} \cdot \mathbf{T}(\mathbf{v}) = \mathbf{T}(\mathbf{w}) \cdot \mathbf{v}$ . For any eigenvector **u** with eigenvalue  $\lambda$ , we have

$$\mathbf{u} \cdot \mathbf{T}(\mathbf{u}) = \lambda \mathbf{u} \cdot \mathbf{u} = \mathbf{T}(\mathbf{u}) \cdot \mathbf{u} = \lambda^* \mathbf{u} \cdot \mathbf{u}.$$
(1.293)

Hence the eigenvalues of a Hermitian transformation are all real numbers. For any two eigenvectors  $\mathbf{u}_i$  and  $\mathbf{u}_j$  of  $\mathbf{T}$ , we have

$$\mathbf{u}_i \cdot \mathbf{T}(\mathbf{u}_j) = \lambda^{(j)} \mathbf{u}_i \cdot \mathbf{u}_j = \mathbf{T}(\mathbf{u}_i) \cdot \mathbf{u}_j = \lambda^{(i)*} \mathbf{u}_i \cdot \mathbf{u}_j = \lambda^{(i)} \mathbf{u}_i \cdot \mathbf{u}_j. \quad (1.294)$$

If  $\lambda^{(i)} \neq \lambda^{(j)}$ , we must have  $\mathbf{u}_i \cdot \mathbf{u}_j = 0$ . In other words, the eigenvectors of a Hermitian transformation are orthogonal to each other if all the eigenvalues are different. This means we can construct a set of basis vectors using these eigenvectors. In the basis formed by the eigenvectors, the Hermitian matrix  $M_{ij}$  is reduced to the diagonal form  $M'_{ij} = \delta_{ij} \lambda^{(i)}$ .

What happens if some of the eigenvalues are the same for a Hermitian transformation? From the fact that  $\mathbf{w} \cdot \mathbf{T}(\mathbf{u}) = \mathbf{T}(\mathbf{w}) \cdot \mathbf{u}$ , it can be seen that if  $\mathbf{u}$  is an eigenvector, we have

$$\mathbf{w} \cdot \mathbf{T}(\mathbf{u}) = \lambda \mathbf{w} \cdot \mathbf{u} = \mathbf{T}(\mathbf{w}) \cdot \mathbf{u}, \qquad (1.295)$$

This means if  $\mathbf{w}$  is orthogonal to  $\mathbf{u}$ , so is  $\mathbf{T}(\mathbf{w})$ . In other words, both  $\mathbf{w}$  and  $\mathbf{T}(\mathbf{w})$  are in the (n-1)-dimensional subspace orthogonal to  $\mathbf{u}$ . Therefore  $\mathbf{T}$  is also a Hermitian transformation in that subspace. By repeating this argument n times, it is seen that we can distill n orthogonal eigenvectors after the original n-dimensional space is exhausted. Therefore, we can construct a set of basis vectors using these eigenvectors regardless whether the eigenvalues are different or not.

It is worth noting that if we use the eigenvectors as the basis vectors, the *j*th eigenvector  $\mathbf{e}'_j$  can be represented by the array  $u'_j = (0, \ldots, 1, \ldots, 0)$ ,

where 1 appears at the *j*th column. Substituting it into Eq. (1.280), we see that in the original basis the *j*th eigenvector is represented by  $u_i = S_{ij}$ . Therefore, after all the eigenvectors  $\mathbf{u}_i$  have been found out from the equation

$$[\mathbf{M} - \lambda^{(j)}\mathbf{I}]\mathbf{u}_j = 0, \qquad (1.296)$$

we obtain the transformation matrix **S** whose column vectors are just  $\mathbf{u}_j$ . Let  $\mathbf{u}_j = a_{kj} \mathbf{e}_k$ , we have

$$S_{kj} = a_{kj}.\tag{1.297}$$

The fact that  $\mathbf{u}_i \cdot \mathbf{u}_j = \delta_{ij}$  means  $a_{ki}^* a_{kj} = \delta_{ij}$ , hence  $S_{ki}^* S_{kj} = \delta_{ij}$ . In the matrix notation this is

$$\mathbf{S}^{\dagger}\mathbf{S} = \mathbf{I}.\tag{1.298}$$

Any matrix satisfying Eq. (1.298) is called a **unitary** matrix. For a unitary matrix we have

$$\mathbf{S}^{\dagger} = \mathbf{S}^{-1},\tag{1.299}$$

hence for a Hermitian transformation Eq. (1.285) can also be written as

$$\mathbf{M}' = \mathbf{S}^{\dagger} \mathbf{M} \mathbf{S}. \tag{1.300}$$

To illustrate the usefulness of the concept of eigenvalue and eigenvector, let us solve an old high-school mathematical problem with the technique we have just learned. Consider the equation  $Ax^2+2Bxy+Cy^2=1$ . Under what conditions this equation represents an ellipse and a hyperbola respectively? To answer this question, let us write the equation in the matrix form

$$\begin{bmatrix} x & y \end{bmatrix} \begin{bmatrix} A & B \\ B & C \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = 1.$$
(1.301)

By changing to another set of basis vectors, we wish to make the equation look like

$$\begin{bmatrix} x' & y' \end{bmatrix} \begin{bmatrix} \lambda^{(1)} & 0 \\ 0 & \lambda^{(2)} \end{bmatrix} \begin{bmatrix} x' \\ y' \end{bmatrix} = \lambda^{(1)} x'^2 + \lambda^{(2)} y'^2 = 1.$$
(1.302)

If  $\lambda^{(1)}$  and  $\lambda^{(2)}$  have the same sign, the equation is a ellipse, otherwise it is a hyperbola. According to Eq. (1.289)  $\lambda^{(1)}$  and  $\lambda^{(2)}$  are determined by

$$\det \begin{bmatrix} A - \lambda & B \\ B & C - \lambda \end{bmatrix} = 0.$$
(1.303)

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Hence we have

$$\lambda^{2} - (A + C)\lambda + (AC - B^{2}) = 0.$$
(1.304)

The condition for the two roots to have the same sign is  $AC - B^2 > 0$ . If  $AC - B^2 > 0$  the equation represents an ellipse, otherwise a hyperbola. In addition, if  $|\lambda^{(1)}| \ge |\lambda^{(2)}|$ , the semi-major axis *a* and semi-minor axis *b* are given by  $a^2 = 1/|\lambda^{(2)}|$ ,  $b^2 = 1/|\lambda^{(1)}|$  respectively.

To find out which transformation matrix reduces Eq. (1.301) to Eq. (1.302), we start from Eq. (1.280).

$$\begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{bmatrix} \begin{bmatrix} x' \\ y' \end{bmatrix}.$$
 (1.305)

Substituting it into Eq. (1.301), we have

$$\begin{bmatrix} x' & y' \end{bmatrix} \begin{bmatrix} S_{11} & S_{21} \\ S_{12} & S_{22} \end{bmatrix} \begin{bmatrix} A & B \\ B & C \end{bmatrix} \begin{bmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{bmatrix} \begin{bmatrix} x' \\ y' \end{bmatrix} = 1.$$
(1.306)

Comparing with Eq. (1.302) we see the problem is reduced to finding a transformation matrix **S** such that

$$\begin{bmatrix} S_{11} & S_{21} \\ S_{12} & S_{22} \end{bmatrix} \begin{bmatrix} A & B \\ B & C \end{bmatrix} \begin{bmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{bmatrix} = \begin{bmatrix} \lambda^{(1)} & 0 \\ 0 & \lambda^{(2)} \end{bmatrix}.$$
 (1.307)

If  $\mathbf{u}$  and  $\mathbf{v}$  are the two eigenvectors that satisfy

$$\begin{bmatrix} A & B \\ B & C \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = \lambda^{(1)} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix},$$
$$\begin{bmatrix} A & B \\ B & C \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \end{bmatrix} = \lambda^{(2)} \begin{bmatrix} v_1 \\ v_2 \end{bmatrix},$$
(1.308)

we may assign  $(S_{11}, S_{21}) = (u_1, u_2), (S_{12}, S_{22}) = (v_1, v_2)$ . With the orthonormal conditions that  $|\mathbf{u}| = |\mathbf{v}| = 1$  and  $\mathbf{u} \cdot \mathbf{v} = 0$ , we see that Eq. (1.307) is satisfied. Therefore

$$\begin{bmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{bmatrix} = \begin{bmatrix} u_1 & v_1 \\ u_2 & v_2 \end{bmatrix}.$$
 (1.309)

The class of matrix that can be diagonalized is much larger than the class of Hermitian matrix. If a matrix satisfies the condition  $\mathbf{M}^{\dagger}\mathbf{M} = \mathbf{M}\mathbf{M}^{\dagger}$ , it

can be diagonalized. To prove, note that if  $\mathbf{M}$  satisfies  $\mathbf{M}^{\dagger}\mathbf{M} = \mathbf{M}\mathbf{M}^{\dagger}$ , so does  $\mathbf{S}^{-1}\mathbf{M}\mathbf{S}$ . Also note by definition we have

$$\mathbf{T}(\mathbf{w}) \cdot \mathbf{v} = \mathbf{T}(w_i \mathbf{e}_i) \cdot (v_j \mathbf{e}_j) = w_i^* M_{ki}^* v_j (\mathbf{e}_k \cdot \mathbf{e}_j)$$
$$= w_i^* M_{ik}^\dagger v_k = \mathbf{w} \cdot \mathbf{T}^\dagger(\mathbf{v}).$$
(1.310)

If **w** is a normalized eigenvector of **M** with eigenvalue  $\lambda$  and **v** is orthogonal to **w**, then  $\mathbf{T}^{\dagger}(\mathbf{v})$  is also orthogonal to **w**. In other words, both **v** and  $\mathbf{T}^{\dagger}(\mathbf{v})$  are in the (n-1)-dimensional subspace orthogonal to **w**. Therefore  $\mathbf{T}^{\dagger}$  is also a linear transformation in that subspace. Let us denote  $\mathbf{T}^{\dagger}$  that are restricted to the (n-1)-dimensional subspace orthogonal to **w** by  $\mathbf{T}^{\dagger}_{(n-1)}$  and its representing matrix by  $\mathbf{M}^{\dagger}_{(n-1)}$ , then  $\mathbf{M}^{\dagger}_{(n-1)}$  satisfies the same condition  $\mathbf{M}^{\dagger}_{(n-1)}\mathbf{M}_{(n-1)} = \mathbf{M}_{(n-1)}\mathbf{M}^{\dagger}_{(n-1)}$ . Let **u** be a normalized eigenvector of  $\mathbf{T}^{\dagger}_{(n-1)}$ . By the same argument we can find an (n-2)-dimensional subspace orthogonal to **u** in which **T** restricted to this (n-2)-dimensional subspace is a linear transformation  $\mathbf{T}_{(n-2)}$  whose representing matrix satisfying  $\mathbf{M}^{\dagger}_{(n-2)}\mathbf{M}_{(n-2)} = \mathbf{M}_{(n-2)}\mathbf{M}^{\dagger}_{(n-2)}$ . Let us assume  $\mathbf{M}_{(n-2)}$  can be diagonalized with a suitable set of normalized eigenvectors  $\mathbf{v}_i$  with eigenvalue  $\lambda_i$   $(i = 3, 4, \ldots n)$ . In the bases formed by  $\mathbf{w}$ ,  $\mathbf{u}$ , and  $\mathbf{v}_i$   $(i = 3, 4, \ldots n)$ , **M** has the following form

$$\mathbf{M} = \begin{bmatrix} \lambda & a_{12} & 0 & \dots & 0 \\ 0 & a_{22} & 0 & \dots & 0 \\ 0 & a_{32} & \lambda_3 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \\ 0 & a_{n2} & 0 & \dots & \lambda_n \end{bmatrix},$$
(1.311)

where the expansion of  $\mathbf{T}(\mathbf{u})$  in the same bases is

$$\mathbf{T}(\mathbf{u}) = a_{12}\mathbf{w} + a_{22}\mathbf{u} + \sum_{i=3}^{n} a_{i2}\mathbf{v}_i.$$
(1.312)

Since

$$\mathbf{M}^{\dagger} = \begin{bmatrix} \lambda^{*} & 0 & 0 & \dots & 0 \\ a_{12}^{*} & a_{22}^{*} & a_{32}^{*} & \dots & a_{n2}^{*} \\ 0 & 0 & \lambda_{3}^{*} & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & & \lambda_{n}^{*} \end{bmatrix}.$$
 (1.313)

The condition  $\mathbf{M}^{\dagger}\mathbf{M} = \mathbf{M}\mathbf{M}^{\dagger}$  implies

$$a_{12} = 0,$$
  
 $a_{i2} = 0 \ (i = 3, 4, \dots n).$  (1.314)

Hence **M** is diagonal. What we have proved is that if  $\mathbf{M}_{(n-2)}$  can be diagonalized, so can **M**. Since the cases for n = 1 and n = 2 are trivially true, by mathematical induction one can see the condition  $\mathbf{M}^{\dagger}\mathbf{M} = \mathbf{M}\mathbf{M}^{\dagger}$  implies that **M** can be diagonalized.

# 1.9 Vector Analysis

In single-variable calculus, the fundamental theorem of calculus relates the integration of f'(x) over [a, b] to f(b) - f(a). In multi-variable calculus, the situation is diverse. First, the integrand can be a multi-variable vector function  $\mathbf{F}(x, y, x)$ , and the integration can be over a curve, a surface, or a solid volume in the three dimensional space. In addition, as we shall see, there are different kinds of derivatives for vector functions. Each of them has a different meaning in physics. Because of such diversity, the fundamental theorem of calculus in the multi-variable case appears in different forms.

The gradient of a scalar function  $\phi(\mathbf{r})$  is defined by

$$\nabla \phi = \left(\frac{\partial \phi}{\partial x}, \frac{\partial \phi}{\partial y}, \frac{\partial \phi}{\partial z}\right). \tag{1.315}$$

Consider the difference of  $\phi$  for two adjacent points  $\mathbf{r} = (x, y, z)$  and  $\mathbf{r} + \Delta \mathbf{s} = (x + \Delta x, y + \Delta y, z + \Delta z)$ .

$$\Delta \phi = \phi(x + \Delta x, y + \Delta y, z + \Delta z) - \phi(x, y, z)$$

$$= \phi(x + \Delta x, y + \Delta y, z + \Delta z) - \phi(x, y + \Delta y, z + \Delta z)$$

$$+ \phi(x, y + \Delta y, z + \Delta z) - \phi(x, y, z + \Delta z)$$

$$+ \phi(x, y, z + \Delta z) - \phi(x, y, z)$$

$$\approx \frac{\partial \phi}{\partial x} \Delta x + \frac{\partial \phi}{\partial y} \Delta y + \frac{\partial \phi}{\partial z} \Delta z = \nabla \phi \cdot \Delta s. \qquad (1.316)$$

Hence we have

$$\phi(\mathbf{r}_2) - \phi(\mathbf{r}_1) = \int_{\mathbf{r}_1}^{\mathbf{r}_2} \nabla \phi \cdot d\mathbf{s}.$$
 (1.317)

For a fixed distance  $|\Delta \mathbf{s}|$ , the difference  $\Delta \phi$  is maximum when  $\Delta \mathbf{s}$  is parallel to  $\nabla \phi$ . Therefore,  $\nabla \phi$  is the direction in which the increase rate of  $\phi$  is the largest.

The divergence of a vector function  $\mathbf{U} = (U_x, U_y, U_z)$  is defined by

$$\nabla \cdot \mathbf{U} = \frac{\partial U_x}{\partial x} + \frac{\partial U_y}{\partial y} + \frac{\partial U_z}{\partial z}.$$
 (1.318)

Consider the outgoing flux of **U** in a small volume element v spanned by three vectors  $(\Delta x, 0, 0), (0, \Delta y, 0), (0, 0, \Delta z)$  at  $(x_0, y_0, z_0)$ . The outgoing flux is defined by

$$\int_{z_0}^{z_0+\Delta z} \int_{y_0}^{y_0+\Delta y} \left[ U_x(x_0+\Delta x, y, z) - U_x(x_0, y, z) \right] dydz$$

$$+ \int_{x_0}^{x_0+\Delta x} \int_{z_0}^{z_0+\Delta z} \left[ U_y(x, y_0+\Delta y, z) - U_y(x, y_0, z) \right] dzdx$$

$$+ \int_{y_0}^{y_0+\Delta y} \int_{x_0}^{x_0+\Delta x} \left[ U_z(x, y, z_0+\Delta z) - U_z(x, y, z_0) \right] dxdy$$

$$\approx \frac{\partial U_x}{\partial x} \Delta x \Delta y \Delta z + \frac{\partial U_y}{\partial y} \Delta x \Delta y \Delta z + \frac{\partial U_z}{\partial z} \Delta x \Delta y \Delta z$$

$$= (\nabla \cdot \mathbf{U}) \Delta x \Delta y \Delta z. \qquad (1.319)$$

We may define the surface element  $\Delta \mathbf{a}$  to be the surface normal vector times the surface area, then the six surface elements  $\Delta \mathbf{a}_j$   $(j = 1, \dots, 6)$  enclosing vare  $\pm \Delta y \Delta z \mathbf{e}_x$ ,  $\pm \Delta x \Delta z \mathbf{e}_y$ , and  $\pm \Delta x \Delta y \mathbf{e}_z$ , where  $\mathbf{e}_x$ ,  $\mathbf{e}_y$ , and  $\mathbf{e}_z$  are the unit vectors in the x, y, and z directions respectively. The product  $\Delta x \Delta y \Delta z$  in Eq. (1.319) is simply the volume of v, and it is customarily written as  $\Delta v$  for simplicity in notation. We can write Eq. (1.319) in a compact and general form

$$\sum_{j=1}^{6} \mathbf{U} \cdot \Delta \mathbf{a}_{j} = \nabla \cdot \mathbf{U} \Delta v.$$
 (1.320)

Imagine that a region V is composed of many small volumes. Summing over all the component v in the region V, we have

$$\sum_{v} \sum_{j=1}^{6} \mathbf{U} \cdot \Delta \mathbf{a}_{j} = \sum_{v} \nabla \cdot \mathbf{U} \Delta v.$$
(1.321)

On the left hand side we find that the outgoing fluxes in adjacent v cancel at the shared interfaces, therefore only the outgoing flux at the boundary surface S is left. Letting  $\Delta x, \Delta y, \Delta z \to 0$ , we may then rewrite the equation as

$$\int_{S} \mathbf{U} \cdot d\mathbf{a} = \int_{V} \nabla \cdot \mathbf{U} \, dv. \tag{1.322}$$

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#### 1.9. VECTOR ANALYSIS

Note that at the boundary surface the surface elements do not need to be perpendicular to one of the coordinate axes. If the area of a surface element is dA and the surface normal vector is **n**, then

$$\mathbf{U} \cdot d\mathbf{a} = (U_x n_x dA + U_y n_y dA + U_z n_z dA). \tag{1.323}$$

Because the projection of dA onto the x-axis is  $n_x dA$ , and similarly for the y and z-axes, we see  $\mathbf{U} \cdot d\mathbf{a}$  is the infinitesimal outgoing flux at the surface element  $d\mathbf{a}$ . Eq. (1.322) is known as **Gauss' theorem**.

The curl of a vector function  $\mathbf{F} = (F_x, F_y, F_z)$  is defined by

$$\nabla \times \mathbf{F} = \left(\frac{\partial F_z}{\partial y} - \frac{\partial F_y}{\partial z}, \frac{\partial F_x}{\partial z} - \frac{\partial F_z}{\partial x}, \frac{\partial F_y}{\partial x} - \frac{\partial F_x}{\partial y}\right).$$
(1.324)

Consider the loop integral of  $\mathbf{F}$  on a rectangular surface element  $\Delta \mathbf{a}$  at  $(x_0, y_0, z_0)$ . Let us choose a coordinate frame relative to the surface element  $\Delta \mathbf{a}$  in which the surface normal vector is in the z-direction. Then we may assume the surface element is spanned by two orthogonal vectors  $(\Delta x, 0, 0), (0, \Delta y, 0)$ . The loop integral is defined by

$$\int_{x_0}^{x_0+\Delta x} F_x(x, y_0, z_0) dx + \int_{y_0}^{y_0+\Delta y} F_y(x_0 + \Delta x, y, z_0) dy$$
  
+ 
$$\int_{x_0+\Delta x}^{x_0} F_x(x, y_0 + \Delta y, z_0) dx + \int_{y_0+\Delta y}^{y_0} F_y(x_0, y, z_0) dy$$
  
$$\approx \left(\frac{\partial F_y}{\partial x} \Delta x\right) \Delta y - \left(\frac{\partial F_x}{\partial y} \Delta y\right) \Delta x$$
  
= 
$$\left(\frac{\partial F_y}{\partial x} - \frac{\partial F_x}{\partial y}\right) \Delta x \Delta y.$$
 (1.325)

The product  $\Delta x \Delta y$  in Eq. (1.325) is simply the area of  $\Delta \mathbf{a}$ . We may define the line element  $\Delta \mathbf{l}$  to be the tangent vector times the line length, then the four line elements  $\Delta \mathbf{l}_j$   $(j = 1, \dots, 4)$  enclosing  $\Delta \mathbf{a}$  are the four vectors connecting the four corners of  $\Delta \mathbf{a}$ . Namely  $\Delta \mathbf{l}_1$  start from  $(x_0, y_0, z_0)$  to  $(x_0 + \Delta x, y_0, z_0)$ ,  $\Delta \mathbf{l}_2$  from  $(x_0 + \Delta x, y_0, z_0)$  to  $(x_0 + \Delta x, y_0 + \Delta y, z_0)$ ,  $\Delta \mathbf{l}_3$ from  $(x_0 + \Delta x, y_0 + \Delta y, z_0)$  to  $(x_0, y_0 + \Delta y, z_0)$ , and  $\Delta \mathbf{l}_4$  from  $(x_0, y_0 + \Delta y, z_0)$ back to  $(x_0, y_0, z_0)$ . In the vector notation Eq. (1.325) can be written as

$$\sum_{j=1}^{4} \int_{\Delta \mathbf{l}_{j}} \mathbf{F} \cdot d\mathbf{s} = (\nabla \times \mathbf{F}) \cdot \Delta \mathbf{a}, \qquad (1.326)$$

where the line integral for each j on the left hand side is along the line element  $\Delta \mathbf{l}_j$ . Note that if a vector identity is true in one coordinate frame,

it is true in all coordinate frames. Therefore Eq. (1.326) is not limited to the special coordinate frame we choose to derive it.

Imagine that a surface A is composed of many small surface elements  $\Delta \mathbf{a}$ . Summing over all the component surface elements  $\Delta \mathbf{a}$ , we have

$$\sum_{\Delta \mathbf{a}} \sum_{j=1}^{4} \int_{\Delta \mathbf{l}_{j}} \mathbf{F} \cdot d\mathbf{s} = \sum_{\Delta \mathbf{a}} (\nabla \times \mathbf{F}) \cdot \Delta \mathbf{a}.$$
(1.327)

On the left hand side we find that the line integrations  $\int_{\Delta \mathbf{l}_j} \mathbf{F} \cdot d\mathbf{s}$  in adjacent  $\Delta \mathbf{a}$  cancel at the shared borders, therefore only the loop integration at the boundary curve C is left. Letting  $\Delta \mathbf{a} \to 0$ , we may rewrite the equation as

$$\oint_C \mathbf{F} \cdot d\mathbf{s} = \int_A (\nabla \times \mathbf{F}) \cdot d\mathbf{a}.$$
(1.328)

This is known as **Stokes' theorem**.

If a vector field  $\mathbf{F}$  satisfies  $\nabla \times \mathbf{F} = 0$  everywhere, then the line integral  $\int \mathbf{F} \cdot d\mathbf{s}$  from a point  $\mathbf{r}_i$  to another point  $\mathbf{r}_f$  is independent of the path of integration. This can be seen from the fact that

$$\int_{\mathbf{r}_{i}}^{\mathbf{r}_{f}} \mathbf{F} \cdot d\mathbf{s} \text{ (along path 1)} + \int_{\mathbf{r}_{f}}^{\mathbf{r}_{i}} \mathbf{F} \cdot d\mathbf{s} \text{ (along path 2)}$$
$$= \oint \mathbf{F} \cdot d\mathbf{s} = 0, \qquad (1.329)$$

which implies

$$\int_{\mathbf{r}_{i}}^{\mathbf{r}_{f}} \mathbf{F} \cdot d\mathbf{s} \text{ (along path 1)} = \int_{\mathbf{r}_{i}}^{\mathbf{r}_{f}} \mathbf{F} \cdot d\mathbf{s} \text{ (along path 2)}.$$
(1.330)

We may define

$$\phi(\mathbf{r}) - \phi(\mathbf{r}_0) \equiv \int_{\mathbf{r}_0}^{\mathbf{r}} \mathbf{F} \cdot d\mathbf{s}, \qquad (1.331)$$

where  $\mathbf{r}_0$  is an arbitrary reference point. Because the line integration is independent of path, such a definition gives a unique  $\phi(\mathbf{r})$ . From the fact that

$$\int_{\mathbf{r}_0}^{\mathbf{r}} \nabla \phi \cdot d\mathbf{s} = \phi(\mathbf{r}) - \phi(\mathbf{r}_0), \qquad (1.332)$$

we have  $\mathbf{F} = \nabla \phi$ . In other words, if  $\nabla \times \mathbf{F} = 0$  everywhere, there exists a scalar field  $\phi$  such that  $\mathbf{F} = \nabla \phi$ .

### 1.10. CALCULUS IN CURVED COORDINATE SYSTEMS

Now we see the fundamental theorem of calculus in the three dimensional vector space has three forms. The first one, Eq. (1.332), relates the line integration of  $\nabla \phi$  to the values of  $\phi$  at the end points of the integration path. The second one, Eq. (1.328), relates the surface integration of  $\nabla \times \mathbf{F}$  to the line integration of  $\mathbf{F}$  along the boundary of the surface. The third one, Eq. (1.322), relates the volume integration of  $\nabla \cdot \mathbf{U}$  to the surface integration of  $\mathbf{U}$  at the boundary.

## 1.10 Calculus in Curved Coordinate Systems

Let us consider general coordinate systems in which the three axes remains orthogonal to each other, but the orientations of the axes and length scale for each axis may be functions of the position. Unlike the rectangular coordinate system, in a general coordinate system the coordinates are no longer simply the length of the projection of the position vector on the fixed coordinate axes. Instead we must make a clear distinguish between the coordinates and the components of the position vector. For example, in the spherical coordinate system a position is marked by the coordinates  $\{r, \theta, \phi\}$ , and the local coordinate axes are  $\mathbf{e}_r$ ,  $\mathbf{e}_{\theta}$ , and  $\mathbf{e}_{\phi}$ , where

$$\begin{aligned}
\mathbf{e}_{r} &= \sin\theta\cos\phi\mathbf{e}_{x} + \sin\theta\sin\phi\mathbf{e}_{y} + \cos\theta\mathbf{e}_{z}, \\
\mathbf{e}_{\theta} &= \cos\theta\cos\phi\mathbf{e}_{x} + \cos\theta\sin\phi\mathbf{e}_{y} - \sin\theta\mathbf{e}_{z}, \\
\mathbf{e}_{\phi} &= -\sin\phi\mathbf{e}_{x} + \cos\phi\mathbf{e}_{y}.
\end{aligned}$$
(1.333)

Clearly, the orientations of  $\mathbf{e}_r$ ,  $\mathbf{e}_{\theta}$ , and  $\mathbf{e}_{\phi}$  are functions of the coordinates  $\theta$ and  $\phi$ . A line element at  $\{r, \theta, \phi\}$  can be written as

$$d\mathbf{l} = dr\mathbf{e}_r + rd\theta\mathbf{e}_\theta + r\sin\theta d\phi\mathbf{e}_\phi, \qquad (1.334)$$

where on the right-hand side r in the second term and  $r \sin \theta$  in the third term are the scale lengths for  $d\theta$  and  $d\phi$  respectively. Clearly the scale lengths are also functions of the coordinates r and  $\theta$ . In a rectangular coordinate system, we specify a point in the space either by the coordinates  $\{x, y, z\}$ or by the position vector  $x\mathbf{e}_x + y\mathbf{e}_y + z\mathbf{e}_z$  which is also written as (x, y, z). Because of this equivalence, we do not distinguish  $\{x, y, z\}$  from (x, y, z). In a non-rectangular coordinate system, the situation is different. For example in the spherical coordinate system we may use the coordinates  $\{r, \theta, \phi\}$  or the position vector  $r\mathbf{e}_r$  to specify a point in the space. In this case the meaning of  $\{r, \theta, \phi\}$  and  $(r, \theta, \phi)$  are different. Let us investigate how a non-rectangular coordinate system changes the appearance of vector analysis. Assume the line element in a general coordinate system is

$$d\mathbf{l} = h_1 dq_1 \mathbf{e}_1 + h_2 dq_2 \mathbf{e}_2 + h_3 dq_3 \mathbf{e}_3, \tag{1.335}$$

where  $\{q_1, q_2, q_3\}$  are the coordinates and  $\{h_1, h_2, h_3\}$  are the scale lengths. Consider the gradient operator  $\nabla u$ . Since

$$du = \nabla u \cdot d\mathbf{l} = \frac{\partial u}{\partial q_1} dq_1 + \frac{\partial u}{\partial q_2} dq_2 + \frac{\partial u}{\partial q_3} dq_3, \qquad (1.336)$$

we have

$$\nabla u = \left(\frac{1}{h_1}\frac{\partial u}{\partial q_1}, \frac{1}{h_2}\frac{\partial u}{\partial q_2}, \frac{1}{h_3}\frac{\partial u}{\partial q_3}\right).$$
(1.337)

In cylindrical coordinate systems  $q_1 = r$ ,  $q_2 = \theta$ ,  $q_3 = z$ ,  $h_1 = 1$ ,  $h_2 = r$ ,  $h_3 = 1$ , hence

$$\nabla u = \frac{\partial u}{\partial r}\hat{\mathbf{r}} + \frac{1}{r}\frac{\partial u}{\partial \theta}\hat{\boldsymbol{\theta}} + \frac{\partial u}{\partial z}\hat{\mathbf{z}}.$$
(1.338)

In spherical coordinate systems  $q_1 = r$ ,  $q_2 = \theta$ ,  $q_3 = \phi$ ,  $h_1 = 1$ ,  $h_2 = r$ ,  $h_3 = r \sin \theta$ , hence

$$\nabla u = \frac{\partial u}{\partial r}\hat{\mathbf{r}} + \frac{1}{r}\frac{\partial u}{\partial \theta}\hat{\boldsymbol{\theta}} + \frac{1}{r\sin\theta}\frac{\partial u}{\partial \phi}\hat{\boldsymbol{\phi}}.$$
(1.339)

Now we consider the divergence operator  $\nabla \cdot \mathbf{F}$ . For a volume element V at  $\{q_1, q_2, q_3\}$ , by Gauss' theorem we have

$$\int_{S} \mathbf{F} \cdot d\mathbf{a} = \int_{V} \nabla \cdot \mathbf{F} dV, \qquad (1.340)$$

where S represents the six surface elements enclosing V. Let us use the subscripts (1+) and (1-) to denote evaluating at  $\{q_1+dq_1, q_2, q_3\}$  and  $\{q_1, q_2, q_3\}$ respectively, and similarly for (2+), (2-) and (3+), (3-). Since

$$d\mathbf{a}_{(1+)} \equiv h_2(q_1 + dq_1, q_2, q_3)h_3(q_1 + dq_1, q_2, q_3)dq_2dq_3\mathbf{e}_1, d\mathbf{a}_{(1-)} \equiv -h_2(q_1, q_2, q_3)h_3(q_1, q_2, q_3)dq_2dq_3\mathbf{e}_1,$$

### 1.10. CALCULUS IN CURVED COORDINATE SYSTEMS

and similarly for  $d\mathbf{a}_{(2)+}, d\mathbf{a}_{(2-)}, d\mathbf{a}_{(3+)}$ , and  $d\mathbf{a}_{(3-)}$ , we have

$$\begin{split} \int_{S} \mathbf{F} \cdot d\mathbf{a} &= \left[ \mathbf{F}_{(1+)} \cdot d\mathbf{a}_{(1+)} + \mathbf{F}_{(1-)} \cdot d\mathbf{a}_{(1-)} \right] \\ &+ \left[ \mathbf{F}_{(2+)} \cdot d\mathbf{a}_{(2+)} + \mathbf{F}_{(2-)} \cdot d\mathbf{a}_{(2-)} \right] \\ &+ \left[ \mathbf{F}_{(3+)} \cdot d\mathbf{a}_{(3+)} + \mathbf{F}_{(3-)} \cdot d\mathbf{a}_{(3-)} \right] \\ &= \left[ (F_1 h_2 h_3)_{(1+)} - (F_1 h_2 h_3)_{(1-)} \right] dq_2 dq_3 \\ &+ \left[ (F_2 h_1 h_3)_{(2+)} - (F_2 h_1 h_3)_{(2-)} \right] dq_1 dq_2 \\ &= \left[ \frac{\partial (F_1 h_2 h_3)}{\partial q_1} dq_1 \right] dq_2 dq_3 \\ &+ \left[ \left( \frac{\partial (F_1 h_2 h_3)}{\partial q_2} dq_2 \right] dq_1 dq_3 \\ &+ \left[ \frac{\partial (F_2 h_1 h_3)}{\partial q_2} dq_2 \right] dq_1 dq_3 \\ &+ \left[ \frac{\partial (F_3 h_1 h_2)}{\partial q_3} dq_3 \right] dq_1 dq_2 \\ &= \left[ \frac{\partial (F_1 h_2 h_3)}{\partial q_1} + \frac{\partial (F_2 h_1 h_3)}{\partial q_2} + \frac{\partial (F_3 h_1 h_2)}{\partial q_3} \right] dq_1 dq_2 dq_3. \end{split}$$

Since

$$dV = h_1 h_2 h_3 \, dq_1 dq_2 dq_3,$$

comparing with the volume integral on the right-hand side of Eq. (1.340)

$$\int_{V} \nabla \cdot \mathbf{F} dV = \nabla \cdot \mathbf{F} h_1 h_2 h_3 \, dq_1 dq_2 dq_3,$$

we have

$$\nabla \cdot \mathbf{F} = \frac{1}{h_1 h_2 h_3} \left[ \frac{\partial \left( h_2 h_3 F_1 \right)}{\partial q_1} + \frac{\partial \left( h_1 h_3 F_2 \right)}{\partial q_2} + \frac{\partial \left( h_1 h_2 F_3 \right)}{\partial q_3} \right].$$
(1.341)

In the cylindrical coordinate system,  $q_1 = r$ ,  $q_2 = \theta$ ,  $q_3 = z$ ,  $h_1 = 1$ ,  $h_2 = r$ ,  $h_3 = 1$ , hence

$$\nabla \cdot \mathbf{F} = \frac{1}{r} \left[ \frac{\partial \left( rF_r \right)}{\partial r} + \frac{\partial F_\theta}{\partial \theta} + \frac{\partial \left( rF_z \right)}{\partial z} \right].$$
(1.342)

In the spherical coordinate system,  $q_1 = r$ ,  $q_2 = \theta$ ,  $q_3 = \phi$ ,  $h_1 = 1$ ,  $h_2 = r$ ,  $h_3 = r \sin \theta$ , hence

$$\nabla \cdot \mathbf{F} = \frac{1}{r^2 \sin \theta} \left[ \frac{\partial \left( r^2 \sin \theta F_r \right)}{\partial r} + \frac{\partial \left( r \sin \theta F_\theta \right)}{\partial \theta} + \frac{\partial \left( r F_\phi \right)}{\partial \phi} \right].$$
(1.343)

Next we consider the Laplacian operator.

$$\nabla^{2} u = \nabla \cdot \nabla u 
= \nabla \cdot \left(\frac{1}{h_{1}} \frac{\partial u}{\partial q_{1}}, \frac{1}{h_{2}} \frac{\partial u}{\partial q_{2}}, \frac{1}{h_{3}} \frac{\partial u}{\partial q_{3}}\right) 
= \frac{1}{h_{1}h_{2}h_{3}} \left[\frac{\partial}{\partial q_{1}} \left(\frac{h_{2}h_{3}}{h_{1}} \frac{\partial u}{\partial q_{1}}\right) 
+ \frac{\partial}{\partial q_{2}} \left(\frac{h_{1}h_{3}}{h_{2}} \frac{\partial u}{\partial q_{2}}\right) + \frac{\partial}{\partial q_{3}} \left(\frac{h_{1}h_{2}}{h_{3}} \frac{\partial u}{\partial q_{3}}\right)\right].$$
(1.344)

In the cylindrical coordinate system,  $q_1 = r$ ,  $q_2 = \theta$ ,  $q_3 = z$ ,  $h_1 = 1$ ,  $h_2 = r$ ,  $h_3 = 1$ , hence

$$\nabla^2 u = \frac{1}{r} \left[ \frac{\partial}{\partial r} \left( r \frac{\partial u}{\partial r} \right) + \frac{\partial}{\partial \theta} \left( \frac{1}{r} \frac{\partial u}{\partial \theta} \right) + \frac{\partial}{\partial z} \left( r \frac{\partial u}{\partial z} \right) \right].$$
(1.345)

In the spherical coordinate system,  $q_1 = r$ ,  $q_2 = \theta$ ,  $q_3 = \phi$ ,  $h_1 = 1$ ,  $h_2 = r$ ,  $h_3 = r \sin \theta$ , hence

$$\nabla^{2} u = \frac{1}{r^{2} \sin \theta} \left[ \frac{\partial}{\partial r} \left( r^{2} \sin \theta \frac{\partial u}{\partial r} \right) + \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial u}{\partial \theta} \right) + \frac{\partial}{\partial \phi} \left( \frac{1}{\sin \theta} \frac{\partial u}{\partial \phi} \right) \right].$$
(1.346)

Finally we consider the curl operator  $\nabla \times$ . For a surface element S at  $\{q_1, q_2, q_3\}$  facing the  $\mathbf{e}_3$  direction, by Stokes' theorem we have

$$\oint_{L} \mathbf{F} \cdot d\mathbf{l} = \int_{S} \nabla \times \mathbf{F} \cdot d\mathbf{a}, \qquad (1.347)$$

where L represents the four line elements enclosing S. Let us use the subscripts (1+) and (1-) to denote evaluating at  $\{q_1+dq_1, q_2, q_3\}$  and  $\{q_1, q_2, q_3\}$ respectively, and similarly for (2+), (2-). We have

$$\begin{aligned} d\mathbf{l}_{(1+)} &= h_{2(1+)} dq_2 \mathbf{e}_2, \\ d\mathbf{l}_{(1-)} &= -h_{2(1-)} dq_2 \mathbf{e}_2, \\ d\mathbf{l}_{(2+)} &= -h_{1(2+)} dq_1 \mathbf{e}_1, \\ d\mathbf{l}_{(2-)} &= h_{1(2-)} dq_1 \mathbf{e}_1, \end{aligned}$$

and

$$dA_3 = h_1 h_2 \, dq_1 dq_2.$$

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Therefore

$$\begin{split} \oint_{L} \mathbf{F} \cdot d\mathbf{l} &= \left[ \mathbf{F}_{(1+)} \cdot d\mathbf{l}_{(1+)} + \mathbf{F}_{(1-)} \cdot d\mathbf{l}_{(1-)} \right] \\ &+ \left[ \mathbf{F}_{(2+)} \cdot d\mathbf{l}_{(2+)} + \mathbf{F}_{(2-)} \cdot d\mathbf{l}_{(2-)} \right] \\ &= \left[ (h_2 F_2)_{(1+)} - (h_2 F_2)_{(1-)} \right] dq_2 \\ &- \left[ (h_1 F_1)_{(2+)} - (h_1 F_1)_{(2-)} \right] dq_1 \\ &= \left[ \frac{\partial (h_2 F_2)}{\partial q_1} - \frac{\partial (h_1 F_1)}{\partial q_2} \right] dq_1 dq_2 \\ &= \frac{1}{h_1 h_2} \left[ \frac{\partial (h_2 F_2)}{\partial q_1} - \frac{\partial (h_1 F_1)}{\partial q_2} \right] dA_3. \end{split}$$

Comparing with the surface integral on the right-hand side of Eq. (1.347), we have

$$(\nabla \times \mathbf{F}) \cdot \mathbf{e}_3 = \frac{1}{h_1 h_2} \left[ \frac{\partial (h_1 F_1)}{\partial q_2} - \frac{\partial (h_2 F_2)}{\partial q_1} \right],$$

and in general

$$\nabla \times \mathbf{F} = \frac{1}{h_2 h_3} \left[ \frac{\partial (h_3 F_3)}{\partial q_2} - \frac{\partial (h_2 F_2)}{\partial q_3} \right] \mathbf{e}_1 + \frac{1}{h_1 h_3} \left[ \frac{\partial (h_1 F_1)}{\partial q_3} - \frac{\partial (h_3 F_3)}{\partial q_1} \right] \mathbf{e}_2 + \frac{1}{h_1 h_2} \left[ \frac{\partial (h_2 F_2)}{\partial q_1} - \frac{\partial (h_1 F_1)}{\partial q_2} \right] \mathbf{e}_3.$$
(1.348)

In the cylindrical coordinate system,  $q_1 = r$ ,  $q_2 = \theta$ ,  $q_3 = z$ ,  $h_1 = 1$ ,  $h_2 = r$ ,  $h_3 = 1$ , hence

$$\nabla \times \mathbf{F} = \frac{1}{r} \left[ \frac{\partial F_z}{\partial \theta} - \frac{\partial (rF_{\theta})}{\partial z} \right] \hat{\mathbf{r}} + \left[ \frac{\partial F_r}{\partial z} - \frac{\partial F_z}{\partial r} \right] \hat{\boldsymbol{\theta}} + \frac{1}{r} \left[ \frac{\partial (rF_{\theta})}{\partial r} - \frac{\partial F_r}{\partial \theta} \right] \hat{\mathbf{z}}$$
(1.349)

In the spherical coordinate system,  $q_1 = r$ ,  $q_2 = \theta$ ,  $q_3 = \phi$ ,  $h_1 = 1$ ,  $h_2 = r$ ,  $h_3 = r \sin \theta$ , hence

$$\nabla \times \mathbf{F} = \frac{1}{r^2 \sin \theta} \left[ \frac{\partial (r \sin \theta F_{\phi})}{\partial \theta} - \frac{\partial (rF_{\theta})}{\partial \phi} \right] \hat{\mathbf{r}} + \frac{1}{r \sin \theta} \left[ \frac{\partial F_r}{\partial \phi} - \frac{\partial (r \sin \theta F_{\phi})}{\partial r} \right] \hat{\boldsymbol{\theta}} + \frac{1}{r} \left[ \frac{\partial (rF_{\theta})}{\partial r} - \frac{\partial F_r}{\partial \theta} \right] \hat{\boldsymbol{\phi}}.$$
(1.350)

## 1.11 Vector Formulas

The following list is a collection of formulas commonly used in vector analysis. It is straightforward to verify these formulas, and they are useful enough that it helps to memorize each of them. If you hate memorizing, it is possible to prove them on the fly by using the following tensor notation

$$\mathbf{a} \cdot \mathbf{b} = a_i b_i, \tag{1.351}$$

$$\mathbf{a} \times \mathbf{b} = \epsilon_{ijk} a_j b_k, \tag{1.352}$$

where the repeated indices are summed over, and

$$\epsilon_{ijk} = \begin{cases} 1 & \text{for even permutations of } i, j, k \\ \text{starting from } (i, j, k) = (1, 2, 3) \\ 0 & \text{if any two indices are equal} \\ -1 & \text{for odd permutations of } i, j, k \\ \text{starting from } (i, j, k) = (1, 2, 3). \end{cases}$$
(1.353)

We will also use the notation

$$\delta_{ij} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases}$$
(1.354)

and the identity

$$\epsilon_{ijk}\epsilon_{lmk} = \delta_{il}\delta_{jm} - \delta_{im}\delta_{jl} \tag{1.355}$$

in the following derivations. To prove the above identity, we note that  $\epsilon_{ijk}\epsilon_{lmk}$  is nonzero only when  $i \neq j \neq k$  and  $l \neq m \neq k$ . This leaves only two possibilities: i = l, j = m or i = m, j = l. In the former case the signs of  $\epsilon_{ijk}$  and  $\epsilon_{lmk}$  are the same, whereas in the latter case they are opposite.  $\delta_{il}\delta_{jm} - \delta_{im}\delta_{jl}$  is just the mathematical expression for these two cases.

$$\mathbf{a} \cdot (\mathbf{b} \times \mathbf{c}) = \mathbf{b} \cdot (\mathbf{c} \times \mathbf{a}) = \mathbf{c} \cdot (\mathbf{a} \times \mathbf{b}).$$
$$a_i \epsilon_{ijk} b_j c_k = b_j \epsilon_{jki} c_k a_i = c_k \epsilon_{kij} a_i b_j.$$
(1.356)

$$\mathbf{a} \times (\mathbf{b} \times \mathbf{c}) = (\mathbf{a} \cdot \mathbf{c})\mathbf{b} - (\mathbf{a} \cdot \mathbf{b})\mathbf{c}.$$
  

$$\epsilon_{ijk}a_j\epsilon_{klm}b_lc_m = \epsilon_{ijk}a_j\epsilon_{lmk}b_lc_m$$
  

$$= \delta_{il}\delta_{jm}a_jb_lc_m - \delta_{im}\delta_{lj}a_jb_lc_m$$
  

$$= a_jc_jb_i - a_jb_jc_i.$$
(1.357)

# 1.11. VECTOR FORMULAS

$$(\mathbf{a} \times \mathbf{b}) \cdot (\mathbf{c} \times \mathbf{d}) = (\mathbf{a} \cdot \mathbf{c})(\mathbf{b} \cdot \mathbf{d}) - (\mathbf{a} \cdot \mathbf{d})(\mathbf{b} \cdot \mathbf{c}).$$

$$\epsilon_{ijk} a_j b_k \epsilon_{ilm} c_l d_m = \delta_{jl} \delta_{km} a_j b_k c_l d_m - \delta_{jm} \delta_{kl} a_j b_k c_l d_m$$

$$= a_j c_j b_k d_k - a_j d_j b_k c_k.$$

$$(1.358)$$

$$\nabla \times (\nabla \psi) = 0.$$
  

$$\epsilon_{ijk} \frac{\partial}{\partial x_j} \frac{\partial \psi}{\partial x_k} = \frac{\epsilon_{ijk} + \epsilon_{ikj}}{2} \frac{\partial}{\partial x_j} \frac{\partial \psi}{\partial x_k} = 0.$$
(1.359)

$$\nabla \cdot (\nabla \times \mathbf{a}) = 0.$$
  

$$\epsilon_{ijk} \frac{\partial}{\partial x_i} \frac{\partial a_k}{\partial x_j} = \frac{\epsilon_{ijk} + \epsilon_{jik}}{2} \frac{\partial}{\partial x_i} \frac{\partial a_k}{\partial x_j} = 0.$$
 (1.360)

$$\nabla \times (\psi \mathbf{a}) = \nabla \psi \times \mathbf{a} + \psi \nabla \times \mathbf{a}.$$
  

$$\epsilon_{ijk} \frac{\partial (\psi a_k)}{\partial x_j} = \epsilon_{ijk} \frac{\partial \psi}{\partial x_j} a_k + \psi \epsilon_{ijk} \frac{\partial a_k}{\partial x_j}.$$
(1.361)

$$\nabla \times (\nabla \times \mathbf{a}) = \nabla (\nabla \cdot \mathbf{a}) - \nabla^2 \mathbf{a}.$$
  

$$\epsilon_{ijk} \frac{\partial}{\partial x_j} \epsilon_{klm} \frac{\partial}{\partial x_l} a_m = \epsilon_{ijk} \frac{\partial}{\partial x_j} \epsilon_{lmk} \frac{\partial}{\partial x_l} a_m$$
  

$$= \frac{\partial}{\partial x_i} \frac{\partial}{\partial x_j} a_j - \frac{\partial}{\partial x_j} \frac{\partial}{\partial x_j} a_i.$$
 (1.362)

$$\nabla \cdot (\psi \mathbf{a}) = (\mathbf{a} \cdot \nabla)\psi + \psi \nabla \cdot \mathbf{a}.$$
  
$$\frac{\partial(\psi a_k)}{\partial x_k} = \frac{\partial \psi}{\partial x_k} a_k + \psi \frac{\partial a_k}{\partial x_k}.$$
 (1.363)

Using the tensor notation to prove the following three equations is left as an exercise.

$$\nabla(\mathbf{a} \cdot \mathbf{b}) = (\mathbf{a} \cdot \nabla)\mathbf{b} + (\mathbf{b} \cdot \nabla)\mathbf{a} + \mathbf{a} \times (\nabla \times \mathbf{b}) + \mathbf{b} \times (\nabla \times \mathbf{a}). \quad (1.364)$$

$$\nabla \cdot (\mathbf{a} \times \mathbf{b}) = \mathbf{b} \cdot (\nabla \times \mathbf{a}) - \mathbf{a} \cdot (\nabla \times \mathbf{b}).$$
(1.365)

$$\nabla \times (\mathbf{a} \times \mathbf{b}) = \mathbf{a}(\nabla \cdot \mathbf{b}) - \mathbf{b}(\nabla \cdot \mathbf{a}) + (\mathbf{b} \cdot \nabla)\mathbf{a} - (\mathbf{a} \cdot \nabla)\mathbf{b}.$$
(1.366)

# 1.12 Multivariable Taylor Expansion

Let  $C^{\infty}$  be the space spanned by all the functions whose derivatives of any order are continuous. A translation operator  $\hat{T}(a)$  is defined by the following relation

$$f(x+a) = \hat{T}(a)f(x),$$
 (1.367)

where f(x) is any function in  $C^{\infty}$ . From the definition we have

$$f(x+a+b) = \hat{T}(a+b)f(x) = \hat{T}(a)\hat{T}(b)f(x) = \hat{T}(b)\hat{T}(a)f(x). \quad (1.368)$$

Differentiate with respect to a, we obtain

$$\hat{T}'(a+b)f(x) = \hat{T}'(a)\hat{T}(b)f(x).$$
 (1.369)

Let a = 0, we have

$$\hat{T}'(b)f(x) = \hat{T}'(0)\hat{T}(b)f(x).$$
 (1.370)

Therefore  $\hat{T}(b)$  satisfies the differential equation

$$\hat{T}'(b) = \hat{T}'(0)\hat{T}(b) \tag{1.371}$$

with the initial condition  $\hat{T}(0) = 1$ . The solution is

$$\hat{T}(b) = e^{\hat{T}'(0)b}.$$
 (1.372)

By definition,

$$\hat{T}'(0)f(x) = \lim_{\epsilon \to 0} \left[ \frac{T(\epsilon) - 1}{\epsilon} \right] f(x)$$
$$= \lim_{\epsilon \to 0} \left[ \frac{f(x+\epsilon) - f(x)}{\epsilon} \right] = \left( \frac{d}{dx} \right) f(x), \qquad (1.373)$$

hence

$$\hat{T}'(0) = \frac{d}{dx} \tag{1.374}$$

and we obtain

$$f(x+a) = \hat{T}(a)f(x) = e^{\left(a\frac{d}{dx}\right)}f(x) = \sum_{n=0}^{\infty} \frac{a^n}{n!} \left(\frac{d}{dx}\right)^n f(x).$$
(1.375)

### 1.13. FINDING EXTREMA UNDER CONSTRAINTS

This is just the Taylor expansion for f(x).

Now we are ready to derive the multivariable Taylor expansion. The translation operator  $\hat{T}(\mathbf{a})$  is defined by

$$f(\mathbf{x} + \mathbf{a}) = \hat{T}(\mathbf{a})f(\mathbf{x}), \qquad (1.376)$$

and we have

$$\hat{T}(\mathbf{a} + \mathbf{b})f(\mathbf{x}) = \hat{T}(\mathbf{a})\hat{T}(\mathbf{b})f(\mathbf{x}).$$
(1.377)

Take the gradient with respect to  $\mathbf{a}$  and then let  $\mathbf{a} = 0$ , we have

$$\nabla \hat{T}(\mathbf{b}) = \nabla \hat{T}(0)\hat{T}(\mathbf{b}) \tag{1.378}$$

with the initial condition  $\hat{T}(0) = 1$ . The solution is

$$\hat{T}(\mathbf{b}) = e^{\nabla \hat{T}(0) \cdot \mathbf{b}}.$$
(1.379)

By definition,

$$\begin{bmatrix} \nabla \hat{T}(0) \cdot \boldsymbol{\epsilon} \end{bmatrix} f(\mathbf{x}) = \lim_{\boldsymbol{\epsilon} \to 0} \begin{bmatrix} \hat{T}(\boldsymbol{\epsilon}) - 1 \end{bmatrix} f(x) \\ = \lim_{\boldsymbol{\epsilon} \to 0} f(\mathbf{x} + \boldsymbol{\epsilon}) - f(\mathbf{x}) = (\boldsymbol{\epsilon} \cdot \nabla) f(\mathbf{x}). \quad (1.380)$$

Hence

$$\nabla \hat{T}(0) = \nabla \tag{1.381}$$

and we obtain

$$f(\mathbf{x} + \mathbf{a}) = \hat{T}(\mathbf{a})f(\mathbf{x}) = e^{(\mathbf{a} \cdot \nabla)}f(\mathbf{x}) = \sum_{n=0}^{\infty} \frac{(\mathbf{a} \cdot \nabla)^n}{n!}f(\mathbf{x}).$$
 (1.382)

This is the multivariable Taylor expansion for  $f(\mathbf{x})$ .

## 1.13 Finding Extrema under Constraints

Consider the problem of finding the extrema of a function  $\phi(\mathbf{x})$  under the *m* constraints  $C_k(\mathbf{x}) = 0, \ k = 1, 2, \dots, m$ , where **x** is an array of *n* variables and m < n. We cannot use the usual criteria

$$\frac{\partial \phi}{\partial x_j} = 0 \tag{1.383}$$

for  $j = 1, 2, \dots, n$  because under the constraints  $x_j$  are no longer independent variables. Eq. (1.383) together with the constraints form n + m equations for the *n* variables **x**, which cannot be satisfied at the same time. To walk around this problem, let us temporarily turn off the constraints and define a new function

$$\Phi(\mathbf{x}) = \phi(\mathbf{x}) + \sum_{k=1}^{m} \lambda_k C_k(\mathbf{x}).$$
(1.384)

The extrema of  $\Phi(\mathbf{x})$  are determined by

$$\frac{\partial \phi}{\partial x_j} + \sum_{k=1}^m \lambda_k \frac{\partial C_k}{\partial x_j} = 0 \tag{1.385}$$

for  $j = 1, 2, \dots, n$ , where  $\lambda_k$  is a set of arbitrary parameters whose values will be determined later. Now let us set  $C_k(\mathbf{x}) = 0$ . Then the extrema of  $\Phi(\mathbf{x})$  is the same as that of  $\phi(\mathbf{x})$ . Again Eq. (1.385) together with the constraints form n + m equations. But this time we have n + m variables, namely the *n* variables  $\mathbf{x}$  and the *m* variables  $\lambda_k$ , therefore  $\mathbf{x}$  can be solved. This is known as the **method of Lagrange multipliers** where  $\lambda_k$  are the Lagrange multipliers.

We may understand Eq. (1.385) from a geometric point of view. Let us denote S the surface defined by the intersection of the k constraints  $C_k(\mathbf{x}) =$ 0. Assume  $\mathbf{x}_0$  is an extremum on S, then for any infinitesimal displacement  $d\mathbf{r}$  on S from  $\mathbf{x}_0$ , we have  $\phi(\mathbf{x}_0) = \phi(\mathbf{x}_0 + d\mathbf{r})$ . In other words,  $\nabla \phi(\mathbf{x}_0) \cdot d\mathbf{r} = 0$ . Hence  $\nabla \phi(\mathbf{x}_0)$  must be perpendicular to the surface S at  $\mathbf{x}_0$ . Because the dimensionality of S is n - m, we know  $\nabla \phi(\mathbf{x}_0)$  is a m-dimensional vector. On the other hand, all the vectors  $\nabla C_k(\mathbf{x}_0)$  are also perpendicular to S because  $C_k(\mathbf{x}_0) = C_k(\mathbf{x}_0 + d\mathbf{r})$ . Assume all the  $\nabla C_k(\mathbf{x}_0)$  are linearly independent, then we may write  $\nabla \phi(\mathbf{x}_0)$  as a linear combination of  $\nabla C_k(\mathbf{x}_0)$ . Namely, we have Eq. (1.385).

### **1.14** More to Know about n!

Consider the gamma function defined by

$$\Gamma(n+1) = \int_0^\infty x^n e^{-x} \, dx \tag{1.386}$$

for n > -1. Integrating by parts leads to

$$\Gamma(n+1) = \int_0^\infty n x^{n-1} e^{-x} \, dx = n \Gamma(n), \qquad (1.387)$$

#### 1.14. More to Know about n!

and  $\Gamma(1) = 1$ . Therefore if n is a positive integer or zero,  $\Gamma(n+1) = n!$ . By changing variables  $x = \alpha y^2$ , we have

$$\Gamma(n) = 2\alpha^n \int_0^\infty y^{2n-1} e^{-\alpha y^2} \, dy = (n-1)! \,. \tag{1.388}$$

Now consider the possibility that  $n = m + \frac{1}{2}$  where m is a positive integer or zero. We have

$$\Gamma\left(m+\frac{1}{2}\right) = 2\alpha^{m+\frac{1}{2}} \int_0^\infty y^{2m} e^{-\alpha y^2} dy$$
  
=  $\left(m-\frac{1}{2}\right) \left(m-\frac{3}{2}\right) \cdots \left(\frac{3}{2}\right) \left(\frac{1}{2}\right) \Gamma\left(\frac{1}{2}\right)$   
=  $\frac{(2n)!}{n! 2^{2n}} \sqrt{\pi},$  (1.389)

where

$$\Gamma\left(\frac{1}{2}\right) = \int_{-\infty}^{\infty} e^{-y^2} \, dy = \sqrt{\pi} \tag{1.390}$$

is the result of Eq. (1.243).

Let us consider the asymptotic expression of

$$n! = \int_0^\infty x^n e^{-x} \, dx \tag{1.391}$$

when  $n \gg 1$ . Since the maximum of  $x^n e^{-x}$  is at x = n, we may expand  $\ln(x^n e^{-x})$  around n in Taylor series.

$$\ln(x^n e^{-x}) \approx (-n + n \ln n) - \frac{1}{2n}(x - n)^2.$$
(1.392)

Changing variables to u = x - n, Eqs. (1.391) and (1.392) can be written together as

$$n! \approx n^n e^{-n} \int_{-n}^{\infty} \exp\left(-\frac{u^2}{2n}\right) du.$$
 (1.393)

Since  $n \gg 1$ , we may extend the lower integration bound from -n to  $-\infty$ . Then we have

$$n! \approx \sqrt{2\pi n} (n^n e^{-n}). \tag{1.394}$$

This is known as the **Stirling formula**.

The gamma function has many useful and interesting applications. Let us use it to calculate the volume  $V_n(R)$  of a sphere of radius R in *n*-dimension. Instead of calculating the volume directly, we first evaluate the surface area  $S_n(R)$  of the sphere. Since  $S_n(R)$  is proportional to  $R^{n-1}$ , we may write  $S_n(R) = c_n R^{n-1}$ . Let us consider the integral

$$I_n = \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} \exp\left(-\sum_{i=1}^n x_i^2\right) \prod_{i=1}^n dx_i$$
$$= \int_0^{\infty} e^{-r^2} c_n r^{n-1} dr$$
$$= c_n \frac{\Gamma(\frac{n}{2})}{2}.$$
(1.395)

On the other hand,

$$I_n = \prod_{i=1}^n \int_{-\infty}^\infty e^{-x_i^2} \, dx_i = (\sqrt{\pi})^n.$$
(1.396)

Hence we have

$$c_n = \frac{2\pi^{\frac{n}{2}}}{\Gamma(\frac{n}{2})},$$
(1.397)

and

$$V_n = \int_0^R c_n r^{n-1} \, dr = \frac{c_n}{n} R^n. \tag{1.398}$$
### 1.15 Exercises

**Exercise 1.1.** Calculate the derivatives of the following functions.

$$x \sin x$$

$$e^{-x^{2}}$$

$$\tan x$$

$$x^{n} \cos nx$$

$$\frac{x}{x^{2}+1}$$

$$\sqrt{x^{2}+4}$$

$$\sec x$$

$$\ln(\sqrt{x^{2}+1})$$

$$\tan^{-1} x$$

**Exercise 1.2.** Which function satisfies f''(x) = -f(x)? Hint:  $\sin x$  does. Is there another one?

**Exercise 1.3.** Which function satisfies f''(x) = f(x)? Hint:  $e^x$  does. Is there another one?

**Exercise 1.4.** Which function satisfies  $f''(x) = -k^2 f(x)$ ? Hint: Use chain rule on the answer of Exercise 1.2.

**Exercise 1.5.** Which function satisfies  $f''(x) = k^2 f(x)$ ? Hint: Use chain rule on the answer of Exercise 1.3.)

**Exercise 1.6.** Whose derivative is  $\ln x$ ? Hint: Calculate the derivative of  $x \ln x$ .

**Exercise 1.7.** Whose derivative is  $\sqrt{x}$ ? Hint: Can it be written as a constant times  $qx^{q-1}$ ?

**Exercise 1.8.** Whose derivative is  $x/(x^2 + 1)$ ? Hint: Can it be written as a constant times f'(g(x))g'(x)?

**Exercise 1.9.** Whose derivative is  $x \sin x$ ? Hint: Check the derivative of  $-x \cos x$ .

**Exercise 1.10.** Whose derivative is  $1/(x^2 - 1)$ ? Hint: How about changing it to 1/(x-1)-1/(x+1)?

**Exercise 1.11.** Integrate  $\int \tan x \, dx$ . Hint: Substitute  $u = \cos x$ .

**Exercise 1.12.** Integrate  $\int e^x \sin x \, dx$ . Hint: Let  $u = e^x$ ,  $dv = \sin x \, dx$ . You have to use a similar substitution once more.

Exercise 1.13. Integrate

$$\int \frac{dx}{1+e^x}.$$

Hint: Try the following.

$$\int \frac{e^{-x} dx}{1 + e^{-x}} \quad \text{or} \quad \int \left(1 - \frac{e^x}{1 + e^x}\right) dx$$

Exercise 1.14. Integrate

$$\int \frac{2x+3}{x^2+x+1} \, dx.$$

Hint: Consider the following.

$$\int \frac{2x+3}{x^2+x+1} \, dx = \int \frac{2x+1}{x^2+x+1} \, dx + \int \frac{2}{x^2+x+1} \, dx$$
$$\int \frac{2}{x^2+x+1} \, dx = 2 \int \frac{dx}{\left(x+\frac{1}{2}\right)^2+\frac{3}{4}}$$

Exercise 1.15. Integrate

$$\int \frac{3x^2 + 2x - 2}{x^3 - 1} \, dx.$$

Hint: Consider the following.

$$\int \frac{3x^2 + 2x - 2}{x^3 - 1} \, dx = \int \frac{dx}{x - 1} + \int \frac{2x + 3}{x^2 + x + 1} \, dx$$

Exercise 1.16. Prove

$$\int_0^y \frac{1}{1+x^2} \, dx = \tan^{-1} y$$

#### 1.15. EXERCISES

not by substituting  $x = \tan \theta$ , but by using

$$\frac{1}{1+x^2} = \frac{1}{2i} \left( \frac{1}{x-i} - \frac{1}{x+i} \right).$$

**Exercise 1.17.** It is well known that

$$1 + 2 + 3 + 4 \dots + n = \frac{n(n+1)}{2},$$
$$1^2 + 2^2 + 3^2 + 4^2 \dots + n^2 = \frac{n(n+1)(2n+1)}{6}$$

You can prove these relations by mathematical induction, but how do you know the closed-form expressions on the right-hand side in the first place? Hint: Let

$$f_k(n) = \sum_{i=1}^n i^k,$$

derive  $f_3(n)$  by using the identity  $C_k^{n+1} - C_k^n = C_{k-1}^n$ .

**Exercise 1.18.** The number  $i^i$  looks like a very complex complex number. But in fact it is a real number. What is it?

**Exercise 1.19.**  $e = e^{1+2\pi i} = e^{1-2\pi i}$ , therefore  $e = (e^{1+2\pi i})^{1-2\pi i} = e^{1+4\pi^2}$ . What goes wrong? Hint:  $u^z$  is defined by  $e^{z \ln u}$ . Let  $u = e^{1+2\pi i}$  and  $z = 1 - 2\pi i$ . Is  $\ln u$  equal to  $1 + 2\pi i$ ?

**Exercise 1.20.** Evaluate the following limits by using the Taylor expansion.

$$\lim_{x \to 0} \frac{1 - \cos x}{x^2}$$
$$\lim_{x \to 0} \frac{1 - e^{-x^2}}{x^2}$$
$$\lim_{x \to 0} \frac{\ln(\cos ax)}{\ln(\cos bx)}$$

**Exercise 1.21.** Show that  $\lim_{n\to\infty} \left(1 + \frac{x}{n}\right)^n = e^x$ .

**Exercise 1.22.** For positive x, evaluate  $\lim_{x\to 0} x^x$ .

**Exercise 1.23.** The volume of an *n*-dimensional cube of side-length L is  $L^n$ . What is the volume of a pyramid in *n*-dimensional space? What is the

volume  $V_n$  of a sphere in *n*-dimensional space? Hint: Assume  $V_n = f(n)r^n$ , where *r* is the radius. Use mathematical induction to find out f(n).

**Exercise 1.24.** In the movie The Da Vinci Code, the Fibonacci series is used to transmit secret messages. The Fibonacci series  $f_n$  satisfies the equation  $f_{n+2} = f_{n+1} + f_n$ . Let us assume  $f_n = r^n$ , find the two solutions of r. Let the two solutions be  $r_1$  and  $r_2$ . Show that the general solution of  $f_n$  is  $f_n = ar_1^n + br_2^n$ , where the constants a and b are determined by  $f_0$  and  $f_1$ .

**Exercise 1.25.** Consider a series  $a_n$  satisfying the equation  $a_{n+2} = 4a_{n+1} - 4a_n$ . If  $a_0 = 1$ ,  $a_1 = 2$ , it is not difficult to find the solution  $a_n = 2^n$ . But what if  $a_0 = 1$ ,  $a_1 = 3$ ? Can you find a solution too?

**Exercise 1.26.** Let x, y, z be three physical quantities satisfying a functional relation f(x, y, z) = 0. Let w be a function of any two of x, y, z. Show that

$$\left(\frac{\partial x}{\partial y}\right)_{w} \left(\frac{\partial y}{\partial z}\right)_{w} = \left(\frac{\partial x}{\partial z}\right)_{w}, \qquad (1.399)$$

$$\left(\frac{\partial x}{\partial y}\right)_z \left(\frac{\partial y}{\partial x}\right)_z = 1, \qquad (1.400)$$

$$\left(\frac{\partial x}{\partial y}\right)_z \left(\frac{\partial y}{\partial z}\right)_x \left(\frac{\partial z}{\partial x}\right)_y = -1.$$
(1.401)

Hint:

$$dz = \left(\frac{\partial z}{\partial x}\right)_y dx + \left(\frac{\partial z}{\partial y}\right)_x dy.$$
(1.402)

$$dy = \left(\frac{\partial y}{\partial x}\right)_z dx + \left(\frac{\partial y}{\partial z}\right)_x dz.$$
(1.403)

Combining Eqs. (1.402) and (1.403) we have

$$dz = \left[ \left( \frac{\partial z}{\partial x} \right)_y + \left( \frac{\partial z}{\partial y} \right)_x \left( \frac{\partial y}{\partial x} \right)_z \right] dx + \left( \frac{\partial z}{\partial y} \right)_x \left( \frac{\partial y}{\partial z} \right)_x dz.$$
(1.404)

Since dz and dx are independent, the coefficient in front of dz must be one, and the coefficient in front of dx must be zero. This gives Eqs. (1.400) and Eqs. (1.401). Eq. (1.399) can be proved in a similar way.

**Exercise 1.27.** Prove Eqs. (1.364)–(1.366) by using Eqs. (1.352)–(1.354).

Exercise 1.28. Show that

$$\nabla\left(\frac{1}{r}\right) = -\frac{\mathbf{r}}{r^3}.$$

# Chapter 2

# Motion of Particles

# 2.1 Space-Time Coordinates and Physical Laws

Physics is an empirical science, which means we build up the knowledge of physics from our experience. We describe the space around us by building a coordinate grid with a standard ruler. We measure the rate of change of physical quantities with a standard clock. But why do we have so much faith on our standard ruler and standard clock? How do we know the ruler will not shrink and the clock will not slow down tomorrow? How do we know the standard ruler measures the same length when it is moved from Taipei to Kaohsiung? How do we know the standard clock runs at the same rate when it is moved from the Earth to the Moon? The answer is we don't, but we assume they do not change until we are forced by experimental data to abandon that assumption.

Take the law of gravitation for example. Empirically we find that the gravitational force F between two objects are described by the following law.

$$F = G \frac{mM}{r^2},\tag{2.1}$$

where m, M are the masses of the two objects, r is the distance between them, and G is a universal constant. Since r is measured by a standard ruler, if the ruler changes with space and time, we will need to make G change with space and time too. This will result in a very complicated and possibly useless law of gravitation. Similarly, if we believe the standard clock is slowing down, we will have to believe that our heart beat and the motion of the Earth around the Sun are also slowing down with the same proportion. This will make the physics very complicated. The fact that a simple equation like Eq. (2.1) can explain all the experimental data actually enhances our faith on the simplicity of the space-time structure around us and the comprehensibility of the laws of physics. We describe the falling of an apple and the orbit of the Moon by the same simple equation. What a triumph it represents!

Even though there can be many different ways of describing the same thing, we tend to think the simplest is the best. It is possible to invent a theory in which the motion of the Moon is pushed by a genie. However, the physics of a genie is obviously more complicated than Eq. (2.1). If Eq. (2.1) serves well the purpose of predicting how an object moves, why do we need the genie?

But we must also admit that our experience has its own limit. Take the Pythagorean theorem for example. It can be easily proved by looking at Fig. 2.1. The figure is part of our common experience. However, if you are careful you will find that this proof has a hidden assumption. It assumes that the figure lies on a flat surface. You will not be able to prove the theorem if you draw the figure on the surface of a basket ball. If all the space we can reach is the 100 meter square around us, the Pythagorean theorem has no problem. But surely a cross-continent aviator will not use the Pythagorean theorem to calculate the distance between two points. Given that we can only derive and verify the laws of physics from experience, there can be no law of physics that is proved to be absolutely right. There are only laws that are good enough.

### 2.2 Inertial Frames

Newton's first law states that in an inertial reference frame an object will maintain its velocity if no force acts on it. There are two points needed to be clarified in this statement: First, what is the definition of reference frame? How do we determine if a reference frame is inertial? Second, what is the definition of force? How do we measure it? The second question also arises in Newton's second law  $\mathbf{F} = m\mathbf{a}$ .

In order to be precise, in physics we only speak of terms that can be measured, at least in principle, directly or indirectly by some procedure of



Fig. 2.1: The Pythagorean theorem is proved by  $(a + b)^2 - 4 \times \frac{ab}{2} = c^2$ .

operation. We speak of time, and time can be measured by a standard clock. We speak of length, and length can be measured by a standard ruler. We are not afraid of talking about specific heat, because specific heat can be measured by some well-defined procedure of operation. We do not talk about the weight of soul, because no one has found a well-defined procedure of operation to measure it. We may say a physical term is defined only by a procedure of operation through which it can be measured, otherwise it does not have a precise meaning. This is the viewpoint of operational definition commonly accepted by physicists. If we agree that operational definition is the only way to define a physical term without ambiguity, then we must define a procedure to determine whether a reference frame is inertial. Unfortunately, no operational definition of inertial frame is known. People in a free falling elevator will not feel the force of gravity. Without knowing how things move outside, they will not know they are in fact in an accelerating frame instead of an inertial one. This equivalence is the spirit of Einstein's general relativity theory, in which there is no fundamental difference between inertial and accelerating frames. One may argue that by putting a particle which is not under the influence of any force in a reference frame, if the acceleration of the particle is zero, the reference frame is inertial. This is cyclic logic, because it turns the first law into the definition of inertial frame. Even if we agree to do that, in such a test if we do detect acceleration of the particle, how can we know in the first place that there is no force acting on the particle?

Similarly, what is the operational definition of force? Again, people in a free falling elevator will not feel the force of gravity. Without knowing how

things move outside, they will not know the gravitational force is acting on them. Therefore the only way we know the existence of a force is by the acceleration it causes in a inertial frame. In other words,  $\mathbf{F} = m\mathbf{a}$  is the operational definition of force rather than a physical law.

The definition of force again involves the concept of inertial frame. But if there is not a reliable procedure to determine whether a reference frame is inertial, how can the concept of inertial frame and the concept of force be useful? Empirically, around us it is easy to find reference frames which seem to be inertial, namely reference frames in which objects maintain their velocity when there appears no force acting on them. In these frames physics is much simpler. That is why the concept of inertial frame is empirically useful. But what is the origin of such an empirical distinction?

In the discussion of inertial frames and force, we have repeatedly mentioned "Without knowing how things move outside ...". How would "knowing how things move outside" changes the picture? Imagining some intelligent beings living near the north pole of some rapidly rotating planet, and imagining that the atmosphere of that planet is not transparent enough for them to see the stars in the universe. These intelligent beings would probably not come up with the idea of inertial frame because they will constantly experience the centrifugal force. They will have to tie themselves to the north pole by some means to prevent from flying away. If they are allowed to see that all other stars are rotating around them in a uniform angular velocity, it would be much easier for them to explain their local experience. So it does help to look out in a rotating frame. In contrast, in a linearly accelerating frame such as a non-rotating free-falling elevator, looking out does not help that much because there is no need to explain the local experience by looking out. According to general relativity the local frame of a free-falling elevator is equivalent to an inertial frame.

Ernst Mach postulated that if a reference frame moves at a constant velocity relative to the center of mass of the universe and does not rotate with respect to the mass distribution of the universe, it is an inertial frame, and this is what distinguishes an inertial frame from non-inertial ones. Looking into the night sky, we see stars rotating around the polar axis slowly, so slow that the centrifugal force at the equator accounts for only 0.3% change of our weight. This tells us that we are approximately in a non-rotating frame. Gazing at the stars does not tell whether we are falling in some direction in a linearly accelerating frame, because the reference points are too far away. We cannot tell the difference just like a person in an accelerating elevator.

#### 2.3. The Cluster Decomposition Postulate

In summary, we have shown that Newton's first and second laws are not really physical laws. Even if Mach's postulate is true, whether a frame is inertial cannot be determined locally, and because one can only measure acceleration to know the existence of force,  $\mathbf{F} = m\mathbf{a}$  is merely an operational definition of force. However, the concept of inertial frame and  $\mathbf{F} = m\mathbf{a}$  is still useful in classical mechanics simply because we are fortunate to be in a frame which is approximately inertial.

# 2.3 The Cluster Decomposition Postulate

The fact that from physical laws one can predict experimental outcome with locally controlled experimental parameters means that things far away from us have no effect on our experiments. If the fall of a rock in some planet of some other galaxy can change the outcome of our experiment on the Earth, we will not be able to predict the experimental outcome at all, because it will be too hard to take into account of all such unknown remote events. Such empirical observation lead us to believe that the interaction between remote systems is not affected by the fine detail of the interaction between the constituents within each system. This is the Cluster Decomposition Postulate.

Let us imagine a system formed by two interacting particles of masses  $m_1$ and  $m_2$  and positions  $\mathbf{r}_1$  and  $\mathbf{r}_2$ . To a remote observer the system behaves like a single particle of mass  $m = m_1 + m_2$  at a center-of-mass position  $\mathbf{r} = (m_1\mathbf{r}_1 + m_2\mathbf{r}_2)/(m_1 + m_2)$ . If the system does not interact with other systems, then to the remote observer  $m\ddot{\mathbf{r}} = 0$ , which means  $m_1\ddot{\mathbf{r}}_1 = -m_2\ddot{\mathbf{r}}_2$ . In other words, the force acting on particle 1 is the opposite of that acting on particle 2. This is Newton's third law. What we have shown is one can derive the third law from the first or the second law using the Cluster Decomposition Postulate. Since the first and the second laws are not real laws, the third law is not a law either. Nevertheless, just as the first and second laws are empirically correct in the approximately inertial frame we live, so is the third law.

For two particles the Cluster Decomposition Postulate leads to Newton's third law. For many particles we have

$$\sum_{i} m_i \ddot{\mathbf{r}}_i = 0. \tag{2.2}$$

This is just the momentum conservation law, which is more useful than

Newton's third law. For example, if we collide two pieces of dough and after the collision the two pieces stick together, then it is hard to tell which acts what force on the other because they have been combined into one piece. Yet, from the momentum conservation law one can still derive the velocity of the combined piece of dough without bothering with Newton's third law.

# 2.4 Equation of Motion

In section 2.2 we discussed the operational definition of force. If  $\mathbf{F} = m\mathbf{a}$  is merely an operational definition, how can it be so useful in predicting how things move? If we define  $\mathbf{G} = m\mathbf{v}$  or  $\mathbf{H} = m\dot{\mathbf{a}}$ , will they be useful too? Surely, mathematically  $\mathbf{G} = m\mathbf{v}$  is equivalent to  $\mathbf{F} = m\mathbf{a}$  if we let  $\mathbf{F} = \dot{\mathbf{G}}$ . So the real question is which quantity conceptualizes the real world in the simplest way.  $\mathbf{F} = m\mathbf{a}$  is extremely useful because in nature many sources of force can be expressed as a function of position, velocity, and time. In other words, we have

$$\mathbf{F}(\mathbf{r}, \dot{\mathbf{r}}, t) = m\ddot{\mathbf{r}}.\tag{2.3}$$

This is a second-order differential equation that describes the motion of an object. When it is solved we will know the trajectory of the object. Without knowing the form of  $\mathbf{F}(\mathbf{r}, \dot{\mathbf{r}}, t)$ ,  $\mathbf{F}$  is useless. The form of  $\mathbf{F}$  is determined by other physical laws in deeper levels. For instance, for gravity  $\mathbf{F} = -GMm\hat{\mathbf{r}}/r^2$  where  $\hat{\mathbf{r}} = \mathbf{r}/r$ , for friction  $\mathbf{F} \approx -\mu\mathbf{v}$ , and for elasticity  $\mathbf{F} \approx -k\mathbf{r}$ . Some of these deeper physical laws are more fundamental and more exact, such as gravity, and some are only approximately true, such as friction and elasticity. But even  $\mathbf{F} = -GMm\hat{\mathbf{r}}/r^2$  is not completely exact, because force cannot propagate faster than the speed of light. In  $\mathbf{F} = -GMm\hat{\mathbf{r}}/r^2$  the gravitational force propagates with infinite speed.

We can go deeper to find out the origin of friction and elasticity, for instance, in terms of the force between atoms and molecules. The macroscopic force laws such as  $\mathbf{F} \approx -\mu \mathbf{v}$  and  $\mathbf{F} \approx -k\mathbf{r}$  are the results of collective or average motion and interaction of the underlying microscopic world. At certain level,  $\mathbf{F} = m\mathbf{a}$  runs out of gas. For instance, in quantum mechanics it is not possible to specify position and velocity simultaneously. Then we have to replace  $\mathbf{F} = m\mathbf{a}$  by other physical laws that govern the microscopic world.

At the level of classical mechanics,  $\mathbf{F} = m\mathbf{a}$  is useful simply because most physical laws at this level can be expressed by a second-order differential equation

$$\mathbf{F}(\mathbf{r}, \dot{\mathbf{r}}, t) = m\ddot{\mathbf{r}},\tag{2.4}$$

not a third-order

$$\mathbf{H}(\mathbf{r}, \dot{\mathbf{r}}, \ddot{\mathbf{r}}, t) = m \frac{d^3 \mathbf{r}}{dt^3}, \qquad (2.5)$$

neither a first-order

$$\mathbf{G}(\mathbf{r},t) = m\dot{\mathbf{r}}.\tag{2.6}$$

Therefore even though  $\mathbf{F} = m\mathbf{a}$  is only the definition of  $\mathbf{F}$ , when  $\mathbf{F}$  can be written as a function of  $\mathbf{r}$ ,  $\dot{\mathbf{r}}$ , and t,  $\mathbf{F} = m\mathbf{a}$  becomes an effective law of physics in the form of a second-order ordinary differential equation. By solving the differential equation  $\mathbf{F}(\mathbf{r}, \dot{\mathbf{r}}, t) = m\ddot{\mathbf{a}}$ , one obtains the trajectory of the particle under the influence of  $\mathbf{F}$ .

### 2.5 Inertial Mass and Gravitational Mass

Under a fixed force, such as the force produced by a spring stretched to a fixed length,  $\mathbf{F} = m\mathbf{a}$  can be used to define the inertial mass of a particle. One can load the standard mass  $m_s$  to the spring and measure its acceleration  $a_s$ , then load the unknown mass  $m_u$  and do the same measurement to determine its mass.

$$\frac{m_u}{m_s} = \frac{a_s}{a_u}.\tag{2.7}$$

Alternatively, one can measure the gravitational mass with a balance and a set of standard weights. It can be shown that these two measurements agree completely with each other, which means for any test particle the acceleration produced by the gravitational force is the same regardless of its mass.

$$\ddot{\mathbf{r}} = -G\frac{M\hat{\mathbf{r}}}{r^2},\tag{2.8}$$

where G is the gravitational constant, M is the mass of the object producing the gravitational force, and r is the distance between the test particle and the object. If there is more than one object producing the gravitational force, we may write

$$\ddot{\mathbf{r}} = -G\sum_{i} \frac{M_i(\mathbf{r} - \mathbf{r}_i)}{|\mathbf{r} - \mathbf{r}_i|^3},\tag{2.9}$$

where  $\mathbf{r}$  is the position vector of the test particle and  $\mathbf{r}_i$  is the position vector of the *i*th object. Eq. (2.9) is a differential equation of  $\mathbf{r}$  independent of the mass of the test particle, therefore its solution which represents the trajectory of the test particle is also independent of its mass.

If the gravitational mass  $m^{(g)}$  were different from the inertial mass  $m^{(i)}$ , it would be possible to use this effect to detect whether one is in an accelerating elevator or in a gravitation field. In an accelerating elevator with acceleration a, an object would have an apparent weight  $m^{(i)}a$ . Therefore two objects of the same weight  $m^{(g)}g$  in a gravitation field would have different apparent weights in the elevator. For the same reason, two objects of the same  $m^{(i)}$ would have different weights in a gravitational field. In a space station orbiting around the Earth, the centrifugal force is balanced by the gravity. If  $m^{(g)} \neq m^{(i)}$ , the balance condition will be

$$\frac{v^2}{r} = G \frac{M}{r^2} \left[ \frac{m^{(g)}}{m^{(i)}} \right],$$
(2.10)

which means different objects will move in different trajectories, and they will not maintain their relative positions. This will lead the astronauts to know that they are not in an inertial frame. On the surface of the Earth, a pendulum of length l will swing at a period

$$T = 2\pi \sqrt{\frac{m^{(i)}l}{m^{(g)}g}}.$$
 (2.11)

If  $m^{(g)} \neq m^{(i)}$ , the period will depend on  $m^{(i)}$ . Experimental investigations have been carried out in this line of thought with great accuracy, and no measurable difference between  $m^{(g)}$  and  $m^{(i)}$  was found.

The fact that  $m^{(g)} = m^{(i)}$  can be easily explained by the Cluster Decomposition Postulate. Let us conduct two free-fall experiments with two objects of the same inertial mass m. In the first experiment, we take the two objects to a height h and let them fall at the same time. The two objects will fall independently to the ground after the same time  $t_m$ . In the second experiment we also take the two objects to a height h and let them fall. However, this time we bind the two object together with a string of negligible mass, so that the mass of the combined object is 2m. The time it takes for the combined object to fall to the ground is  $t_{2m}$ . If  $t_{2m} \neq t_m$ , we have  $m^{(g)} \neq m^{(i)}$ . If that does happen, we can weaken and weaken the strength of the string and do the experiments again and again, until the binding effect of the string becomes negligible. Then we must have  $t_{2m} = t_m$  in this limiting case because it is practically the same as letting the two objects fall independently. To a distant observer, this experimental result means the acceleration of the combined object depends on their internal interaction, namely how strongly they are bound together. This is at odds with the Cluster Decomposition Postulate.

### 2.6 Work and Potential Energy

Let us denote the kinetic energy of a particle by  $T(t) = m\mathbf{v}(t) \cdot \mathbf{v}(t)/2$ , and investigate how it changes with time under the influence of an external force **F**. Let the process starts at  $t_i$  and ends at  $t_f$ . We have

$$\frac{m\mathbf{v}_{f}^{2}}{2} - \frac{m\mathbf{v}_{i}^{2}}{2} = T(t_{f}) - T(t_{i})$$

$$= \int_{t_{1}}^{t_{2}} T'(t) dt$$

$$= \int_{t_{i}}^{t_{f}} m\mathbf{v}(t) \cdot \mathbf{a}(t) dt$$

$$= \int_{t_{i}}^{t_{f}} \mathbf{F}(t) \cdot \mathbf{v}(t) dt$$

$$= \int_{\mathbf{r}_{i}}^{\mathbf{r}_{f}} \mathbf{F}(\mathbf{r}) \cdot d\mathbf{r},$$
(2.12)

where in the last step we have changed the variable of integration from t to **r**. The integral  $\int_{\mathbf{r}_i}^{\mathbf{r}_f} \mathbf{F}(\mathbf{r}) \cdot d\mathbf{r}$  is called the work done by the external force on the particle. Therefore we say the increase of the kinetic energy of a particle is equal to the work done on it. Note that the work may depend on the path. For example, under the influence of frictional force,

$$\int_{\mathbf{r}_{i}}^{\mathbf{r}_{f}} \mathbf{F}(\mathbf{r}) \cdot d\mathbf{r} \quad (\text{along a long path})$$

$$\neq \int_{\mathbf{r}_{i}}^{\mathbf{r}_{f}} \mathbf{F}(\mathbf{r}) \cdot d\mathbf{r} \quad (\text{along a short path}). \quad (2.13)$$

A conservative force is one that can be derived from a potential function  $V(\mathbf{r})$  by

$$\mathbf{F}(\mathbf{r}) = -\nabla V(\mathbf{r}). \tag{2.14}$$

Examples of conservative force are the gravitational force

$$-G\frac{Mm}{r^2}\hat{\mathbf{r}} = -\nabla\left(-G\frac{Mm}{r}\right),\tag{2.15}$$

and the force produced by a spring

$$-k\mathbf{r} = -\nabla \frac{kr^2}{2}.\tag{2.16}$$

Multiplying the equation of motion by the integrating factor  $\mathbf{v}$ ,

$$m\dot{\mathbf{v}}\cdot\mathbf{v} = -\nabla V(\mathbf{r})\cdot\mathbf{v},\tag{2.17}$$

and integrating both sides with respect to t, we have

$$\frac{m\mathbf{v}_f^2}{2} - \frac{m\mathbf{v}_i^2}{2} = -\int_{\mathbf{r}_i}^{\mathbf{r}_f} \nabla V(\mathbf{r}) \cdot d\mathbf{r}.$$
(2.18)

From Stokes theorem, the integration on the right-hand side is independent of path. Therefore

$$\frac{m\mathbf{v}_{f}^{2}}{2} - \frac{m\mathbf{v}_{i}^{2}}{2} = V(\mathbf{r}_{i}) - V(\mathbf{r}_{f}).$$
(2.19)

In Eq. (2.19)  $V(\mathbf{r})$  represents the potential energy at position  $\mathbf{r}$ . It is seen that if the motion is driven by conservative forces, the kinetic energy plus the potential energy is conserved.

If we apply an external force  $\mathbf{F}$  to a particle which is already under the influence of a conservative force, the equation of motion becomes

$$m\dot{\mathbf{v}} = -\nabla V(\mathbf{r}) + \mathbf{F}(\mathbf{r}). \tag{2.20}$$

Multiplying both sides with  $\mathbf{v}$  and integrating with respect to t, we have

$$\frac{m\mathbf{v}_f^2}{2} - \frac{m\mathbf{v}_i^2}{2} = V(\mathbf{r}_i) - V(\mathbf{r}_f) + \int_{\mathbf{r}_i}^{\mathbf{r}_f} \mathbf{F}(\mathbf{r}) \cdot d\mathbf{r}.$$
 (2.21)

Which means the change of the kinetic energy plus the change of the potential energy is equal to the work done by the external force.

# 2.7 Separating out Internal Motion

If we watch an object move in a distance, the object moves like a point particle. The constituents of the object may interact with each other and make relative movements, but according to the Cluster Decomposition Postulate the velocity of the center of mass does not change. Therefore it will make the physics more clear if one can separate the motion of the center of mass from the motion of the constituents relative to it. Indeed, this can be done as shown below.

Let  $\mathbf{r}_i = \mathbf{r}'_i + \mathbf{r}$ ,  $\mathbf{v}_i = \mathbf{v}'_i + \mathbf{v}$ , where  $\mathbf{r}$  is the center-of-mass position defined by

$$\mathbf{r} = \frac{\sum_{i} m_{i} \mathbf{r}_{i}}{\sum_{i} m_{i}} = \frac{\sum_{i} m_{i} \mathbf{r}_{i}}{M}, \qquad (2.22)$$

and  $\mathbf{v} = \dot{\mathbf{r}}$ . The separation of linear momentum is trivial, since

$$\sum_{i} m_{i} \mathbf{v}_{i} = \sum_{i} m_{i} (\mathbf{v} + \mathbf{v}'_{i}) = M \mathbf{v} + \sum_{i} m_{i} \mathbf{v}'_{i} = M \mathbf{v}.$$
 (2.23)

The total force experienced by all the particles is

$$\mathbf{F} = \sum_{i} \mathbf{F}_{i} = \sum_{i} m_{i} \dot{\mathbf{v}}_{i} = M \dot{\mathbf{v}}, \qquad (2.24)$$

which is the total mass times the acceleration of the center of mass.

Next we consider the angular momentum of the system

$$\mathbf{L} = \sum_{i} \mathbf{r}_{i} \times \mathbf{p}_{i} = \sum_{i} \mathbf{r}_{i} \times m_{i} \mathbf{v}_{i}, \qquad (2.25)$$

where  $\mathbf{r}_i$  is the position vector and  $m_i \mathbf{v}_i$  is momentum of the *i*th particle.

$$\mathbf{L} = \sum_{i} \mathbf{r} \times m_{i} \mathbf{v} + \sum_{i} \mathbf{r}_{i}' \times m_{i} \mathbf{v}_{i}' + \left(\sum_{i} m_{i} \mathbf{r}_{i}'\right) \times \mathbf{v} + \mathbf{r} \times \sum_{i} m_{i} \mathbf{v}_{i}'.$$
 (2.26)

The last two terms are zero, because  $\sum_i m_i \mathbf{r}'_i = 0$ . Therefore

$$\mathbf{L} = \sum_{i} \mathbf{r} \times m_i \mathbf{v} + \sum_{i} \mathbf{r}'_i \times m_i \mathbf{v}'_i.$$
(2.27)

The total angular momentum is the angular momentum of the object as a whole at the center of mass plus the angular momentum of the internal motion relative to the center of mass. Similarly, the total torque experienced by all the particles is

$$\boldsymbol{\tau} = \sum_{i} \mathbf{r}_{i} \times m_{i} \dot{\mathbf{v}}_{i} = \sum_{i} \mathbf{r} \times m_{i} \dot{\mathbf{v}} + \sum_{i} \mathbf{r}_{i}^{\prime} \times m_{i} \dot{\mathbf{v}}_{i}^{\prime}, \qquad (2.28)$$

which is the torque applied to the center of mass plus the internal torques with respect to the center of mass.

Finally we consider the kinetic energy. The total kinetic energy is

$$\mathbf{T} = \frac{1}{2} \sum_{i} m_i (\mathbf{v} + \mathbf{v}'_i) \cdot (\mathbf{v} + \mathbf{v}'_i)$$
$$= \frac{1}{2} \sum_{i} m_i v^2 + \frac{1}{2} \sum_{i} m_i v'_i^2 + \mathbf{v} \cdot \left(\sum_{i} m_i \mathbf{v}'_i\right). \quad (2.29)$$

The last term is zero, therefore

$$\mathbf{T} = \frac{1}{2}Mv^2 + \frac{1}{2}\sum_{i}m_i {v'}_i^2.$$
 (2.30)

Again, the total kinetic energy is the kinetic energy of the object as a whole at the center of mass plus the kinetic energy of the internal motion relative to the center of mass.

### 2.8 The Angular Velocity Pseudovector

Angular velocity is an important concept in rotational motion. Consider the transformation of a vector under rotation about the x-, y-, and z-axes with angles  $\xi$ ,  $\phi$ , and  $\psi$  respectively. The transformation matrices are

$$\mathbf{T}_{1}(\xi) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos \xi & -\sin \xi \\ 0 & \sin \xi & \cos \xi \end{bmatrix}, \\
\mathbf{T}_{2}(\phi) = \begin{bmatrix} \cos \phi & 0 & \sin \phi \\ 0 & 1 & 0 \\ -\sin \phi & 0 & \cos \phi \end{bmatrix}, \\
\mathbf{T}_{3}(\psi) = \begin{bmatrix} \cos \psi & -\sin \psi & 0 \\ \sin \psi & \cos \psi & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$
(2.31)

#### 2.8. The Angular Velocity Pseudovector

For finite  $\xi$ ,  $\phi$ , and  $\psi$  these three matrices do not commute, therefore the orientation of the transformed vector depends on the order of  $\mathbf{T}_1(\xi)$ ,  $\mathbf{T}_2(\phi)$ , and  $\mathbf{T}_3(\psi)$ . However,  $\mathbf{T}_1(\xi)$ ,  $\mathbf{T}_2(\phi)$ , and  $\mathbf{T}_3(\psi)$  commute with each other as  $\xi$ ,  $\phi$ , and  $\psi$  approach zero. This means for infinitesimal rotations  $d\xi$  along the *x*-axis,  $d\phi$  along the *y*-axis, and  $d\psi$  along the *z*-axis, the order of rotation around different axes does not matter. To see this, we note that for infinitesimal rotations we have

$$\begin{aligned} \mathbf{T}_{1}(d\xi) &= I + d\xi \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix} \equiv I + d\xi \mathbf{M}_{1}, \\ \mathbf{T}_{2}(d\phi) &= I + d\phi \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{bmatrix} \equiv I + d\phi \mathbf{M}_{2}, \\ \mathbf{T}_{3}(d\psi) &= I + d\psi \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \equiv I + d\psi \mathbf{M}_{3}. \end{aligned}$$
(2.32)

Therefore to the first order of  $d\xi$ ,  $d\phi$ , and  $d\psi$ ,

$$\mathbf{T}_1(d\xi)\mathbf{T}_2(d\phi)\mathbf{T}_3(d\psi) = \mathbf{I} + d\xi\mathbf{M}_1 + d\phi\mathbf{M}_2 + d\psi\mathbf{M}_3, \qquad (2.33)$$

which is independent of the order of rotation. For a vector  $\mathbf{A} = (A_1, A_2, A_3)$ under infinitesimal rotation we have

$$\begin{bmatrix} A_1 \\ A_2 \\ A_3 \end{bmatrix}' = \begin{bmatrix} 1 & -d\psi & d\phi \\ d\psi & 1 & -d\xi \\ -d\phi & d\xi & 1 \end{bmatrix} \begin{bmatrix} A_1 \\ A_2 \\ A_3 \end{bmatrix}, \qquad (2.34)$$

where ' denotes the vector after rotation. Let  $\mathbf{e}_1 = (1, 0, 0)$ ,  $\mathbf{e}_2 = (0, 1, 0)$ , and  $\mathbf{e}_3 = (0, 0, 1)$  be the unit vectors in the *x*-, *y*-, and *z*-axes. Substituting them into Eq. (2.34), it can be seen that they transform according to:

$$e'_1 = \mathbf{e}_1 + d\psi \mathbf{e}_2 - d\phi \mathbf{e}_3, 
 e'_2 = -d\psi \mathbf{e}_1 + \mathbf{e}_2 + d\xi \mathbf{e}_3, 
 e'_3 = d\phi \mathbf{e}_1 - d\xi \mathbf{e}_2 + \mathbf{e}_3.$$
(2.35)

Let us consider the time derivative of a vector  $\mathbf{A}$  attached to a rotating frame. Because the unit vectors in the rotating frame are also rotating, we must take into account the time derivatives of the unit vectors.

$$\frac{d\mathbf{A}}{dt} = \frac{dA_1}{dt}\mathbf{e}_1 + \frac{dA_2}{dt}\mathbf{e}_2 + \frac{dA_3}{dt}\mathbf{e}_3 + A_1\frac{d\mathbf{e}_1}{dt} + A_2\frac{d\mathbf{e}_2}{dt} + A_3\frac{d\mathbf{e}_3}{dt}.$$
 (2.36)

Using Eq. (2.35), we have

$$\frac{d\mathbf{e}_{1}}{dt} = \frac{\mathbf{e}_{1}^{\prime} - \mathbf{e}_{1}}{dt} = \frac{d\psi}{dt}\mathbf{e}_{2} - \frac{d\phi}{dt}\mathbf{e}_{3},$$

$$\frac{d\mathbf{e}_{2}}{dt} = \frac{\mathbf{e}_{2}^{\prime} - \mathbf{e}_{2}}{dt} = \frac{-d\psi}{dt}\mathbf{e}_{1} + \frac{d\xi}{dt}\mathbf{e}_{3},$$

$$\frac{d\mathbf{e}_{3}}{dt} = \frac{\mathbf{e}_{3}^{\prime} - \mathbf{e}_{3}}{dt} = \frac{d\phi}{dt}\mathbf{e}_{1} - \frac{d\xi}{dt}\mathbf{e}_{2}.$$
(2.37)

Hence

$$\frac{d\mathbf{A}}{dt} = \frac{dA_1}{dt}\mathbf{e}_1 + \frac{dA_2}{dt}\mathbf{e}_2 + \frac{dA_3}{dt}\mathbf{e}_3 
+ A_1\left(\frac{d\psi}{dt}\mathbf{e}_2 - \frac{d\phi}{dt}\mathbf{e}_3\right) 
+ A_2\left(\frac{-d\psi}{dt}\mathbf{e}_1 + \frac{d\xi}{dt}\mathbf{e}_3\right) 
+ A_3\left(\frac{d\phi}{dt}\mathbf{e}_1 - \frac{d\xi}{dt}\mathbf{e}_2\right).$$
(2.38)

Let us define an infinitesimal pseudovector  $d\theta \equiv (d\xi, d\phi, d\psi)$  and the angular velocity pseudovector  $\omega \equiv d\theta/dt$ . Both  $d\theta$  and  $\omega$  are pseudovectors because unlike real vectors, they do not reverse their directions when the *x*-, *y*-, and *z*-axes are inverted. In terms of  $\omega$ , Eq. (2.38) can be written as

$$\frac{d\mathbf{A}}{dt} = \left(\frac{d\mathbf{A}}{dt}\right)_{r} + \frac{d\boldsymbol{\theta}}{dt} \times \mathbf{A} \\
= \left(\frac{d\mathbf{A}}{dt}\right)_{r} + \boldsymbol{\omega} \times \mathbf{A},$$
(2.39)

where

$$\left(\frac{d\mathbf{A}}{dt}\right)_{r} \equiv \frac{dA_{1}}{dt}\mathbf{e}_{1} + \frac{dA_{2}}{dt}\mathbf{e}_{2} + \frac{dA_{3}}{dt}\mathbf{e}_{3}$$
(2.40)

represents the time derivative of  $\mathbf{A}$  seen by an observer in the rotating frame because it has not taken into account the rotation of the unit vectors.

# 2.9 Motion in a Rotating Frame

In a rotating frame of constant angular velocity  $\boldsymbol{\omega}$ , how is the appearance of  $\mathbf{F} = m\mathbf{a}$  changed? Setting  $\mathbf{A} = \mathbf{r}$  in Eq. (2.39), we have

$$\mathbf{v}_f = \mathbf{v}_r + \boldsymbol{\omega} \times \mathbf{r},\tag{2.41}$$



Fig. 2.2: Coordinate axes for the analysis of the Foucault pendulum.

where  $\mathbf{v}_f$  is the velocity seen by an observer in the fixed frame, and  $\mathbf{v}_r$  is the velocity seen by an observer in the rotating frame. Applying Eq. (2.39) to  $\mathbf{v}_f$  in Eq. (2.41), we have

$$\begin{pmatrix} d\mathbf{v}_f \\ dt \end{pmatrix}_f = \left( \frac{d\mathbf{v}_f}{dt} \right)_r + \boldsymbol{\omega} \times \mathbf{v}_f$$
  
=  $(\dot{\mathbf{v}}_r + \boldsymbol{\omega} \times \dot{\mathbf{r}})_r + \boldsymbol{\omega} \times (\mathbf{v}_r + \boldsymbol{\omega} \times \mathbf{r})$   
=  $\dot{\mathbf{v}}_r + 2\boldsymbol{\omega} \times \mathbf{v}_r + \boldsymbol{\omega} \times (\boldsymbol{\omega} \times \mathbf{r}).$  (2.42)

The first term on the right-hand side is the acceleration seen in the rotating frame, the second term is the Coriolis acceleration, and the third term is the centrifugal acceleration.

### 2.10 Foucault Pendulum

A Foucault pendulum is simply a two dimensional pendulum set at latitude  $\theta$ . The pendulum is allowed to swing in a plane parallel to the surface of the Earth, and the slow rotation of its swing direction provides a proof that the Earth is rotating. If we set the x-axis pointing to the east and the y-axis pointing to the north, as shown in Fig. 2.2, than the angular velocity  $\Omega$  of the rotating Earth can be written as  $(0, \Omega \cos \theta, \Omega \sin \theta)$ . Let  $\mathbf{r} = (x, y, 0)$  be the small displacement of the pendulum from its equilibrium point, the equation of motion for the pendulum in the rotating frame is

$$\ddot{\mathbf{r}} = -\frac{g}{l}\mathbf{r} - 2\mathbf{\Omega} \times \dot{\mathbf{r}} - \mathbf{\Omega} \times (\mathbf{\Omega} \times \mathbf{r}).$$
(2.43)

Let  $\omega^2 = g/l$ . Since  $|\dot{\mathbf{r}}|$  is approximately  $\omega |\mathbf{r}|$  and  $\omega \gg \Omega$ , we have

$$\left|\frac{g}{l}\mathbf{r}\right| \gg |2\mathbf{\Omega} \times \dot{\mathbf{r}}| \gg |\mathbf{\Omega} \times (\mathbf{\Omega} \times \mathbf{r})|.$$
(2.44)

Therefore we can ignore the last term on the right-hand side of Eq. (2.43), and the equation becomes

$$\ddot{x} = -\frac{g}{l}x + 2\dot{y}\Omega\sin\theta,$$
  
$$\ddot{y} = -\frac{g}{l}y - 2\dot{x}\Omega\sin\theta.$$
 (2.45)

We look for an approximate solution of the following form.

$$x = A(t) \cos \omega t,$$
  

$$y = B(t) \cos \omega t,$$
(2.46)

where A(t), B(t) are slowly varying functions. Substituting into Eq. (2.45), we have

$$\ddot{A}\cos\omega t - 2\omega\dot{A}\sin\omega t = 2\eta(\dot{B}\cos\omega t - B\omega\sin\omega t), \ddot{B}\cos\omega t - 2\omega\dot{B}\sin\omega t = -2\eta(\dot{A}\cos\omega t - A\omega\sin\omega t),$$
(2.47)

where  $\eta = \Omega \sin \theta$ . Assume  $\ddot{A}$  is of the order  $\eta^2 A$ ,  $\dot{A}$  is of the order  $\eta A$ , and similarly for B. Since  $\eta \ll \omega$ , we may drop the first terms on both sides of the equations. Compare the coefficients of  $\sin \omega t$ , we have

$$\dot{A} = \eta B, 
\dot{B} = -\eta A.$$
(2.48)

The solution is  $A(t) = C \sin(\eta t + \phi)$  and  $B(t) = C \cos(\eta t + \phi)$ , namely the pendulum rotates at an angular velocity  $-\eta$ . This is a way we know the spin angular velocity of the Earth without referring to the stars in the sky.

### 2.11 Moment of Inertia

To discuss the rotational motion of a rigid body, it is more convenient to use the angular velocity than the velocity as the dynamic variable, because at different distant from the rotation axis, the velocity is different. Let us express the angular momentum in terms the angular velocity.

$$\mathbf{L} = \sum_{i} m_{i} \mathbf{r}_{i} \times \mathbf{v}_{i}$$
$$= \sum_{i} m_{i} \mathbf{r}_{i} \times (\boldsymbol{\omega} \times \mathbf{r}_{i}). \qquad (2.49)$$

#### 2.11. Moment of Inertia

Using the formula  $\mathbf{a} \times (\mathbf{b} \times \mathbf{c}) = \mathbf{b}(\mathbf{a} \cdot \mathbf{c}) - \mathbf{c}(\mathbf{a} \cdot \mathbf{b})$ , we have

$$\mathbf{L} = \sum_{i} m_{i} [\boldsymbol{\omega} r_{i}^{2} - \mathbf{r}_{i} (\mathbf{r}_{i} \cdot \boldsymbol{\omega})]. \qquad (2.50)$$

The x-component is

$$L_x = \sum_{i} \omega_x m_i (r_i^2 - x_i^2) - \omega_y m_i x_i y_i - \omega_z m_i x_i z_i, \qquad (2.51)$$

and similarly for other components. Therefore we can write

$$\mathbf{L} = \mathbf{I} \cdot \boldsymbol{\omega}, \qquad (2.52)$$

where I is a rank-2 tensor (which looks like a  $3 \times 3$  matrix) with components

$$I_{xx} = \sum_{i} m_{i}(r_{i}^{2} - x_{i}^{2}),$$
  

$$I_{xy} = \sum_{i} -m_{i}x_{i}y_{i},$$
  

$$I_{xz} = \sum_{i} -m_{i}x_{i}z_{i},$$
(2.53)

and similarly for other components. In tensor notation, repeated indices are summed over automatically to save space. For examples,  $r_i r_i$  means  $\sum_i r_i^2 = r_1^2 + r_2^2 + r_3^2$  and  $a_{ij}r_j$  means  $\sum_j a_{ij}r_j = a_{i1}r_1 + a_{i2}r_2 + a_{i3}r_3$ . In this notation the moment of inertia can be written as

$$I_{ij} = \sum_{\alpha} m_{\alpha} \left[ \delta_{ij} r_k^{(\alpha)} r_k^{(\alpha)} - r_i^{(\alpha)} r_j^{(\alpha)} \right], \qquad (2.54)$$

where  $\alpha$  is the particle label,  $r_i^{(\alpha)}$  is the *i*th component of the position vector of the particle labeled by  $\alpha$ , the repeated index k are summed over from 1 to 3, and  $\delta_{ij}$  is defined by

$$\delta_{ij} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j. \end{cases}$$
(2.55)

In tensor notation Eq. (2.52) can be written as

$$L_i = I_{ij}\omega_j. \tag{2.56}$$

By choosing suitable axes of the coordinate frame, it is possible to simplify  $I_{ij}$  such that it becomes diagonal.

$$I_{ij} = \begin{bmatrix} I_{xx} & 0 & 0\\ 0 & I_{yy} & 0\\ 0 & 0 & I_{zz} \end{bmatrix}.$$
 (2.57)

For example, by choosing the symmetry axes as the coordinate axes, it can be seen readily that  $I_{xy} = I_{yz} = I_{zx} = 0$ , because they are odd functions of x, y, and z respectively when the other two components are held fix. The axes that diagonalize  $I_{ij}$  are called the principal axes. In the frame of principal axes

$$L_x = I_{xx}\omega_x,$$
  

$$L_y = I_{yy}\omega_y,$$
  

$$L_z = I_{zz}\omega_z.$$
(2.58)

One may wonder if angular momentum is conserved, how a falling cat can always land on its feet, or how a diver can adjust the body angle of entering the water. The secret is that a diver is not a rigid body. He can change his body shape to alter  $I_{ij}$ . By doing that, even with a fixed angular momentum he can change the angular velocity. With good timing it is possible to control the posture as long as the initial angular momentum is not zero. In the case of a falling cat, even if the initial angular momentum is zero the cat can still adjust its posture by rotating the front part and the rear part of the body separately, since it has an extremely flexible body. By changing the front-part  $I_{ij}$  and the rear-part  $I_{ij}$  separately, it can flip its body by 180° while maintaining zero angular momentum in the whole process, as shown in Fig. 2.3.

Now we shall express the kinetic energy in terms of  $\boldsymbol{\omega}$ .

$$T = \frac{1}{2} \sum_{i} m_{i} \mathbf{v}_{i} \cdot (\boldsymbol{\omega} \times \mathbf{r}_{i})$$

$$= \frac{1}{2} \sum_{i} m_{i} \boldsymbol{\omega} \cdot (\mathbf{r}_{i} \times \mathbf{v}_{i})$$

$$= \frac{1}{2} \boldsymbol{\omega} \cdot \mathbf{L}$$

$$= \frac{1}{2} I_{ij} \omega_{i} \omega_{j}.$$
(2.59)

In the coordinate system spanned by the principal axes,

$$T = \frac{1}{2} (I_{xx} \omega_x^2 + I_{yy} \omega_y^2 + I_{zz} \omega_z^2).$$
 (2.60)

The moment-of-inertia tensor can be written in the vector form as

$$I_{ij} = \sum_{\alpha} m_{\alpha} [\delta_{ij} |\mathbf{r}_{\alpha}|^2 - (\mathbf{r}_{\alpha} \cdot \mathbf{e}_i) (\mathbf{r}_{\alpha} \cdot \mathbf{e}_j)], \qquad (2.61)$$



Fig. 2.3: A cat rotates itself in the midair. Figures on the left are the side views, and figures on the right are the front views. The cat first retracts its front feet to reduce the moment of inertia of the front body. Then it rotates the front body clockwise with a large angle. Because the rear body has a much larger moment of inertia, it rotates counter-clockwise correspondingly with a small angle. Next the cat extends its front feet and retracts its rear feet. Then it rotates the front body counter-clockwise with a small angle. Because now the rear body has a much smaller moment of inertia, it rotates clockwise correspondingly with a large angle. The result is a 90° rotation of the whole body.

where  $\alpha$  is the particle label. If the center of mass is located at **b**, the position vector with respect to the center of mass is

$$\mathbf{r}' = \mathbf{r} - \mathbf{b}.\tag{2.62}$$

With respect to the center of mass, the moment-of-inertia tensor is

$$I'_{ij} = \sum_{\alpha} m_{\alpha} \{ \delta_{ij} | \mathbf{r}_{\alpha} - \mathbf{b} |^{2} - [(\mathbf{r}_{\alpha} - \mathbf{b}) \cdot \mathbf{e}_{i}] [(\mathbf{r}_{\alpha} - \mathbf{b}) \cdot \mathbf{e}_{j}] \}$$
  

$$= \sum_{\alpha} m_{\alpha} [\delta_{ij} r_{\alpha}^{2} - (\mathbf{r}_{\alpha} \cdot \mathbf{e}_{i}) (\mathbf{r}_{\alpha} \cdot \mathbf{e}_{j})]$$
  

$$+ \sum_{\alpha} m_{\alpha} [-\delta_{ij} 2\mathbf{r}_{\alpha} \cdot \mathbf{b} + (\mathbf{r}_{\alpha} \cdot \mathbf{e}_{i}) (\mathbf{b} \cdot \mathbf{e}_{j}) + (\mathbf{b} \cdot \mathbf{e}_{i}) (\mathbf{r}_{\alpha} \cdot \mathbf{e}_{j})]$$
  

$$+ \sum_{\alpha} m_{\alpha} [\delta_{ij} b^{2} - (\mathbf{b} \cdot \mathbf{e}_{i}) (\mathbf{b} \cdot \mathbf{e}_{j})]. \qquad (2.63)$$

Because

$$\sum_{\alpha} m_{\alpha} \mathbf{r}_{\alpha} = M \mathbf{b}, \qquad (2.64)$$

where  $M = \sum_{\alpha} m_{\alpha}$ , the second term on the right-hand side of Eq. (2.63) is simply -2 times the third term. Hence we have

$$I'_{ij} = I_{ij} - M[\delta_{ij}b^2 - (\mathbf{b} \cdot \mathbf{e}_i)(\mathbf{b} \cdot \mathbf{e}_j)].$$
(2.65)

The second term on the right-hand-side is simply the moment of inertia of a particle of mass M at location **b**. Eq. (2.65) is known as the **parallel axis theorem** for moment of inertia.

In Eq. (2.31) we have already shown how a vector transforms under rotation. If we rotate the coordinate frame instead of the vector itself, the vector transforms the same way as in Eq. (2.31), except that we reverse the angles  $\xi$ ,  $\phi$ , and  $\psi$ . The transformation matrix  $\mathbf{S} = \mathbf{T}_1(-\xi)\mathbf{T}_2(-\psi)\mathbf{T}_3(-\psi)$  satisfies the unitary condition  $\mathbf{S}^{\dagger} = \mathbf{S}^{-1}$ . Let us investigate how  $I_{ij}$  transforms under the rotation of the coordinate frame. By Eq. (2.54), in the new coordinate frame we have

$$I'_{ij} = \sum_{\alpha} m_{\alpha} \left[ \delta_{ij} r'^{(\alpha)}_{k} r'^{(\alpha)}_{k} - r'^{(\alpha)}_{i} r'^{(\alpha)}_{j} \right].$$
(2.66)

Substituting  $r_i^{\prime(\alpha)} = S_{ij} r_j^{(\alpha)}$  into Eq. (2.66), we have

$$I'_{ij} = \sum_{\alpha} m_{\alpha} \left[ \delta_{ij} S_{kl} r_l^{(\alpha)} S_{km} r_m^{(\alpha)} - S_{jm} r_m^{(\alpha)} S_{ik} r_k^{(\alpha)} \right]$$
$$= \sum_{\alpha} m_{\alpha} \left[ \delta_{ij} r_l^{(\alpha)} S_{lk}^{\dagger} S_{km} r_m^{(\alpha)} - S_{ik} r_k^{(\alpha)} r_m^{(\alpha)} S_{mj}^{\dagger} \right].$$
(2.67)



Fig. 2.4: Calculating the gravitational potential from a mass sphere.

Since  $S_{lk}^{\dagger}S_{km} = \delta_{lm}$ ,

$$I'_{ij} = \sum_{\alpha} m_{\alpha} \left[ \delta_{ij} r_l^{(\alpha)} \delta_{lm} r_m^{(\alpha)} - S_{ik} r_k^{(\alpha)} r_m^{(\alpha)} S_{mj}^{\dagger} \right]$$
$$= \delta_{ij} \left( \sum_{\alpha} m_{\alpha} r_m^{(\alpha)} r_m^{(\alpha)} \right) - S_{ik} \left( \sum_{\alpha} m_{\alpha} r_k^{(\alpha)} r_m^{(\alpha)} \right) S_{mj}^{\dagger}.$$
(2.68)

The first term is already diagonalized, and in Section 1.8 we show that the second term can also be diagonalized if we choose the column vectors of  $\mathbf{S}^{\dagger}$  to be the eigenvectors of the matrix  $M_{km} = \sum_{\alpha} m_{\alpha} r_k^{(\alpha)} r_m^{(\alpha)}$ . In other words,  $I_{ij}$  can always be written as Eq. (2.57) in some coordinate frame.

## 2.12 The Shell Theorem of Gravity

Consider the gravitational potential field produced by a spherical uniform mass shell of radius R. We shall calculate the potential field at a position  $\mathbf{r}$  from the center of the shell. Let us choose  $\mathbf{r}$  to be the  $\theta = 0$  direction, such that the shell can be divided into surface elements  $2\pi R^2 \sin \theta d\theta$  as shown in Fig. 2.4. The distances from the surface elements to the position  $\mathbf{r}$  are  $\sqrt{r^2 + R^2 - 2rR\cos\theta}$ . The potential field is

$$\phi(r) = -G \int_0^{\pi} \frac{\rho 2\pi R^2 \sin \theta \, d\theta}{\sqrt{r^2 + R^2 - 2rR \cos \theta}},$$
(2.69)

where  $\rho$  is the surface mass density. Let us define  $y = \cos \theta$  and x = r/R. We have

$$\phi(r) = 2\pi G \rho R \int_{1}^{-1} \frac{dy}{\sqrt{x^{2} + 1 - 2xy}}$$

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$$= \frac{2\pi G\rho R}{-x} \sqrt{x^2 + 1 - 2xy} \Big|_{y=1}^{y=-1}.$$
 (2.70)

If x > 1, the position **r** is outside of the shell. We have

$$\phi(r) = \frac{2\pi G\rho R}{-x} [x+1-(x-1)] = -\frac{4\pi G\rho R}{x} = -\frac{GM}{r}, \qquad (2.71)$$

where  $M = 4\pi\rho R^2$  is the total mass of the shell. The potential field is the same as that produced by a point of mass M at the center of the shell. If x < 1, the position **r** is inside of the shell. We have

$$\phi(r) = \frac{2\pi G\rho R}{-x} [x + 1 - (1 - x)] = -4\pi G\rho R = -\frac{GM}{R}.$$
 (2.72)

In this case the potential is a constant. Therefore there is no gravitational force in the shell.

### 2.13 The Kepler Problem

Let us now discuss the Kepler's laws in terms of Newton's law of universal gravitation. In the 17th century, Kepler wrote down three empirical laws based on his analysis of observational data on the motion of planets. The laws are:

- 1. Planets move in elliptical obits, with the Sun at one of the foci.
- 2. A line connecting a planet and the Sun sweeps out an area at a constant rate.
- 3. The square of the obit period is proportional to the third power of the planet's average distance from the Sun.

The great success of Newton's law of universal gravitation is that Kepler's laws can be derived completely from it.

Let us consider a general central force f(r). The equation of motion is

$$\dot{\mathbf{p}} = f(r)\frac{\mathbf{r}}{r},\tag{2.73}$$

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where in our notation  $r = |\mathbf{r}|$ . The angular momentum follows the following equation

$$\dot{\mathbf{L}} = \frac{d}{dt}(\mathbf{r} \times \mathbf{p}) = \dot{\mathbf{r}} \times \mathbf{p} + \mathbf{r} \times \dot{\mathbf{p}}$$
$$= \dot{\mathbf{r}} \times m\dot{\mathbf{r}} + \mathbf{r} \times f(r)\frac{\mathbf{r}}{r} = 0, \qquad (2.74)$$

hence is a constant vector. The cross product of  $\dot{\mathbf{p}}$  with the constant angular momentum  $\mathbf{L}$  can be expanded as

$$\dot{\mathbf{p}} \times \mathbf{L} = f(r)\frac{\mathbf{r}}{r} \times m(\mathbf{r} \times \dot{\mathbf{r}}) = \frac{mf(r)}{r}[\mathbf{r} \times (\mathbf{r} \times \dot{\mathbf{r}})]$$
$$= \frac{mf(r)}{r}[\mathbf{r}(\mathbf{r} \cdot \dot{\mathbf{r}}) - r^{2}\dot{\mathbf{r}}].$$
(2.75)

Since

$$\mathbf{r} \cdot \dot{\mathbf{r}} = \frac{1}{2} \frac{d}{dt} (\mathbf{r} \cdot \mathbf{r}) = r\dot{r}, \qquad (2.76)$$

we may replace  $\mathbf{r} \cdot \dot{\mathbf{r}}$  in Eq. (2.75) by  $r\dot{r}$  to obtain

$$\frac{d}{dt}(\mathbf{p} \times \mathbf{L}) = -mf(r)r^2 \left(\frac{\dot{\mathbf{r}}}{r} - \frac{\mathbf{r}\dot{r}}{r^2}\right)$$
(2.77)

$$= -mf(r)r^2\frac{d}{dt}\left(\frac{\mathbf{r}}{r}\right). \qquad (2.78)$$

Substituting in the force of gravity  $f(r) = -k/r^2$ , we can define

$$\mathbf{A} \equiv \mathbf{p} \times \mathbf{L} - mk\frac{\mathbf{r}}{r},\tag{2.79}$$

and immediately we see  $\dot{\mathbf{A}} = 0$ , namely  $\mathbf{A}$  is a conserved vector like the angular momentum. It is known as the Laplace-Runge-Lenz vector. The magnitude of  $\mathbf{A}$  can be derived from

$$\mathbf{A} \cdot \mathbf{A} = \left( \mathbf{p} \times \mathbf{L} - mk\frac{\mathbf{r}}{r} \right) \cdot \left( \mathbf{p} \times \mathbf{L} - mk\frac{\mathbf{r}}{r} \right)$$
$$= \left( \mathbf{p} \times \mathbf{L} \right) \cdot \left( \mathbf{p} \times \mathbf{L} \right) - \frac{2mk}{r} \mathbf{r} \cdot \left( \mathbf{p} \times \mathbf{L} \right) + m^2 k^2.$$
(2.80)

Using the formula  $(\mathbf{a} \times \mathbf{b}) \cdot (\mathbf{c} \times \mathbf{d}) = (\mathbf{a} \cdot \mathbf{c})(\mathbf{b} \cdot \mathbf{d}) - (\mathbf{a} \cdot \mathbf{d})(\mathbf{b} \cdot \mathbf{c})$ , and noting that

$$\mathbf{r} \cdot (\mathbf{p} \times \mathbf{L}) = \mathbf{L} \cdot (\mathbf{r} \times \mathbf{p}) = L^2,$$
 (2.81)

Eq. (2.80) can be reduced to

$$\mathbf{A} \cdot \mathbf{A} = p^2 L^2 - \frac{2mk}{r} \mathbf{L} \cdot (\mathbf{r} \times \mathbf{p}) + m^2 k^2$$
$$= 2m L^2 \left(\frac{p^2}{2m} - \frac{k}{r}\right) + m^2 k^2$$
$$= 2m L^2 E + m^2 k^2, \qquad (2.82)$$

where E is the total energy of the system.

From the definition of **A**, it is clear that

$$\mathbf{A} \cdot \mathbf{L} = 0, \tag{2.83}$$

Therefore **A** must be a fixed vector lying in the plane of planet motion. Let the direction of **A** be the  $\theta = 0$  axis in the polar coordinate system. We have

$$\mathbf{r} \cdot \mathbf{A} = Ar \cos \theta = \mathbf{r} \cdot (\mathbf{p} \times \mathbf{L}) - mkr.$$
(2.84)

From Eq. (2.81), Eq. (2.84) is

$$Ar\cos\theta = L^2 - mkr. \tag{2.85}$$

Writing Eq. (2.85) in rectangular coordinates, we have

$$x^{2} + y^{2} = \left(\frac{L^{2} - Ax}{mk}\right)^{2},$$
(2.86)

or

$$\left(1 - \frac{A^2}{m^2 k^2}\right) \left[x + \frac{L^2 A/(m^2 k^2)}{1 - A^2/(m^2 k^2)}\right]^2 + y^2 = \frac{L^4/(m^2 k^2)}{1 - A^2/(m^2 k^2)}.$$
 (2.87)

Set

$$a^{2} = \frac{L^{4}/(m^{2}k^{2})}{[1 - A^{2}/(m^{2}k^{2})]^{2}} = \frac{k^{2}}{4E^{2}},$$
 (2.88)

$$b^{2} = \frac{L^{4}/(m^{2}k^{2})}{1 - A^{2}/(m^{2}k^{2})} = \frac{L^{2}}{-2mE},$$
(2.89)

$$c = \frac{L^2 A / (m^2 k^2)}{1 - A^2 / (m^2 k^2)} = \frac{A}{-2mE},$$
(2.90)

then

$$\frac{(x+c)^2}{a^2} + \frac{y^2}{b^2} = 1.$$
 (2.91)

#### 2.13. The Kepler Problem

From Eq. (2.82) and Eqs.(2.88)–(2.90), it can be seen that  $a^2 - b^2 = c^2$ , therefore the origin (0,0) is one of the foci. If E < 0, the planet is bounded by the gravity. In this case both  $a^2$  and  $b^2$  are positive and Eq. (2.91) is the equation for an ellipse, which gives Kepler's first law. For the unbound case we have E > 0, then  $a^2$  is still positive but  $b^2$  becomes negative, and the trajectory is a hyperbola. Eqs. (2.82) and (2.91) yield

$$\left(\frac{4E}{k^2}\right)x^2 - \left(\frac{4A}{mk^2}\right)x - \left(\frac{2m}{L^2}\right)y^2 = -\left(\frac{2L^2}{mk^2}\right).$$
(2.92)

If  $E \to 0$ , we have the critically bounded case in which Eq. (2.92) reduces to

$$\left(\frac{4}{k}\right)x + \left(\frac{2m}{L^2}\right)y^2 = \left(\frac{2L^2}{mk^2}\right),\tag{2.93}$$

or

$$y^{2} = -\frac{2L^{2}}{mk} \left( x - \frac{L^{2}}{2mk} \right).$$
 (2.94)

This is a parabola with the focus at the origin.

Conservation of the angular momentum means

$$m \left| \mathbf{r} \times \frac{d\mathbf{r}}{dt} \right| = L = \text{constant.}$$
 (2.95)

Because  $|\mathbf{r} \times d\mathbf{r}|$  is the area spanned by  $\mathbf{r}$  and  $d\mathbf{r}$ , we see the vector  $\mathbf{r}$  sweeps an area with a constant rate. This is Kepler's second law. Let us integrate the area S(t) swept by the vector  $\mathbf{r}$  for one period T.

$$S(T) = \int_0^T \frac{1}{2} \left| \mathbf{r} \times \frac{d\mathbf{r}}{dt} \right| dt \qquad (2.96)$$

$$= \frac{LT}{2m} = \pi ab. \tag{2.97}$$

Substituting in the expressions for a and b in Eqs. (2.88) and (2.89), we have

$$T = \frac{2m\pi ab}{L} = \frac{2\pi L^3 / (mk^2)}{[1 - A^2 / (m^2k^2)]^{3/2}} = 2\pi \sqrt{\frac{m}{k}} a^{3/2}$$
$$= \frac{2\pi}{\sqrt{GM}} a^{3/2}.$$
(2.98)

Since in an ellipse the sum of the distances to the two foci is 2a, the average distance to one of the focus is a. Eq. (2.98) gives Kepler's third law.



Fig. 2.5: A rod hanging on a wall.

#### 2.14 Exercises

**Exercise 2.1.** A fish can swim at a speed of 3 m/s on still water. It wants to cross a river while spending the shortest possible time. In what direction should it go with respect to the bank if the speed of water is (1) 2 m/s, (2) 4 m/s? Assume that the speed of the water is the same everywhere.

**Exercise 2.2.** A fish can swim at a speed of 3 m/s on still water. It wants to cross a river while traveling the shortest possible distance. In what direction should it go with respect to the bank if the speed of water is (1) 2 m/s, (2) 4 m/s? Assume that the speed of the water is the same everywhere.

**Exercise 2.3.** A rod of mass m is hanging on the wall as shown in Fig. 2.5. One end of the rod is pulled by a string fixed to the wall at point A, and the other end is pushed against the wall at point B by gravity. The distance between A and B is equal to the length of the rod, and the angle between the rod and the wall is  $\theta$ . If the force exerted by the wall to the rod at point B is  $\mathbf{F}$ , what is  $|\mathbf{F}|$  as a function of  $\theta$ ?

**Exercise 2.4.** A spring with a uniform mass density  $\rho$  has a spring constant k. When the spring is placed horizontally on a table without being stretched, its length is L. What is its length when it is hung vertically and stretched by the gravitational force? Note that when the spring is hung vertically, its mass density is no longer uniform, because the upper part is stretched more than the lower part.

**Exercise 2.5.** A fishing boat had lost its direction on a foggy sea. The captain decided to sail in a fixed direction at a constant speed  $v_t$  in the

#### 2.14. EXERCISES

hope that the boat would eventually reach the shore. At the same time, he reported to the police through radio the position of the boat and the speed and direction of sailing. However, the radio broke down during the transmission, so that the police only knew the position and the speed, not the direction. Nevertheless, a speedboat capable of sailing at  $v_p$  was dispatched to search for this fishing boat. When the speedboat arrived at the reported position, a time  $\Delta t$  had passed. Because the police did not know in what direction the fishing boat went, it seemed that there was no way to continue. However, because the captain of the speedboat learned calculus well, he figured out a reliable plan to catch the fishing boat. If you were the captain, what would be your plan? How long would it take? What was the distance the speedboat traveled before catching the fishing boat, there may be some parameters of random choice in your plan. The answer will of course depend on these parameters, instead of being a fixed number.

**Exercise 2.6.** There are four ants in the four corners of a square room of length l. Ant A is at the south-east corner, and B is at the north-east corner, ant C is at the north-west corner, and ant D is at the south-west corner. Starting at t = 0, and A moves toward its target and B, and B moves toward its target ant C, and C moves toward its target ant D, and ant D moves toward its target ant A. All the ants move at a fixed speed v in the direction pointing to their respective targets. Eventually, the four ants collide in the center of the room. How far has each ant traveled? How long does it take? What are the coordinates of ant A as functions of time? (Hint: If you use the real time t as the variable for the equation of motion, the equation becomes highly nonlinear. Choose a suitable variable s, which is a function of t, to reduce the equation of motion to a linear form. You do not need to know s(t) explicitly to begin with; you only need to define s through a relation between ds and dt, namely ds/dt = f(t). Neither do you need to know what is f(t) in the beginning. After the problem is solved in the variable s, f(t)will become obvious.)

**Exercise 2.7.** Landslide can occur if the coefficient of static friction  $\mu_s$  between soil is reduced by heavy rain. For a 45° slope, what is the minimum value of  $\mu_s$  before landslide occurs?

**Exercise 2.8.** Two identical balls A and B are in contact with each other. Their centers are on the *y*-axis and the contact point is at the origin. A third identical ball C moving at a speed of 10 m/s along the *x*-axis collides elastically with A and B. Find the velocities of all three balls after collision.



Fig. 2.6: A shifted stack of blocks.

**Exercise 2.9.** Consider how to stack N blocks of unit length to make the top block extend farthest out without falling, as shown in Fig. 2.6. The (n+1)th block is shifted relative to the nth block beneath it by a distance  $d_n$ . What is the formula for  $d_n$ ?

**Exercise 2.10.** Consider a small projectile fired by a gun with a 45° angle of elevation at earth surface. The initial velocity is  $\mathbf{v}_0$ . Assume the density of air is small enough such that the drag force  $\mathbf{F}_d$  is proportional to the velocity of the projectile, namely  $\mathbf{F}_d = -\beta \mathbf{v}$ . Calculate the position of the projectile as a function of time before it falls back to the ground.

**Exercise 2.11.** A car of mass m climbs up and down a small hill with a constant speed v. The shape of the hill is described by

$$z = he^{-ax^2},$$

where z is the vertical coordinate, x is the horizontal coordinate, and h is the height of the hill. If v is too large, at the peak of the hill the wheels of the car may loose contact with the road. This is of course dangerous. What is the speed limit if such risk is to be avoided?

**Exercise 2.12.** A vertically free falling ball is slowed down by a drag force from the air. The initial velocity of the ball is zero. Assuming the drag force is proportional to the square of the velocity, the equation of motion for the ball becomes

$$m\frac{dv}{dt} = mg - \gamma v^2.$$

Solve this equation of motion.

**Exercise 2.13.** A thin rope of mass m and length L is put on a table as shown in Fig. 2.7. Half of the rope lies flat on the table, and the other half



Fig. 2.7: A rope falling from a table.

hangs vertically through a hole near the edge. As gravity pulls the rope down, what is the position of the center of the rope relative to the table as a function of time? Assume there is no friction between the rope and the table.

**Exercise 2.14.** A bicycle is constructed in such a way that the radius of the wheels is 30 cm and the distance between the axes of the wheels is 1 m. When a 60-kg rider is riding the bicycle on flat ground, the center of mass for the rider and the bicycle as a whole is at equal distance from the axes of the wheels and at a height of 60 cm from the ground. After a while the rider encounters a  $30^{\circ}$  down slope. As the bicycle goes down the slope it picks up a speed of 40 km/hr. At this moment the rider decides to pull the front break. This is of course dangerous, because the bicycle may turn over. At what deceleration, the rear wheel starts to loose contact with the ground?

**Exercise 2.15.** An observer on the Earth finds a motionless uniform rope hanging vertically from the sky. One end of the rope is just above the ground, and the other end extends high up into the sky beyond the visual range. If he had not learned physics, he might think the rope is hanging from a spaceship sent by extra-terrestrial beings. However, it is possible for a bare rope to hang from the space just like the Moon hangs on the sky. How long should the rope be? In this exercise we assume the Earth does not have an atmosphere.

Exercise 2.16. A transparent vacuum tunnel was built to test a magnetic-

levitated prototype train powered by hydrogen fuel cells. Peter, who was standing by the tunnel, observed that at the first stage the train used x liters of fuel to accelerate from 0 to 100 km/hr, and at the second stage the train used 3x liters more of fuel to accelerate from 100 to 200 km/hr. Because the motion of the train has almost no friction, Peter figured that all the energy of the fuel was converted to the kinetic energy of the train. That is why in the first stage the fuel consumption was x liters while in the second stage the fuel consumption was 3x liters. Another observer Paul, who was on an ordinary train moving at a speed of 100 km/hr in the opposite direction, also witnessed the event. From his point of view, in the first stage the speed of the speed increased from 200 to 300 km/hr. Therefore Paul figured in the second stage the fuel consumption should be  $(3^2 - 2^2)/(2^2 - 1^2)x = (5/3)x$  liters. Who is right, Peter or Paul? If one is right, the other must have made a mistake in his calculation. Do the correct calculation for the wrong one.

**Exercise 2.17.** A sniper at a latitude of  $30^{\circ}$  north is aiming at a small target 1 km away in the north. The speed of the bullet is 800 m/s. If the sniper does not take into account the rotation of the Earth, by how far to the east or the west will the bullet miss the target? In this exercise we assume the Earth does not have an atmosphere.

**Exercise 2.18.** A powerful rail gun located at the Equator is aimed at the horizontal direction toward east. With the aid from the spin of the Earth, the gun is capable of launching a projectile to the escape velocity of the Earth, so that the projectile has just enough energy to break loose from the gravitational pull of the Earth and travel to a place that is infinitely far away. Because the spin of the Earth adds velocity to the projectile, when the gun is placed at the Equator and aimed at the horizontal direction toward east minimum energy from the power supply of the gun is required. However, because of a mistake in the calculation, the energy stored into the power supply of the gun is only 95% of this minimum energy. Assuming all the energy stored into the power supply of the projectile, how long after the launch will the projectile return to the Earth? In this exercise we assume the Earth does not have an atmosphere. We also ignore the influence from the Moon, the Sun, and other planets.

**Exercise 2.19.** A dumb-bell sits on a horizontal frictionless table, not moving or rotating, as shown in Fig. 2.8. The dumb-bell can be considered as two point masses M joined by a massless rod of length L. A ball of mass


Fig. 2.8: A dumb-bell hit by a ball.



Fig. 2.9: Falling into a mine.

m < M moving in the -x direction with velocity v makes a head-on elastic collision with one of the mass point of the dumb-bell and bounces back in the x-direction. After the collision, what is the center-of-mass motion and the rotational motion of the dumb-bell? What is the velocity of the ball after the collision?

**Exercise 2.20.** A crazy mining company has dug up a tunnel from the surface of the Earth all the way down to the center of the Earth. At the midpoint of the tunnel it has dug up a spherical cavity of radius R/4, where R is the radius of the Earth, as shown in Fig. 2.9. An unfortunate worker falls into the tunnel. What is the impact velocity when the worker hits the end of the tunnel? In this exercise we assume the Earth does not have an atmosphere.

**Exercise 2.21.** The mass of Jupiter is  $1.9 \times 10^{27}$  kg and its speed relative to the Sun is 13 km/s. A spacecraft of 3000 kg approaches Jupiter with a speed of 3 km/s relative to the Sun. The trajectory of the spacecraft is bent by

the gravitational force from Jupiter such that in a reference frame fixed to Jupiter the spacecraft comes in with a velocity  $\mathbf{v}$  and leaves with a velocity  $\mathbf{u}$ . The angle between  $\mathbf{v}$  and  $\mathbf{u}$  is  $\theta$ . Show that the final speed of the spacecraft relative to the Sun after this soft encounter can be much larger than its initial velocity 3 km/s. Find the final speed of the spacecraft as a function of  $\theta$ .

**Exercise 2.22.** On the line connecting the Earth and the Sun there is a point rotating with the same angular velocity as that of the Earth around the Sun, where the gravitational forces from the Earth and the Sun and the centrifugal force cancel each other. This is called the first Lagrange point. How far is this point from the center of the Earth? Give a numerical answer. Consider the shape of the effective potential function at this point in a rotating frame in which the origin is at the center of the Sun and the position vector of the Earth is  $\mathbf{r}$ . The frame rotates with the same angular velocity as that of the Earth around the Sun. Does the potential function has a minimum in the  $\hat{\mathbf{r}}$ -direction? Does the potential function has a minimum in the  $\boldsymbol{\theta}$ -direction (the direction perpendicular to r)? Hint: Define  $\alpha \equiv m/M \ll 1$ , where m is the mass of the Earth and M the mass of the Sun, and  $\beta \equiv l/L$ , where l is the distance from the Earth to the first Lagrange point and L the distance from the Earth to the Sun. Write the equilibrium condition in terms of  $\alpha$  and  $\beta$ . Assuming  $\beta \ll 1$  for the time being, one can throw away high-order terms of both  $\alpha$  and  $\beta$  to simplify the equation. After solving the equation, verify  $\beta \ll 1$  for consistency. How many terms to throw away is your own choice. Here we only ask for a numerical answer that is accurate to the second digit.

**Exercise 2.23.** Consider a base-ball bat shown in Fig. 2.10. Point c is the center of mass. Point a is the position to hold the bat when striking. If the bat is pivoted about a horizontal frictionless axis through a to form a physical pendulum, its frequency of small oscillation is  $\omega$ . Point b is chosen such that if the bat is pivoted about a horizontal frictionless axis through b to form a physical pendulum, its frequency of small oscillation is also  $\omega$ . Show that, if the hitter strikes the base ball at b with the velocity of the incoming ball perpendicular to the axis of the bat, his hands at a do not feel the reaction force. In this problem we assume the surface of the bat around point b is cylindrical and it is parallel to the axis of the bat. Hint: If the strike point is at the opposite end of a from c, the bat tends to rotate in addition to recoiling back. If the strike point is far enough from c, the rotation can make point a move in the opposite direction of the incoming ball. Hence in between there is an ideal strike point for which a does not move.



Fig. 2.10: The best point to strike a base ball.



Fig. 2.11: Tilting a rotating ball.

**Exercise 2.24.** A solid ball of mass m and radius r is rotating around a horizontal shaft parallel to the *x*-axis. The angular velocity is  $\omega \hat{\mathbf{x}}$  where  $\omega > 0$ . The shaft is supported by two vertical poles that are parallel to the *z*-axis and separated by a distance d. The ball is at an equal distance d/2 from the poles. If the shaft is tilted by a small angle  $\theta \ll 1$  as shown in Fig. 2.11, what is the impulse acted on each pole? Note that impulse is an vector, so you should include the direction of the impulse in your answer.

**Exercise 2.25.** Consider a particle moving in the *x-y* plane under the gravitational force from a massive thin wire in the *z*-axis. The wire extends from  $z = -\infty$  to  $z = \infty$ . The mass per unit length is  $\rho$ . Show that for any initial position and initial velocity, it is not possible to escape from this gravitational system. As usual, here "escape" means to go as far as one wants.

**Exercise 2.26.** In the outer space there is a uniform massive thin shell of radius R with a small round opening of radius  $r \ll R$  on the top. The mass per unit area of the shell is  $\rho$ . A particle is released at the center of the

shell with zero initial velocity. What is the final velocity of the particle as it collides with the shell?

**Exercise 2.27.** Oil companies search underground pocket of oil by detecting the minute change of gravitational force at the Earth surface. Assume the detector is right above an underground spherical pocket of oil. The radius of the pocket is r and the center of the pocket is at a depth d. If the change of gravitational acceleration can be written as

$$\Delta g = g - g_0 = a - bx^2,$$

where  $g_0 = 9.8 \text{ m/s}^2$  and x is a small horizontal displacement of the detector from the position right above the pocket at the Earth surface, what is r and d in terms of a and b? In this problem we assume the Earth is a uniform solid sphere of density  $\rho_e$  without spin and the oil has a uniform density  $\rho_o$ . Note that we assume  $x \ll r < d$  and  $d \ll R$ , where R is the radius of the Earth.

**Exercise 2.28.** A 10-g marble is launched vertically by a sling-shot with an initial velocity of 20 m/s. Assume the drag force F from the air is given by  $F = \gamma v^2$ , where v is the velocity of marble and  $\gamma = 8 \times 10^{-5}$  kg/m. How long does it take for the marble to reach the maximum height? What is the maximum height? In this problem we assume the Earth has no spin.

**Exercise 2.29.** A roller coaster runs with a constant speed v along a track described by  $h(x) = h_0(\tanh x + 1)$ , where h is the height of the track, x is the horizontal coordinate, and  $h_0$  is a constant. During a run from x = -100 to x = 100, the maximum acceleration experienced by the roller coaster is  $a_{\text{max}}$ . If in the next run the speed is changed to 2v, what will be the maximum acceleration?

**Exercise 2.30.** A top is made of a solid ball attached to a pin of negligible mass. The mass of the ball is 0.25 kg and the radius is 2 cm. The top is spinning at a rate of 1200 rpm. The the distance between center of the sphere and the end of the pin, where the top is supported, is 4 cm. The angle between the top's rotation axis and the vertical axis is 15°. Due to the torque produced by the gravitational force, the angular momentum rotates slowly around the vertical axis, as shown in Fig. 2.12. This rotation is known as the gyroscopic precession. What is the rate of precession? In your calculation does the precession change the angle between the angular momentum and the vertical axis? If not, how can a top fall eventually as it slows down?

Exercise 2.31. A short section of round pipe made of honeycomb composite



Fig. 2.12: Gyroscopic precession of a top.



Fig. 2.13: A rolling pipe.

material is rolling on a flat surface without slipping, driven by a boy of mass 30 kg running inside of it, as shown in Fig. 2.13. The inner radius of the pipe is 1.5 m and the outer radius is 1.7 m. The mass density of the pipe is  $100 \text{ kg/m}^3$  and the length is 1 m. The boy maintains his angular position at  $30^{\circ}$  from the vertical axis by running on the slope of the pipe. What is the acceleration of the pipe?

**Exercise 2.32.** A way to launch a satellite without using a rocket is by releasing it from a high tower at the equator. If the tower is not high enough, the satellite will crash into the Earth. Show that the minimum height of the tower h satisfies an equation of the following form.

$$(h+R)^4 + a_3(h+R)^3 + a_2(h+R)^2 + a_1(h+R) + a_0 = 0,$$

where R is the radius of the Earth. What are the four coefficients  $a_0$ ,  $a_1$ ,  $a_2$ , and  $a_3$ ? In this problem we assume the Earth is a perfect sphere with no atmosphere and the tower has no mass.

Exercise 2.33. In 1909 Ernest Rutherford's research team discovered that

the scattering angle of an alpha particle by gold foil can be unexpectedly large. This led to the postulate that atoms have a highly concentrated nucleus that contains all the positive charges. Considering an alpha particle flying toward a gold nucleus with a velocity of  $1.8 \times 10^7$  m/s. The Coulomb repulsive force will bend the trajectory, such that the alpha particle will leave the gold nucleus at an angle  $\theta$  with respect to the incoming direction. Let d be the smallest distance between the alpha particle and the gold nucleus during the encounter. As one can imagine, a smaller d yields a larger  $\theta$ . If  $\theta = 90^\circ$ , how small is d? In this problem we assume the mass ratio between the alpha particle and the gold nucleus does not move. We also assume that the electrons around the gold nucleus have no effect on the alpha particle because they are evenly distributed in a much larger space. Note that the atomic number of gold is 79.

## Chapter 3

# **Oscillators and Waves**

## 3.1 Driven Harmonic Oscillators

An ideal simple harmonic oscillator can oscillate indefinitely. However, in reality there is always some friction that damps the oscillation. Therefore continuous oscillation must be driven by external forces. The equation of motion for a driven harmonic oscillator with damping is

$$m\ddot{x} + \mu\dot{x} + kx = F(t), \qquad (3.1)$$

where  $-\mu \dot{x}$  represents the damping force, -kx the restoring force, and F(t) the external driving force. It is more convenient to use the following form

$$\ddot{x} + \gamma \dot{x} + \omega_0^2 x = f(t), \qquad (3.2)$$

where  $\gamma = \mu/m$  and f(t) = F(t)/m. First, let us consider the case in which f(t) = 0. The solutions are

$$x(t) = a_1 e^{\lambda_+ t} + a_2 e^{\lambda_- t}, \tag{3.3}$$

where  $a_1$  and  $a_2$  are determined by the initial conditions, and

$$\lambda_{\pm} = \frac{-\gamma \pm \sqrt{\gamma^2 - 4\omega_0^2}}{2}.$$
(3.4)

If  $\gamma > 2\omega_0$ , the oscillator is called an overdamped oscillator. The solutions are just exponentially decaying functions, and there is no oscillation at all.

If  $\gamma < 2\omega_0$ , the oscillator is called an underdamped oscillator. It oscillates at a frequency  $\omega = \sqrt{\omega_0^2 - \gamma^2/4}$  with an exponentially decaying amplitude  $e^{-\gamma t/2}$ . If we choose the coefficients in Eq. (3.3) to be  $a_1 = a_2 = b_1/2$  or  $a_1 = -a_2 = b_2/(2i)$ , the two solutions for an underdamped oscillator can be expressed as

$$x(t) = b_1 e^{-\gamma t/2} \cos \omega t \tag{3.5}$$

or

$$x(t) = b_2 e^{-\gamma t/2} \sin \omega t. \tag{3.6}$$

If  $\gamma = 2\omega_0$ , the oscillator is called a critically damped oscillator. In this case the two independent solutions can be found by taking the limit of  $\omega \to 0$  in Eqs. (3.5) and (3.6) regardless of the constant coefficients in front of them, which will be determined by the initial condition anyway. Hence the solutions for a critically damped oscillator are  $e^{-\omega_0 t}$  and  $te^{-\omega_0 t}$ .

Next, let us assume f(t) is nonzero only between t = 0 and t = T. We need to find a special solution to add to the solutions in Eq. (3.3). Let us write x(t) and f(t) in terms of their Fourier transforms.

$$x(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \tilde{x}(\omega) e^{i\omega t} d\omega, \qquad (3.7)$$

$$f(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \tilde{f}(\omega) e^{i\omega t} d\omega.$$
(3.8)

Both x(t) and f(t) can be thought of as a superposition of many frequency components  $\cos \omega t$  and  $\sin \omega t$ , and  $\tilde{x}(\omega)$  and  $\tilde{f}(\omega)$  represent the amplitude of the  $\omega$ -component. Substituting Eqs. (3.7) and (3.8) into Eq. (3.2). We have

$$\int_{-\infty}^{\infty} (-\omega^2 + i\gamma\omega + \omega_0^2)\tilde{x}(\omega)e^{i\omega t}d\omega = \int_{-\infty}^{\infty} \tilde{f}(\omega)e^{i\omega t}d\omega.$$
(3.9)

Comparing both sides, we obtain

$$\tilde{x}(\omega) = \frac{\tilde{f}(\omega)}{-\omega^2 + i\gamma\omega + \omega_0^2}.$$
(3.10)

Now that we know  $\tilde{x}(\omega)$ , we can calculate x(t) by the inverse Fourier transform. Alternatively we may use the convolution theorem of Fourier transform and Eq. (1.254) to obtain

$$x(t) = \frac{1}{\beta} \int_{-\infty}^{t} f(t') e^{-\gamma(t-t')/2} \sin[\beta(t-t')] dt', \qquad (3.11)$$

where

$$\beta = \sqrt{\omega_0^2 - \frac{\gamma^2}{4}}.\tag{3.12}$$

In Eq. (3.11), the displacement x(t) at time t can be interpreted as the linear response to the external force f(t') at time t'. Since the response is not instantaneous, x(t) is a linear combination of all the f(t') with coefficient  $\frac{1}{\beta}e^{-\gamma(t-t')/2}\sin[\beta(t-t')]$ . The function g(t) that satisfies the equation

$$x(t) = \int_{-\infty}^{\infty} f(t')g(t-t') dt$$
 (3.13)

is known as the **Green's function**. By setting  $f(t') = \delta(t')$  in Eq. (3.13), it can be seen that the Green's function g(t) is the solution of the equation

$$\ddot{x} + \gamma \dot{x} + \omega_0^2 x = \delta(t). \tag{3.14}$$

The solution in Eq. (3.11) shows that

$$g(t) = \begin{cases} \frac{1}{\beta} e^{-\gamma t/2} \sin \beta t & \text{when } t \ge 0\\ 0 & \text{when } t < 0. \end{cases}$$
(3.15)

For the special case where

$$f(t) = A \cos \omega t$$
  
=  $\frac{A}{2}e^{i\omega t} + \frac{A}{2}e^{-i\omega t},$  (3.16)

we may assume the solution has the following form:

$$x(t) = Be^{i\omega t} + B^* e^{-i\omega t}.$$
(3.17)

Substituting into Eq. (3.2), we obtain

$$B = \frac{A/2}{-\omega^2 + i\gamma\omega + \omega_0^2}.$$
(3.18)

Set

$$\frac{1}{-\omega^2 + i\gamma\omega + \omega_0^2} = |\chi|e^{i\phi},\tag{3.19}$$

where

$$\begin{aligned} |\chi| &= \frac{1}{|-\omega^2 + i\gamma\omega + \omega_0^2|},\\ e^{i\phi} &= \frac{|-\omega^2 + i\gamma\omega + \omega_0^2|}{-\omega^2 + i\gamma\omega + \omega_0^2|}, \end{aligned} (3.20)$$

one obtains

$$x(t) = \frac{A}{2} \left( |\chi| e^{i\phi} e^{i\omega t} + |\chi| e^{-i\phi} e^{-i\omega t} \right)$$
  
=  $A|\chi| \cos(\omega t + \phi).$  (3.21)

When the driving frequency  $\omega$  is much smaller than the resonance frequency  $\omega_0$ , we have  $\phi \to 0$ , which shows the oscillator is **in phase** with the driving force. When the driving frequency  $\omega$  is equal to the resonance frequency  $\omega_0$ , we have  $\phi = -\pi/2$ , which shows the oscillator is **delayed by 90 degrees** with respect to the driving force. When the driving frequency  $\omega$  is much larger than the resonance frequency  $\omega_0$ , we have  $\phi \to -\pi$ , which shows the oscillator is **out of phase** with the driving force.

If the oscillator is weakly damped,  $\gamma \ll \omega_0$ . Then  $\tilde{x}(\omega)$  has a resonance peak at  $\omega = \omega_0$ . Near the resonance peak,  $\omega_0^2 - \omega^2 \approx 2\omega(\omega_0 - \omega)$ , we have

$$\tilde{x}(\omega) \approx \frac{\tilde{f}(\omega)/(2\omega)}{\omega_0 - \omega + i\gamma/2},$$
(3.22)

and

$$|\tilde{x}(\omega)|^2 \approx \frac{|\tilde{f}(\omega)|^2/(4\omega^2)}{(\omega_0 - \omega)^2 + \gamma^2/4}.$$
 (3.23)

If we define the width of the resonance peak to be the difference between the two values of  $\omega$  that reduce  $|\tilde{x}(\omega)|^2$  by half, then the width is  $\gamma$ .

Let us go back to see what trick the Fourier transform does to the equation that allows us to get the solution without much effort. In the time domain Eq. (3.2) is a differential equation. Fourier transform turns it into an algebraic equation in the frequency domain, Eq. (3.10), which is much easier to solve. This is why spectral analysis by Fourier transform is a powerful tool for linear differential equations.

#### **3.2** Harmonic Generation in Nonlinear Oscillators

Consider a particle in a potential well V(x). The equation of motion is

$$m\ddot{x} = -\frac{dV}{dx}.$$
(3.24)

#### 3.2. HARMONIC GENERATION IN NONLINEAR OSCILLATORS

If we assume that V(x) = V(-x) and the minimum of V(x) is at x = 0, we may expand V(x) in Taylor series.

$$V(x) = V(0) + \frac{V''(0)}{2}x^2 + \frac{V^{(4)}(0)}{24}x^4 + \cdots$$
 (3.25)

For small oscillation, namely the motion of the particle is not far from x = 0, the equation of motion is approximately

$$\ddot{x} = -\omega_0^2 x - \alpha x^3, \tag{3.26}$$

where  $\omega_0^2 = k/m = V''(0)/m$  and  $\alpha = V^{(4)}(0)/(6m)$ . If  $\alpha x^3$  is omitted, we get the simple harmonic oscillator. Therefore if the amplitude of oscillation is small enough such that  $\alpha x^3 \ll \omega_0^2 x$ , we should obtain a solution that is only slightly different from the solution of the simple harmonic oscillator. Now let us see how  $\alpha x^3$  changes the solution of the simple harmonic oscillator. Assuming the initial conditions are  $x(0) \neq 0$  and x'(0) = 0, let us try the following function as the first-order guess.

$$x(t) = a_1 \cos(\omega t) + a_3 \cos(3\omega t). \tag{3.27}$$

Because the solution should be close to the simple harmonic oscillator, we assume  $a_3 \ll a_1$ . Substituting it into Eq. (3.26), we obtain

$$\left( -a_1\omega^2 + a_1\omega_0^2 + \frac{3}{4}\alpha a_1^3 + \frac{3}{4}\alpha a_1^2 a_3 + \frac{3}{2}\alpha a_1 a_3^2 \right) \cos(\omega t)$$

$$+ \left( -a_39\omega^2 + a_3\omega_0^2 + \frac{1}{4}\alpha a_1^3 + \frac{3}{2}\alpha a_1^2 a_3 + \frac{3}{4}\alpha a_3^3 \right) \cos(3\omega t)$$

$$+ \left( \frac{3}{4}\alpha a_1^2 a_3 + \frac{3}{4}\alpha a_1 a_3^2 \right) \cos(5\omega t)$$

$$+ \frac{3}{4}\alpha a_1 a_3^2 \cos(7\omega t) + \frac{1}{4}\alpha a_3^3 \cos(9\omega t) = 0.$$

$$(3.28)$$

Since we assume  $a_3 \ll a_1$ , the coefficient of  $\cos(\omega t)$  gives

$$\omega^2 \approx \omega_0^2 + \frac{3}{4}\alpha a_1^2, \qquad (3.29)$$

and the coefficient of  $\cos(3\omega t)$  gives

$$a_3 = \frac{\frac{1}{4}\alpha a_1^3}{9\omega^2 - \omega_0^2 - \frac{3}{2}\alpha a_1^2} \approx \frac{\frac{1}{4}\alpha a_1^3}{8\omega_0^2 + \frac{21}{4}\alpha a_1^2}.$$
(3.30)

Because for small oscillation  $\alpha a_1^2 \ll \omega_0^2$ ,

$$\frac{a_3}{a_1} \approx \frac{\alpha a_1^2}{32\omega_0^2}.$$
 (3.31)

Here we see indeed  $a_3 \ll a_1$ , which is consistent with our assumption in the beginning. Note that  $a_3$  is proportional to the first order of  $\alpha$ . If we keep terms only up to the first order of  $\alpha$ , we can ignore the  $\cos(5\omega t)$ ,  $\cos(7\omega t)$  and  $\cos(9\omega t)$  terms. Therefore Eq. (3.27) is only an approximation up to the first order of  $\alpha$ . We can improve the approximation by adding a term  $a_5 \cos(5\omega t)$  to our guess solution, then we will be able to obtain solutions up to the second order of  $\alpha$ , only with more complicated calculation.

Eq. (3.29) tells us how the frequency of the nonlinear oscillator changes with its amplitude, and Eq. (3.30) gives the amplitude of the third harmonic generated from the nonlinear term. The oscillation speeds up for positive  $\alpha$ and vice versa as expected. The ratio of the third harmonic power to the fundamental power is proportional to the square of the fundamental power, namely

$$\frac{a_3^2}{a_1^2} \propto a_1^4. \tag{3.32}$$

This means the fraction of harmonic distortion of the oscillator increases quadratically with the fundamental power.

Let us look back at the process we employed to obtain the approximate solution. The  $\alpha x^3$  term in the equation of motion can be thought of as a frequency mixer. Let  $x(t) = \cos(\omega_1 t) + \cos(\omega_2 t)$ . The  $\alpha x^3$  term will generate terms of frequencies  $3\omega_1$ ,  $3\omega_2$ ,  $2\omega_2 \pm \omega_1$ , and  $2\omega_1 \pm \omega_2$  with amplitudes proportional to  $\alpha$ . If we start from the solution of the harmonic oscillator  $x(t) = a_1 \cos(\omega t)$ , the  $\alpha x^3$  term will generate a term  $\alpha a_1^3 \cos(3\omega t)/4$ . Therefore we must add to the solution a term proportional to  $\cos(3\omega t)$  to cancel it. Let the added term be  $a_3 \cos(3\omega t)$ . The linear response of the added term gives a contribution of  $(9\omega^2 - \omega_0^2)a_3 \cos(3\omega t)$ . Therefore

$$a_3 = \frac{\alpha a_1^3 / 4}{9\omega^2 - \omega_0^2} \approx \frac{\alpha a_1^3}{32\omega_0^2}.$$
 (3.33)

Now that we have the  $\cos(3\omega t)$  term in the solution, mixing the  $\cos(\omega t)$  term and the  $\cos(3\omega t)$  by  $\alpha x^3$  leads to the  $\cos(5\omega t)$  term. Because the  $\cos(3\omega t)$ term is proportional to  $\alpha$ , the  $\cos(5\omega t)$  term is proportional to  $\alpha^2$ . Continuing this process, we find the solution contains an infinite sequence of odd harmonics  $\cos[(2n + 1)\omega t]$  with decreasing amplitudes proportional to  $\alpha^n a_1^{2n+1}/\omega_0^{2n}$ . In this process,  $\ddot{x} = -\omega_0^2 x$  is called the zeroth-order equation and  $a_1 \cos(\omega t)$  the zeroth-order solution. The term  $\alpha x^3$  is called the perturbation term of the zeroth-order equation. We add a first-order solution

#### 3.2. HARMONIC GENERATION IN NONLINEAR OSCILLATORS

 $a_3 \cos(3\omega t)$  to cancel the terms generated from the zeroth-order solution by the perturbation term of the equation of motion. But the first-order solution together with the zeroth-order solution generate again new terms through the perturbation term of the equation of motion. Therefore we have to add a second-order term to cancel them. If the perturbation term is small enough, correction for each order will be smaller than that for the previous order. The process will converge, and we can have an approximate solution as close to the real solution as we want. Such a procedure of finding approximate solutions is known as the **perturbation expansion**.

Next we consider a weakly damped asymmetric nonlinear oscillator driven by an external force  $mf(t) = mA\cos(\omega t)$ . Any initial oscillation that is not driven by the external force will be damped out in the long run, therefore we look for the steady state solution in which the oscillation amplitude does not change with time. Again, for small oscillation the equation of motion is approximately

$$\ddot{x} = -\gamma \dot{x} - \omega_0^2 x - \beta x^2 + A\cos(\omega t), \qquad (3.34)$$

where  $\beta = V''(0)/(2m)$ . Treating  $\beta x^2$  as the perturbation term, we shall use the following trial solution.

$$x(t) = a_0 + a_1 \cos(\omega t) + b_1 \sin(\omega t) + a_2 \cos(2\omega t) + b_2 \sin(2\omega t) + a_3 \cos(3\omega t) + b_3 \sin(3\omega t),$$
(3.35)

where  $a_2 \cos(2\omega t) + b_2 \sin(2\omega t)$  is the first-order correction, and  $a_3 \cos(3\omega t) + b_3 \sin(3\omega t)$  is the second-order correction. Substituting into Eq. (3.34), one has

$$a_{0}\omega_{0}^{2} + \beta \left(a_{0}^{2} + \frac{a_{1}^{2}}{2} + \frac{b_{1}^{2}}{2} + \frac{a_{2}^{2}}{2} + \frac{b_{2}^{2}}{2} + \frac{a_{3}^{2}}{2} + \frac{b_{3}^{2}}{2}\right)$$

$$+ \left[-a_{1}\omega^{2} + \gamma b_{1}\omega + a_{1}\omega_{0}^{2} + \beta \left(2a_{0}a_{1} + a_{1}a_{2} + b_{1}b_{2} + a_{2}a_{3} + b_{2}b_{3}\right) - A\right]\cos(\omega t)$$

$$+ \left[-b_{1}\omega^{2} - \gamma a_{1}\omega + b_{1}\omega_{0}^{2} + \beta \left(2a_{0}b_{1} + a_{1}b_{2} - b_{1}a_{2} + a_{2}b_{3} - b_{2}a_{3}\right)\right]\sin(\omega t)$$

$$+ \left[-4a_{2}\omega^{2} + 2\gamma b_{2}\omega + a_{2}\omega_{0}^{2} + \beta \left(\frac{a_{1}^{2}}{2} - \frac{b_{1}^{2}}{2} + 2a_{0}a_{2} + a_{1}a_{3} + b_{1}b_{3}\right)\right]\cos(2\omega t)$$

$$+ \left[-4b_{2}\omega^{2} - 2\gamma a_{2}\omega + b_{2}\omega_{0}^{2} + \beta \left(2a_{0}b_{2} + a_{1}b_{1} + a_{1}b_{3} - b_{1}a_{3}\right)\right]\sin(2\omega t)$$

$$+ \left[-9a_{3}\omega^{2} + 3\gamma b_{3}\omega + a_{3}\omega_{0}^{2} + \beta \left(2a_{0}b_{3} + a_{1}a_{2} - b_{1}b_{2}\right)\right]\cos(3\omega t)$$

$$+ \left[-9b_{3}\omega^{2} - 3\gamma a_{3}\omega + b_{3}\omega_{0}^{2} + \beta \left(2a_{0}b_{3} + a_{1}b_{2} + b_{1}a_{2}\right)\right]\sin(3\omega t) = 0. \quad (3.36)$$

#### CHAPTER 3. OSCILLATORS AND WAVES

Let us assume  $a_0$  is of the same order as  $\beta a_1^2, \beta b_1^2$  and  $a_n, b_n$  are of the same order as  $\beta^{n-1}a_1^n, \beta^{n-1}b_1^n$ . We shall justify these assumptions later. If  $\beta$  is small we can include only terms of the lowest-order correction. That is

$$a_0(\omega_0^2 + \beta a_0) + \beta \left(\frac{a_1^2}{2} + \frac{b_1^2}{2}\right) = 0, \qquad (3.37)$$

$$-a_1\omega^2 + \gamma b_1\omega + a_1\omega_0^2 - A = 0, \qquad (3.38)$$

$$-b_1\omega^2 - \gamma a_1\omega + b_1\omega_0^2 = 0, \qquad (3.39)$$

$$-4a_2\omega^2 + 2\gamma b_2\omega + a_2\omega_0^2 + \beta \left(\frac{a_1^2}{2} - \frac{b_1^2}{2}\right) = 0, \qquad (3.40)$$

$$-4b_2\omega^2 - 2\gamma a_2\omega + b_2\omega_0^2 + \beta a_1b_1 = 0, \qquad (3.41)$$

$$-9a_3\omega^2 + 3\gamma b_3\omega + a_3\omega_0^2 + \beta \left(a_1a_2 - b_1b_2\right) = 0, \qquad (3.42)$$

$$-9b_3\omega^2 - 3\gamma a_3\omega + b_3\omega_0^2 + \beta \left(a_1b_2 + b_1a_2\right) = 0.$$
(3.43)

Therefore

$$a_0 = -\frac{\beta(a_1^2 + b_1^2)}{2(\omega_0^2 + \beta a_0)},\tag{3.44}$$

$$a_1 = \frac{-(\omega^2 - \omega_0^2)}{\gamma^2 \omega^2 + (\omega^2 - \omega_0^2)^2} A,$$
(3.45)

$$b_1 = \frac{\gamma \omega}{\gamma^2 \omega^2 + (\omega^2 - \omega_0^2)^2} A,$$
 (3.46)

$$a_{2} = \beta \frac{2a_{1}b_{1}\gamma\omega + \left(\frac{a_{1}^{2}}{2} - \frac{b_{1}^{2}}{2}\right)(4\omega^{2} - \omega_{0}^{2})}{4\gamma^{2}\omega^{2} + (4\omega^{2} - \omega_{0}^{2})^{2}},$$
(3.47)

$$b_2 = \beta \frac{a_1 b_1 (4\omega^2 - \omega_0^2) - \gamma \omega (a_1^2 - b_1^2)}{4\gamma^2 \omega^2 + (4\omega^2 - \omega_0^2)^2},$$
(3.48)

$$a_3 = \beta \frac{3\gamma\omega \left(a_1b_2 + b_1a_2\right) + \left(9\omega^2 - \omega_0^2\right)\left(a_1a_2 - b_1b_2\right)}{9\gamma^2\omega^2 + \left(9\omega^2 - \omega_0^2\right)^2}, \qquad (3.49)$$

$$b_3 = \beta \frac{(a_1 b_2 + b_1 a_2) \left(9\omega^2 - \omega_0^2\right) - 3\gamma\omega \left(a_1 a_2 - b_1 b_2\right)}{9\gamma^2 \omega^2 + (9\omega^2 - \omega_0^2)^2}.$$
 (3.50)

As we can see from the solutions of  $a_0, a_1, a_2, a_3$  and  $b_1, b_2, b_3$ , indeed our assumptions that  $a_0$  is of the same order as  $\beta a_1^2, \beta b_1^2$  and  $a_n, b_n$  are of the same order as  $\beta^{n-1}a_1^n, \beta^{n-1}b_1^n$  are satisfied. The process can be continued by adding a next-order correction  $a_4 \cos(4\omega t) + b_4 \sin(\omega t)$  to the perturbation expansion Eq. (3.34), then a more and more accurate solution can be obtained.



Fig. 3.1: Two harmonic oscillators coupled by a spring.

## 3.3 Normal Modes of Coupled Oscillators

Consider the two harmonic oscillators shown in Fig. 3.1. The equations of motion for the two harmonic oscillators are

$$\begin{array}{lll} m\ddot{x}_1 &=& -kx_1 - k'(x_1 - x_2), \\ m\ddot{x}_2 &=& -kx_2 - k'(x_2 - x_1). \end{array}$$
(3.51)

Clearly,  $x_1$  and  $x_2$  are not independent of each other, and the solutions are not obvious. The equations can be much simplified by choosing another set of variables.

$$u_1 \equiv (x_1 + x_2), u_2 \equiv (x_1 - x_2).$$
(3.52)

Then the equations become

$$\begin{aligned} m\ddot{u}_1 &= -ku_1, \\ m\ddot{u}_2 &= -(k+2k')u_2. \end{aligned}$$
 (3.53)

The new set of variables changes the coupled equations into uncoupled ones. Therefore  $x_1 + x_2$  and  $x_1 - x_2$  are the two independent modes of oscillation for this system of oscillators. Such independent modes of oscillation are known as **normal modes**.

## 3.4 Swinging a Swing

When you were a child, you probably had the experience of playing with a swing. You might have noticed that by moving your body up and down in synchronization with the swing, you could make the amplitude of the swing grow by yourself, without someone else pushing the swing. In an ideal swing, no matter how you change the height of the center of mass of your body, you can only exert a force in the radial direction, and the force is balanced by the tension of the swing. How can you affect the rotational motion of the swing without an external torque? In this section we shall analyze this problem.

Consider an ideal swing in which the player can move his/her center of mass up and down by a small distance  $y = y_0 \cos(\Omega t)$ , as shown in Fig. 3.2. The equation of motion is

$$m(l+y)^2\dot{\theta} = -2m(l+y)\dot{y}\dot{\theta} - mg(l+y)\theta, \qquad (3.54)$$

where l is the length of the swing and m is the mass of the player. The first term on the right-hand side is the Coriolis force. Dividing by m(l + y), Eq. (3.54) becomes

$$(l+y)\ddot{\theta} = -2\dot{y}\dot{\theta} - g\theta. \tag{3.55}$$

Assume the solution we are looking for has the following form:

$$\theta(t) = a(t)\cos(\omega t) + b(t)\sin(\omega t), \qquad (3.56)$$

where  $\omega = \sqrt{g/l}$  is the resonance frequency of the swing, and a(t), b(t) are the slow-varying amplitudes. Because a(t) and b(t) vary slowly,  $\dot{a}$  and  $\dot{b}$  are first-order small quantities. Remember that we have also assumed y is a first-order small quantity, therefore  $\ddot{a}, \ddot{b}, \dot{a}y, \dot{a}y, \dot{b}y$ , and  $\dot{b}y$  are all secondorder small quantities. Ignoring all the second-order small quantities when substituting the trial solution Eq. (3.56) into Eq. (3.55), we obtain

$$l \left[ -2\dot{a}\omega\sin(\omega t) + 2\dot{b}\omega\cos(\omega t) - a\omega^{2}\cos(\omega t) - b\omega^{2}\sin(\omega t) \right] + y \left[ -a\omega^{2}\cos(\omega t) - b\omega^{2}\sin(\omega t) \right] = -2\dot{y} \left[ -a\omega\sin(\omega t) + b\omega\cos(\omega t) \right] - g \left[ a\cos(\omega t) + b\sin(\omega t) \right]. \quad (3.57)$$

Since  $l\omega^2 = g$ , it is

$$l\left[-2\dot{a}\omega\sin(\omega t) + 2\dot{b}\omega\cos(\omega t)\right] + y\left[-a\omega^2\cos(\omega t) - b\omega^2\sin(\omega t)\right]$$
  
=  $-2\dot{y}\left[-a\omega\sin(\omega t) + b\omega\cos(\omega t)\right].$  (3.58)

If the swing is driven resonantly,  $\Omega$  must be an integer multiple of  $\omega$ . When  $\Omega = 2\omega$ , namely  $y = y_0 \cos(2\omega t)$ , we obtain

$$\begin{bmatrix} -2\dot{a}\omega l + \frac{1}{2}b\omega^2 y_0 \end{bmatrix} \sin(\omega t) + \begin{bmatrix} 2\dot{b}\omega l - \frac{1}{2}a\omega^2 y_0 \end{bmatrix} \cos(\omega t)$$
$$-\frac{1}{2}b\omega^2 y_0 \sin(3\omega t) - \frac{1}{2}a\omega^2 y_0 \cos(3\omega t)$$
$$= 2b\omega^2 y_0 \sin(\omega t) - 2a\omega^2 y_0 \cos(\omega t)$$
$$+ 2b\omega^2 y_0 \sin(3\omega t) + 2a\omega^2 y_0 \cos(3\omega t).$$
(3.59)



Fig. 3.2: A model of an ideal swing.

Both sides of the equation contain the lowest power of  $\cos(\omega t)$  and  $\sin(\omega t)$ . Comparing coefficients, we have

$$\dot{a} = \frac{-3\omega y_0}{4l}b,\tag{3.60}$$

$$\dot{b} = \frac{-3\omega y_0}{4l}a.\tag{3.61}$$

But what about the coefficients of  $\cos(3\omega t)$  and  $\sin(3\omega t)$ ? Just like what we did in treating the nonlinear oscillators, they can be taken care of by including higher-order terms such as  $a_3(t)\cos(3\omega t)$  and  $b_3(t)\sin(3\omega t)$  in the trial solution Eq. (3.56). For simplicity, here we work out the lowest-order solution first. Combining Eqs. (3.60) and (3.61), one has

$$\ddot{a} = \left(\frac{3\omega y_0}{4l}\right)^2 a. \tag{3.62}$$

Assume  $y_0 > 0$  and let  $\lambda = 3\omega y_0/(4l)$ , the solution is then

$$a(t) = a_{+}e^{\lambda t} + a_{-}e^{-\lambda t}, \qquad (3.63)$$

and from Eq. (3.60)

$$b(t) = -a_{+}e^{\lambda t} + a_{-}e^{-\lambda t}.$$
(3.64)

The decaying solution associated with  $a_{-}$  can be ignored in the long run, and the growing solution associated with  $a_{+}$  is what we are interested in. Namely

$$\theta(t) = a_{+}[\cos(\omega t) - \sin(\omega t)]e^{\lambda t}, \qquad (3.65)$$



Fig. 3.3: A model of longitudinal mechanical waves.

From the solution we see that in order to make a swing swing, one must have an initial oscillation first, and the player should raise and lower his/her center of mass at twice of the resonant frequency of the swing. When the swing is at an phase angle of  $\pi/4$ , the player should position his/her center of mass at the lowest point and start to stand up, until the swing is at an phase angle of  $3\pi/4$ . At this point the player should have the highest center of mass. Then the player should start to lower down again, until the swing reverse to an phase angle of  $5\pi/4$ , which is equivalent to  $\pi/4$  in the reverse direction.

We may now add a correction term  $a_3 \cos(3\omega t) + b_3 \sin(3\omega t)$  to  $\theta(t)$  so that Eq. (3.55) is satisfied better. This additional term generates

$$-8l\omega^{2}[a_{3}\cos(3\omega t) + b_{3}\sin(3\omega t)]$$
(3.66)

in Eq. (3.55) plus higher order terms in  $\cos(5\omega t)$  and  $\sin(5\omega t)$  as well as small correction terms in  $\cos(\omega t)$  and  $\sin(\omega t)$ . To cancel the  $\cos(3\omega t)$  and  $\sin(3\omega t)$  terms, we have

$$a_{3} = -\frac{ay_{0}}{4l},$$
  

$$b_{3} = -\frac{by_{0}}{4l}.$$
(3.67)

Because  $y_0 \ll l$ , the correction term is indeed small compared with a(t)and b(t). To obtain more and more accurate solutions, this process can be continued by adding correction terms  $a_5 \cos(5\omega t) + b_5 \sin(5\omega t)$ ,  $a_7 \cos(7\omega t) + b_7 \sin(7\omega t)$ , and so on.

### 3.5 Waves on a String

In classical mechanics, wave is a simple form of collective motion whose closest analogy is vibration. Consider a one-dimensional string of bounded

#### 3.5. Waves on a String

particles in which each particle's motion is influenced by its two nearest neighbors, as shown in Fig. 3.3. If the motion of the particles around its equilibrium point is small, one can assume the force acting on each particle is proportional to the separation between the particles. The equation of motion reads:

$$m\ddot{a}_{l} = \eta(a_{l-1} - a_{l}) + \eta(a_{l+1} - a_{l}), \qquad (3.68)$$

where *m* is the mass of the particles,  $a_l$  the displacement of the *l*th particle from the equilibrium point, and  $\eta$  the spring constant. Because the string is fixed at both end points (l = 0 and l = N) we have  $a_0(t) = a_N(t) = 0$ . This system of linear equations can be solved by a change of variable (Fourier transformation)

$$a_{l}(t) = \sum_{k} u_{k}(t)\sin(kls) + v_{k}(t)\cos(kls), \qquad (3.69)$$

where s is the distance between neighboring particles. The boundary condition  $a_0(t) = 0$  sets  $v_k(t) = 0$ , and the possible values of k is determined by the other boundary condition  $a_N(t) = 0$ , which yields  $kNs = n\pi$  or  $kL = n\pi$ , where L is the length of the string and n is a positive integer. Substituting

$$a_l(t) = \sum_k u_k(t)\sin(kls) \tag{3.70}$$

into Eq. (3.68), we have

$$\sum_{k} m \ddot{u}_k \sin(kls) = 2\eta \sum_{k} [\cos(ks) - 1] u_k \sin(kls).$$
(3.71)

Comparing coefficients, we have

$$m\ddot{u}_k = 2\eta[\cos(ks) - 1]u_k, \tag{3.72}$$

hence

$$u_k(t) = u_k(0)\cos(\omega_k t) + \frac{\dot{u}_k(0)}{\omega_k}\sin(\omega_k t), \qquad (3.73)$$

where  $m\omega_k^2 = 2\eta[1 - \cos(ks)]$  is called the dispersion relation of the wave. Under the new variables  $u_k$ , the equations of motion are decoupled. Each degree of freedom  $u_k$  is an independent harmonic oscillator. Each such collective harmonic motion, labelled by k, is called a mode. In a continuous system,  $s \to 0$ , the dispersion relation becomes  $\omega_k = k\sqrt{\eta s^2/m}$ . We note that m/s is the mass density  $\rho$  of the string and  $\eta s$  is the tension T of the string. Therefore we have  $\omega_k = k\sqrt{T/\rho}$  and the phase velocity  $\omega_k/k$  is independent of k. In the continuum limit, Eq. (3.69) becomes

$$a(x,t) = \sum_{k} u_k(t) \sin(kx),$$
 (3.74)



Fig. 3.4: A model of transverse mechanical waves.

where we have changed from the discrete label l to the continuous label x = ls. It is seen that the displacement of the particle at x is a superposition of various modes (waves)  $\sin(kx)$  and the amplitudes of these modes  $u_k(t)$  are harmonic oscillators. Substituting  $u_k(t)$  in Eq. (3.73), we can write Eq. (3.74) in another form.

$$a(x,t) = \sum_{k} \left\{ \frac{u_k(0)}{2} \left[ \sin(kx - \omega t) + \sin(kx + \omega t) \right] + \frac{\dot{u}_k(0)}{2\omega_k} \left[ \cos(kx - \omega t) - \cos(kx + \omega t) \right] \right\}.$$
(3.75)

In the above analysis we have considered the longitudinal wave, where the particle displacement is in the same direction of wave propagation. The analysis of the transverse wave is similar. Consider the transverse displacement shown in Fig. 3.4. For a small transverse displacement  $a_l$ , the restoring force  $F_l$  is

$$F_{l} = T(\sin \theta_{l-1} - \sin \theta_{l}) \approx T\left(\frac{a_{l} - a_{l-1}}{s} - \frac{a_{l+1} - a_{l}}{s}\right),$$
(3.76)

where s is the distance between neighboring particles. Since the spring constant  $\eta$  is equal to T/s, the equation of motion for the *l*th particle is the same as Eq. (3.68).

### 3.6 Solutions of the Wave Equation

Consider the continuous limit of Eq. (3.68). Dividing both sides by s, we have

$$\frac{m}{s}\ddot{a}_{l} = \eta s \frac{(a_{l-1} - a_{l}) + (a_{l+1} - a_{l})}{s^{2}}.$$
(3.77)

#### 3.6. Solutions of the Wave Equation

In the limit  $s \to 0$ , we change from the discrete label l to the continuous label x = ls. Eq. (3.77) becomes

$$\rho \frac{\partial^2 a}{\partial t^2} = T \frac{\partial^2 a}{\partial x^2},\tag{3.78}$$

where  $\rho = m/s$  is the mass density of the string and  $T = \eta s$  is the tension of the string. Eq. (3.78) is a special case of the wave equation called the nondispersive wave equation, which can be written as

$$\frac{\partial^2 a}{\partial x^2} - \frac{1}{v^2} \frac{\partial^2 a}{\partial t^2} = 0, \qquad (3.79)$$

where  $v = \sqrt{T/\rho}$  is the phase velocity of the wave. To find the solution of Eq. (3.79), we note that it can be written as

$$\left(\frac{\partial}{\partial x} - \frac{1}{v}\frac{\partial}{\partial t}\right)\left(\frac{\partial}{\partial x} + \frac{1}{v}\frac{\partial}{\partial t}\right)a = 0, \qquad (3.80)$$

or

$$\left(\frac{\partial}{\partial x} + \frac{1}{v}\frac{\partial}{\partial t}\right)\left(\frac{\partial}{\partial x} - \frac{1}{v}\frac{\partial}{\partial t}\right)a = 0.$$
(3.81)

Changing variables by

$$u = x + vt,$$
  

$$w = x - vt,$$
(3.82)

we have

$$\frac{\partial}{\partial u}\frac{\partial}{\partial w}a = 0, \tag{3.83}$$

or

$$\frac{\partial}{\partial w}\frac{\partial}{\partial u}a = 0. \tag{3.84}$$

Therefore the general solution is

$$a(x,t) = f(x - vt) + g(x + vt)$$
(3.85)

for any functions f and g. The actual f and g are determined by the initial conditions a(x,0) and  $b(x,0) \equiv \partial a(x,t)/\partial t|_{t=0}$ . Namely

$$a(x,0) = f(x) + g(x),$$
  

$$b(x,0) = -vf'(x) + vg'(x).$$
(3.86)

Differentiating the first equation, we have

$$a'(x,0) = f'(x) + g'(x),$$
  

$$b(x,0) = -vf'(x) + vg'(x).$$
(3.87)

From these two equations we can solve f'(x) and g'(x) in terms of the known functions a'(x,0) and b(x,0), and then by integration we have f(x) and g(x) up to the constants of integration.

Alternatively, we may use a technique called separation of variables to solve Eq. (3.79). Let us assume the solution has the form

$$a(x,t) = f(x)g(t).$$
 (3.88)

Substituting into Eq. (3.79), and dividing by f(x)g(t), we have

$$\frac{f''(x)}{f(x)} = \frac{1}{v^2} \frac{g''(t)}{g(t)}.$$
(3.89)

Since the left hand side is a function of x and the right-hand side is a function of t, they must equal to the same constant independent of x and t. Let us denote the constant  $-k^2$  Then we have

$$f(x) = e^{\pm ikx}$$
  

$$g(t) = e^{\pm i\omega t},$$
(3.90)

and  $\omega/k = v$ .

$$a(x,t) = \sum_{k} \left[ c_{1}(k)e^{i(kx-\omega t)} + c_{2}(k)e^{i(kx+\omega t)} + c_{3}(k)e^{-i(kx-\omega t)} + c_{4}(k)e^{-i(kx+\omega t)} \right]$$
  
= 
$$\sum_{k} \left[ \alpha_{1}(k)\sin(kx)\sin(\omega t) + \alpha_{2}(k)\sin(kx)\cos(\omega t) + \alpha_{3}(k)\cos(kx)\sin(\omega t) + \alpha_{4}(k)\cos(kx)\cos(\omega t) \right], \quad (3.91)$$

where  $c_i(k)$  or  $\alpha_i(k)$  (i = 1, 2, 3, 4) are constants to be determined by the initial conditions or the boundary conditions.

If the solution is specified by the initial conditions a(x,0) and  $b(x,0) \equiv \partial a(x,t)/\partial t|_{t=0}$ , we have

$$a(x,0) = \sum_{k} [\alpha_2(k)\sin(kx) + \alpha_4(k)\cos(kx)], \qquad (3.92)$$

$$b(x,0) = \sum_{k} [\omega \alpha_1(k) \sin(kx) + \omega \alpha_3(k) \cos(kx)].$$
 (3.93)

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#### 3.7. Energy Density of String Waves

These are the Fourier expansion of a(x,0) and b(x,0), hence  $\alpha_i(k)$  (i = 1,2,3,4) can be uniquely determined.

If in addition the solution is also specified at the boundary points, for instance a(0,t) = a(L,t) = 0, which represents a string tied down at x = 0 and x = L, we have

$$a(x,t) = \sum_{k} [\alpha_1(k)\sin(kx)\sin(\omega t) + \alpha_2(k)\sin(kx)\cos(\omega t)], \qquad (3.94)$$

where the boundary condition at x = L requires that  $k = n\pi/L$ . Again the initial condition a(x, 0) will determine  $\alpha_2(k)$  and b(x, 0) will determine  $\alpha_1(k)$ .

## 3.7 Energy Density of String Waves

The time-averaged energy of the string wave is

$$\overline{E} = \sum_{l} \frac{m \overline{\dot{a}_{l}^{2}}}{2} + \frac{\eta \overline{(a_{l+1} - a_{l})^{2}}}{2}.$$
(3.95)

In the continuum limit,

$$\overline{E} = \int \left[\frac{\rho}{2}\overline{\left(\frac{\partial a}{\partial t}\right)^2} + \frac{T}{2}\overline{\left(\frac{\partial a}{\partial x}\right)^2}\right] dx.$$
(3.96)

For standing waves, substituting

$$a(x,t) = \sum_{k} u_k \cos(\omega t + \phi) \sin(kx)$$
(3.97)

into Eq. (3.96), we have

$$\overline{E} = L \sum_{k} \left( \frac{\rho}{8} \omega^2 u_k^2 + \frac{T}{8} k^2 u_k^2 \right) = \frac{LT}{4} \sum_{k} k^2 u_k^2.$$
(3.98)

For a particular mode represented by k, the energy stored in the mode is

$$\overline{E}_k = \frac{LT}{4} k^2 u_k^2. \tag{3.99}$$

For traveling waves, substituting

$$a(x,t) = \sum_{k} \frac{u_k}{\sqrt{2}} \cos(kx - \omega t - \phi)$$
(3.100)

into Eq. (3.96), we have

$$\overline{E} = L \sum_{k} \left( \frac{\rho}{4} \omega^2 u_k^2 + \frac{T}{4} k^2 u_k^2 \right) = \frac{LT}{2} \sum_{k} k^2 u_k^2.$$
(3.101)

For a particular mode represented by k, the energy stored in the mode is

$$\overline{E}_k = \frac{LT}{2} k^2 u_k^2. \tag{3.102}$$

### **3.8** Wave Propagation through an Interface

Imagine a composite string made of two different strings by joining them at x = 0. Let us consider the propagation of string waves through the interface between the two strings when a tension T is applied to the composite string. As the wave goes though the interface, part of the wave will be transmitted and part will be reflected. As we shall see, this is required by the boundary conditions at the interface. Let the incident wave be

$$a_i(x,t) = \alpha_i \exp i(k_i x - \omega t), \qquad (3.103)$$

and the transmitted wave be

$$a_t(x,t) = \alpha_t \exp i(k_t x - \omega t). \tag{3.104}$$

At x = 0 the mass element must oscillate synchronously, hence the transmitted wave must have the same frequency as the incident wave. Yet  $k_i \neq k_t$ because the two waves have different phase velocities. The amplitudes must be continuous across the interface, that is

$$a_i(0,t) = a_t(0,t), (3.105)$$

otherwise the position of the interface is undefined. The forces acted on the mass elements at both sides of the interface must also be continuous, otherwise the interface will experience an infinite acceleration. As the separation s between the mass elements approaches zero, the force on the x < 0 side is

$$\eta \Delta a_i = \frac{T}{s} \Delta a_i \to T \frac{\partial a_i}{\partial x}, \qquad (3.106)$$

and force on the x > 0 side is

$$\eta \Delta a_t = \frac{T}{s} \Delta a_t \to T \frac{\partial a_t}{\partial x}.$$
(3.107)

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Therefore we have

$$\frac{\partial a_i}{\partial x} = \frac{\partial a_t}{\partial x}.$$
(3.108)

These boundary conditions lead to

$$\alpha_i = \alpha_t,$$
  

$$k_i \alpha_i = k_t \alpha_t.$$
(3.109)

Obviously there is a contradiction because  $k_i \neq k_t$ . The contradiction is removed if there is a reflected wave

$$a_r(x,t) = \alpha_r \exp i(-k_i x - \omega t). \tag{3.110}$$

With the addition of a reflected wave, we have

$$\alpha_i + \alpha_r = \alpha_t,$$
  

$$k_i \alpha_i - k_i \alpha_r = k_t \alpha_t.$$
(3.111)

The solution is

$$\alpha_t = \frac{2k_i}{k_t + k_i} \alpha_i,$$
  

$$\alpha_r = \frac{k_i - k_t}{k_t + k_i} \alpha_i.$$
(3.112)

If the wave incidences from a medium of larger phase velocity to a medium of smaller phase velocity, we have  $k_i < k_t$ . In this case the reflected wave is  $\pi$  out of phase with the incident wave. In the opposite case the the reflected wave is in phase with the incident wave. The transmitted wave is always in phase with the incident wave.

We have shown in Eq. (3.102) that the energy density of a string wave is

$$\overline{\frac{E}{L}} = \frac{T}{2}k^2 u_k^2. \tag{3.113}$$

Therefore the energy-density flux flowing toward the interface is

$$\frac{T}{2}v_ik_i^2\alpha_i^2 = \frac{T\omega}{2}k_i\alpha_i^2,$$

and that flowing out of the interface is

$$\frac{T\omega}{2}(k_t\alpha_t^2 + k_i\alpha_r^2).$$

Substituting  $\alpha_t$  and  $\alpha_r$  in Eq. (3.112), we see the incoming energy-density flux is the same as the outgoing flux, as expected from the energy conservation law.



Fig. 3.5: Oscillating marble in a bowl.

## 3.9 Exercises

**Exercise 3.1.** A round marble of mass m and radius r is placed at the bottom of a round bowl of radius R. The marble can roll in the bowl without slipping. If the marble is placed slightly off the center of the bowl, as shown in Fig. 3.5. What is its oscillation frequency under the influence of gravity? In this exercise we assume the amplitude of oscillation is so small that the restoring force is proportional to the angle of displacement and the friction of air is negligible.

**Exercise 3.2.** The mass of the moon is  $7.36 \times 10^{22}$  kg, its radius is  $1.74 \times 10^{6}$  m. Assume the mass distribution is a uniform sphere. We dig a tunnel from the moon surface to the other side of the surface through the center of the moon, then drop a baseball of 0.2 kg into the tunnel. The initial velocity of the ball is zero. Ignore the gravity from other planets and consider only the gravity of the moon. When the baseball reaches the other end, how much time has passed? Hint: Use the shell theorem.

**Exercise 3.3.** Continue with the last exercise. We fill the tunnel with viscous liquid, so that the motion of the baseball is damped. Assume the damping force is proportional to its velocity, i.e.,  $f_d = -\gamma v$ . If we wish that the farthest position the ball can reach is the center of the moon (regardless how long it will take). What is the minimum value of  $\gamma$ ?

**Exercise 3.4.** On a frictionless table, a weight of mass m is tied to a thin post at the center of the table by a spring. The spring and the weight can rotate freely around the post without friction. The spring constant is k.



Fig. 3.7: An inverted cycloid.

Show that if the initial displacement is in the x-direction while the initial velocity is in the y-direction or the initial displacement is in the y-direction while the initial velocity is in the x-direction, the trajectory of the weight can be an ellipse. In these cases, if the total energy of the system is E, and the angular momentum is L, what is the semi-major axis and semi-minor axis of the ellipse as functions of E and L? In this exercise we assume the mass of the spring is negligible and the length of the spring is zero when unstretched.

**Exercise 3.5.** If a disk of radius R is rolled horizontally, a point at the edge of the disk traces out a curve shown in Fig. 3.6. This curve is known as a cycloid. (a) What is the equation that describes the curve? (b) Consider a bead sliding along an inverted cycloid as shown in Fig. 3.7. The bead is released from a height a with zero initial velocity. Show that the time it takes for the bead to reach the bottom is independent of a.

**Exercise 3.6.** A small ball of mass m is connected to two identical unstretched springs as shown in Fig. 3.8. The springs have a length l when



Fig. 3.8: A soft oscillator.

they are not stretched or compressed. The spring constant is k. If the ball is displaced in the direction perpendicular to the springs by a distance  $d \ll l$  and released with zero initial velocity, the oscillation period is T. If the displacement is 2d, what will be the oscillation period?

**Exercise 3.7.** A coupled oscillator is shown in Fig. 3.9, in which  $k_1 = k_3 = 1$ ,  $k_2 = 3$ ,  $m_1 = 1$ , and  $m_2 = 2$ . Show that the motion of both weights can be described by linear combinations of two oscillatory motions known as the normal modes. What are the frequencies of the two normal modes? (Note: You do not need to solve the equation of motion to know the frequencies. If the displacement of the two weights are  $x_1(t)$  and  $x_2(t)$ , You may simplify the equation of motion by changing variables to  $y_1(t)$  and  $y_2(t)$  according to

$$y_1 = a_{11}x_1 + a_{12}x_2, y_2 = a_{21}x_1 + a_{22}x_2,$$
(3.114)

where  $a_{ij}$  are coefficients of linear combinations. If you choose these coefficients wisely,  $y_1(t)$  and  $y_2(t)$  will be solutions of independent simple harmonic oscillators.

**Exercise 3.8.** A 2-gram guitar string is stretched to hold a tension of 100 newtons. The distance between the two bridges that fixes the two ends of the string is 80 cm. What is the fundamental oscillation frequency f of the string? If the string is pulled up at the center by 1 cm and suddenly released, as shown in Fig. 3.10, what is the amplitude ratio among the waves of frequencies f, 2f, and 3f?



Fig. 3.9: Coupled oscillators.



Fig. 3.10: A guitar string pulled up at the center.

**Exercise 3.9.** A mechanical toy telephone can be made by connecting the bottoms of two plastic cups with a stretched elastic string. As a person speaks toward one cup, the sound wave is converted to the vibration of the cup, and the vibration is transmitted by the string to the other cup in which it is converted back to sound. The string has a linear mass density of 5 g/m when it is not stretched. When stretched, its fractional increase of length is 0.1% per newton. How much tension must be applied to the string in order to make the transmission faster than talking through the air directly? The speed of sound in the air is 346 m/s. For simplicity in this exercise we ignore the effect of gravity on the string.

**Exercise 3.10.** A string is stretched under a tension of 100 newtons. The linear mass density  $\rho$  of the string is a function of x.

$$\rho(x) = \begin{cases} 1 \text{ g/m} & x < 0, \\ 4 \text{ g/m} & 0 \le x \le L, \\ 1 \text{ g/m} & x > L, \end{cases}$$

where L is 1 m. A wave incidents from the region of x < 0 and transmits to the region of x > L. The amplitude of the transmitted wave depends on the frequency of the wave. If the amplitude of the incident wave in the region of x < 0 is  $A_i$  and the amplitude of the transmitted wave in the region of x > L is  $A_t$ , the transmittance T is defined by

$$T = \frac{A_t^2}{A_i^2}.$$



Fig. 3.11: Two coupled springs.

Find the frequency of the wave such that the transmittance is 1, i.e., no wave is reflected.

**Exercise 3.11.** Two equal masses are connected with two identical massless springs of spring constant k, as shown in Fig. 3.11. Considering motion in the vertical direction only, what are the angular frequencies of the two normal modes? Find the ratio of amplitudes of the two masses in each of the two modes.

**Exercise 3.12.** It is well known that the oscillation period of a simple harmonic oscillator is independent of its oscillation amplitude. This is because the restoring force of a simple harmonic oscillator is always proportional to the length of stretching, no matter how long it is stretched. However, in the real world a spring can break when it is stretched too much, therefore a more realistic spring may be represented by the following potential function:

$$V(x) = a(e^{-2\alpha x} - 2e^{-\alpha x}),$$

where a and  $\alpha$  are positive constants. The minimum of V(x) is at x = 0, hence the position of the mass can oscillate around x = 0. When  $x \to \infty$ ,  $V(x) \to 0$ , which means there is no restoring force when the spring is stretched too much. In other words, it is broken. Calculate the oscillation period of this oscillator as a function of the total energy E, a, and  $\alpha$ .

## Chapter 4

## Statistical and Thermal Physics

## 4.1 Thermodynamic Variables and Processes

Thermodynamics is the physics about the change of state for macroscopic systems as a result of energy transfer. A macroscopic system may consist of many particles, and these particles can be atoms and molecules, or even stars in a galaxy. Because it is impractical to describe the motion of so many particles individually, we are concerned only with the state of the macroscopic system as a whole. The state of a macroscopic system is described by thermodynamic variables such as the pressure P, the volume V, the internal energy U, the temperature T etc. These variables are well defined only when the macroscopic system is in an equilibrium state. For instance, if we divide a bottle in vacuum into two cells and put gas into one of them, after a while the gas will reach a state of equilibrium in which we can measure its temperature, pressure, volume, etc. If we suddenly remove the dividing wall between the two cells, the gas will rush into the other cell. After a while a new equilibrium is reached and we have a new pressure, temperature, and volume. In this process we know the initial state and the final state of the gas, but not the states in between. It is not possible to describe the state of the gas between the initial state and the final state because before reaching the equilibrium the pressure and temperature of the gas are likely to be different at each different position. In this case we call the process irreversible. The word "irreversible" does not mean we cannot go back from the final state to the initial state. It only means we cannot follow the path from the initial state to the final state reversely, because we do not know the path

in the first place. To know the path, every state of the macroscopic system in between must be well defined. In order to meet this condition, we must keep the system in equilibrium all the time. A possible way of doing this is by changing the system very slowly, so that the system has enough time to maintain equilibrium all the time. Then the path can be well defined.

A macroscopic system can be described by different thermodynamic variables in different ways. Thermodynamic variables are not necessarily independent of each others. They can be related by some equations of state. For instance, for the ideal gas we have the equation of state PV = NkT, which relates P and V to T. Therefore any two of the three variables P, V, and T are sufficient to specify the state of the ideal gas. The existence of the equation of state allows us to treat one thermodynamic variable as an implicit function of other thermodynamic variables, hence in analyzing a thermodynamic problem we may use freely the most convenient variables. For instance, if the thermodynamic process is under the condition of constant temperature, then choosing temperature to be one of the independent variables should greatly simplify the analysis.

In physics of few particles, a particle can have kinetic energy and potential energy, and the energy can be changed by the work of external forces. In a macroscopic system we must consider an additional form of energy known as the internal energy. Consider the energy of a bottle of gas. Even though the bottle itself is not moving, the gas molecules in the bottle is still moving fast in all directions and thus have kinetic energy. If there are forces between the molecules, the molecules also have potential energy. The energy of the molecules is called the internal energy. The fast moving molecules also give rise to a gas pressure, which can be used to do work. Because energy is conserved, if the gas does some work to the outside world, it loses some of its internal energy. But doing work is not the only way for the bottle of gas to lose energy. If we put the bottle into cold water, the internal energy can decrease without doing apparent work. Energy can flow out of the bottle by heat conduction. Taking into consideration of heat conduction, the law of energy conservation reads

$$dQ = dU + dW, (4.1)$$

where dQ is the infinitesimal amount of heat transferred to the system, dU is the infinitesimal increase of internal energy, and dW is the infinitesimal amount of work done to the outside world. This is known as **the first law** of thermodynamics.

#### 4.2. Entropy in Thermodynamics

In addition to the energy conservation law, it is found empirically that heat cannot be transferred from a low-temperature object to a high-temperature one without importing work from the outside world. This is known as **the second law of thermodynamics**. Imagine how different the world would be if the second law of thermodynamics could be broken. Then one would be able to connect a machine between a chunk of ice and a tank of boiling water to make the ice colder and the water hotter. The machine would not need any fuel because no work would be required. The boiling water could be utilized to drive a steam engine doing as much work as we desire, and the ice could be used to cool our rooms and refrigerators. What a wonderful world!

Since the work done by the system to the outside world is

$$\Delta W = \int_{i}^{f} P \, dV, \tag{4.2}$$

it depends on the path from the initial state i to the final state f. As shown in Fig. 4.1, the system does more work going through path A than going through path B. Consequently the amount of heat  $\Delta Q$  absorbed by the system also depends on the path from the initial state to the final state. For this reason neither W nor Q can be treated as a thermodynamic variable. To be qualified as a thermodynamic variable, the variable must depend only on the state of the system, not the path leading to the state. Because heat transfer is the central problem of thermodynamics, the fact that Q is not a thermodynamic variable causes great inconvenience. As we shall see, this problem can be solved by introducing a new variable S known as the entropy, which is qualified as a thermodynamic variable.

#### 4.2 Entropy in Thermodynamics

The concept of entropy was first developed from the study of the efficiency of Carnot engines. The construction of a Carnot engine is shown in Fig. 4.2. The engine takes heat  $Q_1$  from a reservoir at temperature  $T_1$ , converts some of the heat to work W, and dumps the rest of the heat into another reservoir at temperature  $T_2$ . After a complete cycle the engine returns to its initial state. Therefore the internal energy U does not change. By the first law of thermodynamics, we have

$$\Delta Q = Q_1 - Q_2 = \Delta U + W = W. \tag{4.3}$$



Fig. 4.1: Two paths with the same initial state and final state but exporting different amount of work.

If W > 0, we must have  $T_1 > T_2$ . Otherwise we can use friction to convert the work back into heat at the reservoir of temperature  $T_2$ . Then the net effect will be transporting heat from a lower-temperature reservoir to a higher-temperature one. This violates the second law.

The efficiency of a Carnot engine is defined by

$$\eta = \frac{W}{Q_1} = \frac{Q_1 - Q_2}{Q_1} = 1 - \frac{Q_2}{Q_1},\tag{4.4}$$

where W is the work done by the engine and  $Q_1$  is the heat absorbed. From the second law of thermodynamics,  $\eta$  must be smaller than 1, otherwise we can use the engine to absorb heat  $Q_1$  from a reservoir and convert all the heat to work. By friction, the work can be converted back to heat at another reservoir which has a higher temperature. Then again the net effect will be transporting heat from a lower-temperature reservoir to a higher-temperature one, which violates the second law.

A reversible Carnot engine is one that can either absorb heat  $Q_1$  at  $T_1$ , release heat  $Q_2$  at  $T_2$ , while exporting work W, or reversely absorb heat  $Q_2$ at  $T_2$ , release heat  $Q_1$  at  $T_1$ , while importing work W. If we connect two identical reversible Carnot engines together and let one export work to drive the other in the reverse direction, the net effect will be nothing happens. However, because friction in the engines will convert some work into heat,



Fig. 4.2: A model of thermal engines.

if we use one Carnot engine to drive another in the reverse direction, it is unavoidable that some heat flows from  $T_1$  to  $T_2$ . This makes the engines irreversible. Therefore in reality there is no reversible engine. Theoretically we can imagine an engine with almost no friction. Such an engine is almost reversible.

Let us combine an irreversible Carnot engine and a reversible Carnot engine, and investigate the efficiency of the combined engine. Let engine A be the irreversible engine and B be the reversible engine running in the reverse direction. All the work produced by engine A will be used to drive engine B reversely, as shown in Fig. 4.3. The heat absorbed by the combined engine at  $T_1$  is  $Q_{A1} - Q_{B1}$ , and the heat released by the combined engine at  $T_2$  is  $Q_{A2} - Q_{B2}$ , while the net production of work is 0. The first law of thermal dynamics requires that  $Q_{A2} - Q_{B2} = Q_{A1} - Q_{B1}$ . Let us assume  $T_1 > T_2$ . Because heat can only flow from the reservoir at temperature  $T_1$  to the reservoir at temperature  $T_2$ , we have  $Q_{A1} \ge Q_{B1}$ , which means

$$\eta_B = \frac{W}{Q_{B1}} \ge \frac{W}{Q_{A1}} = \eta_A. \tag{4.5}$$

In other words, the efficiency of a reversible Carnot engine is higher than that of any irreversible Carnot engine. If engine A is also reversible, we can reverse the roles of the two engines to obtain  $\eta_A \ge \eta_B$ . Therefore any two reversible Carnot engines have the same efficiency.



Fig. 4.3: A reversible engine driven by an irreversible engine.

Let us use the compression and expansion of the ideal gas to construct an ideal Carnot engine, and see how large the efficiency can be. The cycle of the engine consists of four stages as shown in Fig. 4.4. In the first stage the gas is kept in thermal contact with a reservoir at  $T_1$ . The heat absorbed from the reservoir makes the gas expand and do positive work. In the second stage the gas is thermally isolated from the environment while continuing expanding and doing positive work. In the third stage the gas is kept in thermal contact with a reservoir at  $T_2$ . The heat released to the reservoir makes the gas compress and do negative work. In the fourth stage the gas is thermally isolated from the environment while continuing compressing and doing negative work.

Experimentally it is found that the ideal monoatomic gas has the following equations of state,

$$PV = NkT, (4.6)$$

$$U = \frac{3}{2}NkT,\tag{4.7}$$

and as we shall see, these equations of state can be well explained by the kinetic theory of gases. Therefore in the first stage the work done by the gas is

$$\int_{V_1}^{V_2} P \, dV = \int_{V_1}^{V_2} \frac{NkT_1}{V} \, dV = NkT_1 \ln\left(\frac{V_2}{V_1}\right). \tag{4.8}$$


Fig. 4.4: A Carnot cycle based on expansion and compression of an ideal gas.

Since the temperature of the gas does not change,  $\Delta U = 0$ . The absorbed heat is also equal to  $NkT_1 \ln(V_2/V_1)$ . In the second state, the volume of the gas continues to increase from  $V_2$  to  $V_3$ . This time we have

$$\int_{V_2}^{V_3} P \, dV = \int_{T_1}^{T_2} -dU = -\int_{T_1}^{T_2} \frac{3}{2} d(NkT) = \frac{3Nk}{2} (T_1 - T_2). \tag{4.9}$$

Similarly, in the third stage the absorbed heat which is equal to the work done is

$$\int_{V_3}^{V_4} P \, dV = NkT_2 \ln(V_4/V_3). \tag{4.10}$$

The work done in the fourth stage is  $3Nk(T_2 - T_1)/2$ , which cancels the work done in the second stage. The efficiency of the engine is

$$\eta = 1 + \frac{T_2 \ln(V_4/V_3)}{T_1 \ln(V_2/V_1)}.$$
(4.11)

During the second and the fourth stages, the gas expands without absorbing heat. The equation for this process is

$$0 = PdV + dU = PdV + \frac{3}{2}d(PV) = \frac{5}{2}PdV + \frac{3}{2}VdP.$$
 (4.12)

By separation of variables, we have

$$\frac{5}{3}\frac{dV}{V} = -\frac{dP}{P}.\tag{4.13}$$

After integration, we have

$$PV^{\frac{3}{3}} = c,$$
 (4.14)

where c is a constant. This is the equation for the adiabatic expansion of the ideal gas. Eq. (4.14) can also be written as

$$NkTV^{\frac{2}{3}} = c.$$
 (4.15)

Hence

$$\ln V = \frac{3}{2} \ln \left(\frac{c}{NkT}\right). \tag{4.16}$$

This gives the relation between  $V_2, V_3$  and  $V_4, V_1$ .

$$\ln V_3 - \ln V_2 = \frac{3}{2} (\ln T_1 - \ln T_2) = -(\ln V_1 - \ln V_4).$$
(4.17)

Substituting in Eq. (4.11), we have

$$\eta = 1 - \frac{T_2}{T_1}.\tag{4.18}$$

Because all the reversible Carnot engines have the same efficiency, this is the universal efficiency of reversible Carnot engines. Because

$$\eta = 1 - \frac{Q_2}{Q_1},\tag{4.19}$$

Eq. (4.18) can also be written as

$$\frac{Q_1}{T_1} = \frac{Q_2}{T_2}.$$
(4.20)

For any Carnot engine we have  $\eta = 1 - Q_2/Q_1 \le 1 - T_2/T_1$ , therefore

$$\frac{Q_1}{T_1} \le \frac{Q_2}{T_2},$$
 (4.21)

where the equal sign applies only to reversible Carnot engines.

Let us define a cyclic process to be one that starts from a thermodynamic state and ends in the same state. Consider a system  $\Gamma$  going through a cyclic process that absorbs heat Q from the environment in which the temperature is not kept constant. Let us construct the process from a sequence of small component processes, such that each component process absorbs heat  $Q_i^{(in)}$ 

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#### 4.2. Entropy in Thermodynamics

or releases heat  $Q_i^{(\text{out})}$  at temperature  $T_i$ . For each component process, let us use a reversible Carnot engine to supply  $Q_i^{(\text{in})}$  or absorb  $Q_i^{(\text{out})}$  as shown in Fig. 4.5. Each reversible Carnot engine is constructed in the following way: If the component process absorbs heat, the engine runs between temperature  $T_1$  and  $T_i$ , where  $T_1$  is the temperature of a reservoir and  $T_1 > T_i$ . On the contrary, if the component process releases heat, the engine runs between temperature  $T_i$  and  $T_2$ , where  $T_2$  is the temperature of another reservoir and  $T_i > T_2$ . Let us separate the two groups of engines and label them by group  $G_1$  and group  $G_2$ . For the  $G_1$  engines, the engine absorbs heat  $Q_i^{(1)}$  from a reservoir kept at  $T_1$ , and releases heat  $Q_i^{(\text{in})}$  to the component process at  $T_i$ . From Eq. (4.21) we have

$$Q_i^{(1)} = T_1 \frac{Q_i^{(\text{in})}}{T_i}.$$
(4.22)

Therefore the total amount of heat absorbed from the reservoir at  $T_1$  is

$$Q^{(1)} = \sum_{i \in G_1} Q_i^{(1)} = T_1 \sum_{i \in G_1} \frac{Q_i^{(in)}}{T_i}.$$
(4.23)

Similarly, for the  $G_2$  engines the engine absorbs heat  $Q_i^{(\text{out})}$  from the component process at  $T_i$  and releases heat  $Q_i^{(2)}$  to a reservoir kept at  $T_2$ . From Eq. (4.21) we have

$$Q_i^{(2)} = T_2 \frac{Q_i^{(\text{out})}}{T_i}.$$
(4.24)

Therefore the total amount of heat released to the reservoir at  $T_2$  is

$$Q^{(2)} = \sum_{i \in G_2} Q_i^{(2)} = T_2 \sum_{i \in G_2} \frac{Q_i^{(\text{out})}}{T_i}.$$
(4.25)

Let us treat  $\Gamma$  and the reversible Carnot engines all together as a composite engine. The net effect of the composite engine is that it absorbs heat  $Q^{(1)}$ from a reservoir at  $T_1$  and releases heat  $Q^{(2)}$  to another reservoir at  $T_2$ . From Eq. (4.21) we have

$$\frac{Q^{(1)}}{T_1} \le \frac{Q^{(2)}}{T_2}.\tag{4.26}$$

We may define a positive  $\Delta Q$  to be the heat absorbed by a system and a negative  $\Delta Q$  to be the heat released. Under this notation we have  $\Delta Q_i =$ 



Fig. 4.5: A thermodynamic cycle in which the heat transfer is supplied by Carnot engines.

 $Q_i^{(\text{in})}$  for  $i \in G_1$  and  $\Delta Q_i = -Q_i^{(\text{out})}$  for  $i \in G_2$ . Then the net result can be written as

$$\sum_{i} \frac{\Delta Q_i}{T_i} \le 0. \tag{4.27}$$

Let the number of component processes approach infinity. We have

$$\oint \frac{dQ}{T} \le 0, \tag{4.28}$$

where the equal sign holds when the composite engine is reversible. Because each engine of the composite engine is reversible, the equal sign holds when the cyclic process of  $\Gamma$  is reversible.

Since

$$\oint \frac{dQ}{T} = 0 \tag{4.29}$$

for a reversible cyclic process, we may define a new variable S, which is a function of the thermodynamic state a, by

$$S(a) = \int_{o}^{a} \frac{dQ}{T},$$
(4.30)

### 4.2. Entropy in Thermodynamics

where o is an arbitrary reference state. From Eq. (4.28) we have

$$\int_{o}^{a} \frac{dQ}{T} + \int_{a}^{b} \frac{dQ}{T} + \int_{b}^{o} \frac{dQ}{T} \le 0$$

$$(4.31)$$

for any integration path connecting o, a, b. Therefore we have

$$S(b) - S(a) \ge \int_{a}^{b} \frac{dQ}{T}$$

$$(4.32)$$

for any two arbitrary states a and b, where the equal sign applies to reversible processes. For an isolated system dQ = 0, we have

$$S(b) \ge S(a). \tag{4.33}$$

This means the entropy of an isolated system can only increase.

We started from the second law of thermodynamics, which states that heat cannot flow from a place of lower temperature to a place of higher temperature in an isolated system, and arrived at the statement that the entropy of an isolated system can only increase. Conversely, if heat Q could flow from a place of lower temperature to a place of higher temperature, we would have

$$\Delta S = \frac{Q}{T_1} - \frac{Q}{T_2} < 0. \tag{4.34}$$

Therefore, that the entropy of an isolated system can only increase is an equivalent statement of the second law of thermodynamics.

As an example, let us calculate  $\Delta S$  for an ideal gas when its volume is changed from  $V_a$  to  $V_b$  while its temperature is changed from  $T_a$  to  $T_b$ . Substituting U = 3NkT/2 and P/T = Nk/V into

$$\Delta S = \int_a^b \frac{dQ}{T} = \int_a^b \frac{dU}{T} + \int_a^b \frac{PdV}{T}, \qquad (4.35)$$

we have

$$\Delta S = \int_{a}^{b} \frac{3Nk}{2} \frac{dT}{T} + \int_{a}^{b} Nk \frac{dV}{V} \\ = \frac{3Nk}{2} (\ln T_{b} - \ln T_{a}) + Nk (\ln V_{b} - \ln V_{a}).$$
(4.36)

In other words,

$$S(T,V) = \frac{3Nk}{2}\ln T + Nk\ln V - C,$$
(4.37)

where C is a constant assigned to be the entropy of the reference state a. We may also write S as a function of U and V,

$$S(U,V) = \frac{3Nk}{2}\ln U + Nk\ln V - C', \qquad (4.38)$$

where again C' is assigned to be the entropy of the reference state a.

From the definition of S we have

$$dQ = TdS. \tag{4.39}$$

This simple relation looks as if Q and S are related by a change of variable. It is not. This is because T is not a function of S only; it depends on other thermodynamic variable too. As we have seen, S is uniquely defined for each thermodynamic state up to a constant, whereas it is not possible to assign a unique Q to a thermodynamic state. How much heat a system has absorbed depends on the history of the system. It is not a conserved quantity because a system can do work to the outside world. Mathematically we can say 1/Tis an integration factor of dQ. By multiplying dQ with 1/T, we obtain an integrable differential form dS.

## 4.3 Thermodynamic Potentials

With dQ = TdS the first law of thermodynamics reads

$$dU = TdS - PdV. (4.40)$$

This is a differential form which signifies that U is a function of S and V. Since

$$dU = \left(\frac{\partial U}{\partial S}\right) dS + \left(\frac{\partial U}{\partial V}\right) dV, \qquad (4.41)$$

by comparison we have

$$\left( \frac{\partial U}{\partial S} \right)_{V} = T,$$

$$\left( \frac{\partial U}{\partial V} \right)_{S} = -P.$$

$$(4.42)$$

#### 4.3. Thermodynamic Potentials

For isolated systems, no work is done and no heat is transported to the outside world, hence dU = 0. If the volume is allowed to change while no heat can flow in or out, we have

$$dU + PdV = 0. \tag{4.43}$$

In analogy to the conversion between potential energy  $\phi$  and work W represented by the equation  $d\phi + dW = 0$ , we see that U is the potential energy of a system when it is thermally isolated.

For open systems, it is not always convenient to choose S and V as the thermodynamic variables because heat can flow in and out and volume can change. As a result, dS and dV are not zero. For example, chemical reaction usually occurs under constant P and T. In order to maintain constant T and P, the system must be allowed to exchange heat with the outside world and adjust its volume. In this case it would be more convenient to use P and T as the thermodynamic variables because they are constants. What will the first law become when P and T are used as the thermodynamic variables? Let us consider first the Helmholtz free energy defined as A = U - TS. From this definition we have

$$dA = dU - TdS - SdT = -dW - SdT = -PdV - SdT.$$

$$(4.44)$$

This is a differential form signifying that A is a function of T and V, and therefore we have

$$\begin{pmatrix} \frac{\partial A}{\partial V} \end{pmatrix}_T = -P, \\ \begin{pmatrix} \frac{\partial A}{\partial T} \end{pmatrix}_V = -S.$$
 (4.45)

For a reversible process that occurs at constant T and V, A does not change. If the volume is allowed to change while temperature is kept constant, we have

$$dA + PdV = 0 \tag{4.46}$$

at constant temperature. In analogy to the conversion between potential energy  $\phi$  and work W represented by the equation  $d\phi + dW = 0$ , we see that A is the potential energy of a system when the temperature of the system is kept constant.

Consider an irreversible process  $p_{ir}$  that brings the system from state  $s_1$  to state  $s_2$  at constant temperature, and the process does an amount of

work  $\Delta W_{ir}$  to the outside world which is also kept at the same constant temperature. The change of Helmholtz free energy is  $A_{s2} - A_{s1} \equiv \Delta A_r$ We may bring the system back from  $s_2$  to  $s_1$  by a reversible process  $p_r$ at the same constant temperature. In this process the work  $\Delta W_r$  done to the outside world plus the change of Helmholtz free energy is zero, hence  $\Delta W_r = -(A_{s1} - A_{s2}) = \Delta A_r$ . To ensure that the temperature does not change, the two processes are carried out under a close contact with a thermal reservoir of temperature T. The work done by the combined process  $p_{ir} + p_r$ is equal to  $\Delta W_{ir} - (A_{s1} - A_{s2})$ . This work cannot be positive because if so we are converting heat drawn from a thermal reservoir at temperature T completely into work. This violates the second law of thermodynamics. Therefore

$$\Delta W_{\rm ir} + \Delta A_{\rm r} \le 0. \tag{4.47}$$

As we have mentioned,  $\Delta W_{ir}$  is the amount of work done to the outside world when the state of the system is changed from  $s_1$  to  $s_2$ . Since the outside world is also kept at a constant temperature T, if we use this amount of work to change the state of the outside world in a reversible way, the change of Helmholtz free energy for the outside world is

$$\Delta A_{\text{outside}} = -(-\Delta W_{\text{ir}}) = \Delta W_{\text{ir}}.$$
(4.48)

Note that in this case the work done by the outside world is  $-\Delta W_{ir}$ . Consequently, the total change of Helmholtz free energy  $\Delta A$  is

$$\Delta A = \Delta A_{\text{outside}} + \Delta A_{\text{r}} \le 0. \tag{4.49}$$

In other words, when a system undergoes an internal irreversible process at a constant temperature T, we have  $\Delta A < 0$ . In comparison, when a system undergoes an internal irreversible process at a constant internal energy U, we have  $\Delta S > 0$ . If a system is not initially in equilibrium, it can move toward equilibrium through irreversible processes. If the irreversible process is carried out under the constraint  $\Delta U = 0$ , we see that the entropy change  $\Delta S$  is positive until the system reaches equilibrium. Therefore we say at equilibrium the entropy S reaches maximum. Similarly, if the irreversible process is carried out under the constraint  $\Delta T = 0$ , we have  $\Delta A < 0$  until the system reaches equilibrium. Therefore we say at equilibrium the Helmholtz free energy A reaches minimum.

We can move a step further to define the Gibbs free energy as G = U - TS + PV. From this definition we have

$$dG = dU - TdS - SdT + PdV + VdP$$

### 4.3. Thermodynamic Potentials

$$= -dW + PdV - SdT + VdP$$
  
= -SdT + VdP. (4.50)

This is a differential form signifying that G is a function of T and P, and therefore we have

$$\left( \frac{\partial G}{\partial T} \right)_P = -S,$$

$$\left( \frac{\partial G}{\partial P} \right)_T = V.$$

$$(4.51)$$

For a reversible process that occurs at constant T and P, G does not change. For an irreversible process, from Eqs. (4.46) and (4.49) we have

$$\Delta A_{\text{outside}} \le -\Delta A_{\text{r}}.\tag{4.52}$$

For constant P,  $\Delta(PV) = P\Delta V$ , hence  $\Delta G = \Delta A + P\Delta V$ . Consequently

$$\Delta A_{\text{outside}} + P\Delta V_{\text{outside}} \le -\Delta A_{\text{r}} - P\Delta V_{\text{system}}, \qquad (4.53)$$

where  $\Delta V_{\text{outside}}$  is the change of volume of the outside world,  $\Delta V_{\text{system}}$  is the change of volume of the system, and  $\Delta V_{\text{outside}} = -\Delta V_{\text{system}}$ . This means the total change of the Gibbs free energy  $\Delta G$  satisfies  $\Delta G \leq 0$ . Therefore we say at equilibrium the Gibbs free energy G reaches minimum when temperature and pressure are both kept constant.

Another useful thermodynamic variable is the enthalpy defined by H = U + PV. From this definition we have

$$dH = dU + PdV + VdP = TdS + VdP.$$
(4.54)

This is a differential form signifying that H is a function of S and P, and therefore we have

$$\left( \frac{\partial H}{\partial S} \right)_P = T,$$

$$\left( \frac{\partial H}{\partial P} \right)_S = V.$$

$$(4.55)$$

At constant pressure dH = TdS = dQ, hence H is commonly used to specify the heat absorbed in chemical reactions under constant pressure.

## 4.4 Kinetic Theory of Ideal Gas

Daniel Bernoulli was the person who first gave a correct analysis of the properties of gases in terms of the motion of their constituent molecules. At that time (1738), the concept of atoms and molecules was far from being mature, and there had been no experimental evidence of their existence. The theory is completely a result of Bernoulli's creative thinking.

Consider the statistical distribution of gas particles in a closed rectangular box. The number of particles with velocity around  $\mathbf{v}$  is

$$\frac{dN}{N} = f(\mathbf{v})d^3\mathbf{v},\tag{4.56}$$

where  $f(\mathbf{v})$  is the distribution function that satisfies

$$\int f(\mathbf{v})d^3\mathbf{v} = 1. \tag{4.57}$$

Assume the length of the box is L and the area of the wall in the x-direction is A. Within a time interval  $\Delta t$ , the impulse produced by this group of particles bouncing against the wall in the x-direction is

$$dF_x \Delta t = 2mv_x dN, \tag{4.58}$$

where  $\Delta t = L/v_x$ . The total force on the wall produced by all particles with all velocities is

$$F_x = \frac{2mN}{L} \int_{v_x>0} v_x^2 f(\mathbf{v}) d^3 \mathbf{v}.$$
(4.59)

Since by symmetry  $f(\mathbf{v}) = f(-\mathbf{v})$ , Eq. (4.59) can be written as

$$F_x = \frac{mN}{L} \int_{\text{all } v_x} v_x^2 f(\mathbf{v}) d^3 \mathbf{v}$$
  
=  $\frac{mN}{L} \overline{v_x^2},$  (4.60)

where  $\overline{v_x^2}$  denotes the average of  $v_x^2$ . Since  $\overline{v^2} = \overline{v_x^2} + \overline{v_y^2} + \overline{v_z^2}$  and  $\overline{v_x^2} = \overline{v_y^2} = \overline{v_z^2}$ , Eq. (4.60) can be written as

$$F_x = \frac{mN}{3L}\overline{v^2}.\tag{4.61}$$

#### 4.4. KINETIC THEORY OF IDEAL GAS

Dividing both sides by A and noting that AL = V is the volume of the gas, we have

$$PV = \frac{2N}{3}\overline{E},\tag{4.62}$$

where  $\overline{E}$  is the average kinetic energy of the gas particles. Comparing with the empirical law of ideal gas

$$PV = NkT, (4.63)$$

we have

$$\overline{E} = \frac{3kT}{2}.\tag{4.64}$$

Eq. (4.64) establishes a connection between heat and the internal motion of matter. This concept was well ahead of its time, as we note that the transformation of mechanical energy to heat by friction had not become clear until a century later.

Let us consider the form of  $f(\mathbf{v})$ . By symmetry  $f(\mathbf{v})$  cannot depend on the direction of  $\mathbf{v}$ , therefore  $f(\mathbf{v}) = f(v^2) = f(v_x^2 + v_y^2 + v_z^2)$ . Since  $v_x, v_y$ , and  $v_z$  are independent random variables, we may decompose the distribution function  $f(v^2)$  into  $g(v_x^2)g(v_y^2)g(v_z^2)$ . By symmetry, the distribution functions of  $v_x^2, v_y^2$ , and  $v_z^2$  are all the same function g. Let  $v_y = v_z = 0$ , we have f = cg, where c is a constant.

$$cg(v_x^2 + v_y^2 + v_z^2) = g(v_x^2)g(v_y^2)g(v_z^2).$$
(4.65)

If a function F satisfies F(x + y) = cF(x)F(y), we may take the derivative of both sides with respect to x, then let x = 0. This leads to F'(y) = cF'(0)F(y). Integrating it with respect to y, we have  $F(y) = ae^{by}$ , where aand b are constants. With this observation in mind, we see  $f(v^2) = ae^{bv^2}$ , where a and b are constants to be determined by the following equations:

$$\int f(v^2)d^3\mathbf{v} = 1. \tag{4.66}$$

$$\int v^2 f(v^2) d^3 \mathbf{v} = \frac{3kT}{m}.$$
(4.67)

Before computing the two integrals in Eqs. (4.66) and (4.67), let us first evaluate

$$I_0 = \int_{-\infty}^{\infty} e^{-x^2} \, dx. \tag{4.68}$$

We may write

$$I_0^2 = \int_{-\infty}^{\infty} e^{-(x^2 + y^2)} \, dx \, dy = \int_0^{\infty} \int_0^{2\pi} e^{-r^2} r \, d\phi \, dr = \pi.$$
(4.69)

Hence  $I_0 = \sqrt{\pi}$ . Then we evaluate

$$I_2 = \int x^2 e^{-x^2} \, dx \tag{4.70}$$

using integration by parts. Let u = x,  $dv = xe^{-x^2} dx$ .

$$\int x^2 e^{-x^2} dx = \int \frac{e^{-x^2}}{2} dx = \frac{\sqrt{\pi}}{2}.$$
(4.71)

From the value of  $I_0$  and  $I_2$ , we have

$$g(v_x) = \sqrt{\frac{m}{2\pi kT}} \exp\left(-\frac{mv_x^2}{2kT}\right), \qquad (4.72)$$

and

$$\int f(\mathbf{v})d^3\mathbf{v} = \int \left(\frac{m}{2\pi kT}\right)^{\frac{3}{2}} \exp\left(-\frac{mv^2}{2kT}\right) d^3\mathbf{v}$$
$$= \int \left(\frac{m}{2\pi kT}\right)^{\frac{3}{2}} \exp\left(-\frac{mv^2}{2kT}\right) 4\pi v^2 dv.$$
(4.73)

This distribution was first derived by James Clerk Maxwell, and now is known as the **Maxwell distribution**. We may express the Maxwell distribution in terms of energy. Then we have  $v = \sqrt{2E/m}$  and

$$f(E) dE = \frac{2}{\sqrt{\pi}} \left(\frac{1}{kT}\right)^{\frac{3}{2}} \sqrt{E} \exp\left(-\frac{E}{kT}\right) dE.$$
(4.74)

Note that f(E) is independent of the mass of the gas particles.

In the discussion above, we have assumed the gas particle distribution is uniform in space. This is true when the gas is not under the influence of an external force. If the gas is pushed by an external force, the particle moves along the direction of the force. As a result, the pressure builds up against the force until the balance is reached. Because the pressure is proportional to density, there will be a density gradient in the direction of the external force. In that case, we may no longer assume the density is independent of position. The law of ideal gas now reads

$$P(\mathbf{r}) = \rho(\mathbf{r})kT. \tag{4.75}$$

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#### 4.5. DIFFUSION

Consider a thin layer of gas pushed by a conservative force  $-\nabla \phi(\mathbf{r})$ . Let us assume the normal vector of the layer is in the same direction as the force. The thickness of the layer is dx and the area is A. At equilibrium we have

$$-N\nabla\phi(\mathbf{r}) = \nabla P(\mathbf{r})Adx = \nabla\rho(\mathbf{r})kTAdx, \qquad (4.76)$$

where N is the total number of gas particles in the layer. Noting that  $N/(Adx) = \rho(\mathbf{r})$ , we have

$$\frac{\nabla\rho(\mathbf{r})}{\rho(\mathbf{r})} = \frac{-\nabla\phi(x)}{kT}.$$
(4.77)

Therefore

$$\rho(\mathbf{r}) = \rho_0 \exp\left[\frac{-\phi(\mathbf{r})}{kT}\right].$$
(4.78)

Combining with Eq. (4.73), we have the phase-space distribution function

$$F(\mathbf{r}, \mathbf{v}) = \rho_0 \left(\frac{m}{2\pi kT}\right)^{\frac{3}{2}} \exp\left[\frac{-\frac{mv^2}{2} - \phi(\mathbf{r})}{kT}\right].$$
(4.79)

## 4.5 Diffusion

In the center of a large room if a droplet of perfume is released, it takes a long while for people at the corner of the room to notice. The farther one is away from the source of the perfume, the later one detects the fragrance. Although the average speed of gas molecule can be as large as several hundred meters per second, the fragrant molecules cannot go straight to the someone's nose. In the process of reaching the nose, the molecules suffer from many random collisions with other gas particles. Each collision randomly changes the direction of moving. Therefore the migration of the molecules is like a random walk, which takes much longer time to go far than straight movement does. As a matter of fact, the transport of fragrant molecules in the real world is mainly by convective air current. If there exists no air current, it would take several hours for a significant fraction of the fragrant molecules to wander a distance of just one meter.

Consider two neighboring regions defined by two slabs. Slab A is at position  $x + \Delta x$  and slab B at position x. Because gas particles in these two slabs move in random directions, the chance for a particle to move from

slab A to slab B is equal to the chance for a particle to move from slab B to slab A. However, if the total number of particles in slab A is different from that in slab B, the net flux from A to B is not zero. The flux from A to B is proportional to  $N_A T_{A\to B}$ , while from B to A is proportional to  $N_B T_{B\to A}$ , where  $N_A$  and  $N_B$  are the number of particles in slab A and slab B respectively, and  $T_{A\to B}=T_{B\to A}$  is the transition probability. The net flux from A to B is simply proportional to  $N_A - N_B$ . In a general mathematical expression one can write

$$\mathbf{J}(\mathbf{r},t) = -D\nabla\rho(\mathbf{r},t),\tag{4.80}$$

where  $\mathbf{J}(\mathbf{r}, t)$  is the flux vector, and  $\rho(\mathbf{r}, t)$  is the density distribution. The proportional constant D is called the diffusion constant.

In the migration process, the number of gas particles in any volume element is conserved. Consider a box at  $\mathbf{r}_0$  with sides equal to  $\Delta x$ ,  $\Delta y$ , and  $\Delta z$ . Within a time  $\Delta t$ , the number of particles flowing into the cell in the *x*-direction is equal to  $J_x(\mathbf{r}_0, t)\Delta y\Delta z\Delta t$ , and the number of particles flowing out of the cell in the *x*-direction is equal to  $J_x(\mathbf{r}_0 + \Delta x, t)\Delta y\Delta z\Delta t$ . The net accumulation of particles is

$$\Delta n = J_x(\mathbf{r}_0, t) \Delta y \Delta z \Delta t - J_x(\mathbf{r}_0 + \Delta x, t) \Delta y \Delta z \Delta t.$$
(4.81)

Dividing both sides by  $\Delta V \equiv \Delta x \Delta y \Delta z$  and  $\Delta t$ , in the infinitesimal limit we have

$$\frac{\partial \rho}{\partial t} = -\frac{\partial J_x}{\partial x}.\tag{4.82}$$

Taking into account the flows in the y- and z-directions, we have

$$\frac{\partial \rho}{\partial t} = -\left(\frac{\partial J_x}{\partial x} + \frac{\partial J_y}{\partial y} + \frac{\partial J_z}{\partial z}\right). \tag{4.83}$$

Namely,

$$\nabla \cdot \mathbf{J}(\mathbf{r}, t) + \frac{\partial \rho(\mathbf{r}, t)}{\partial t} = 0.$$
(4.84)

This is known as the **continuity equation**. Combining Eqs. (4.80) and (4.84), we have

$$-D\nabla^2 \rho(\mathbf{r}, t) + \frac{\partial \rho(\mathbf{r}, t)}{\partial t} = 0.$$
(4.85)

### 4.5. DIFFUSION

### This is known as the **diffusion equation**.

Given an initial density distribution  $\rho(\mathbf{r}, 0)$ , what is the density distribution  $\rho(\mathbf{r}, t)$ ? The problem can be solved by Fourier analysis. Let

$$\rho(\mathbf{r},t) = \left(\frac{1}{\sqrt{2\pi}}\right)^3 \int \tilde{\rho}(\mathbf{k},t) \exp(i\mathbf{k}\cdot\mathbf{r}) d^3\mathbf{k}.$$
(4.86)

Substituting it into the diffusion equation, we have

$$Dk^{2}\tilde{\rho}(\mathbf{k},t) = -\frac{\partial\tilde{\rho}(\mathbf{k},t)}{\partial t}.$$
(4.87)

Hence

$$\tilde{\rho}(\mathbf{k},t) = \tilde{\rho}(\mathbf{k},0)e^{-Dk^2t}.$$
(4.88)

Because  $\tilde{\rho}(\mathbf{k}, 0)$  can be obtained from the initial condition  $\rho(\mathbf{r}, 0)$ ,  $\tilde{\rho}(\mathbf{k}, t)$  is solved. Namely

$$\tilde{\rho}(\mathbf{k},t) = \left(\frac{1}{\sqrt{2\pi}}\right)^3 \int \rho(\mathbf{r},0) \exp(-i\mathbf{k}\cdot\mathbf{r}) d^3\mathbf{r} \cdot e^{-Dk^2t}.$$
(4.89)

Let us assume the initial distribution of the fragrant gas is

$$\rho(\mathbf{r},0) = \frac{\rho_0}{(2\pi)^{\frac{3}{2}}\sigma^3} \exp\left(-\frac{r^2}{2\sigma^2}\right).$$
(4.90)

Then

$$\tilde{\rho}(\mathbf{k},0) = \frac{\rho_0}{(2\pi)^{\frac{3}{2}}\sigma^3} \left(\frac{1}{\sqrt{2\pi}}\right)^3 \int \exp\left(-\frac{r^2}{2\sigma^2}\right) \exp(-i\mathbf{k}\cdot\mathbf{r}) d^3\mathbf{r}$$
$$= \frac{\rho_0}{(2\pi)^{\frac{3}{2}}} \exp\left(-\frac{k^2\sigma^2}{2}\right).$$
(4.91)

$$\tilde{\rho}(\mathbf{k},t) = \frac{\rho_0}{(2\pi)^{\frac{3}{2}}} \exp\left[-k^2 \left(\frac{\sigma^2}{2} + Dt\right)\right].$$
(4.92)

$$\rho(\mathbf{r},t) = \left(\frac{1}{\sqrt{2\pi}}\right)^3 \int \frac{\rho_0}{(2\pi)^{\frac{3}{2}}} \exp\left[-k^2 \left(\frac{\sigma^2}{2} + Dt\right)\right] \exp(i\mathbf{k}\cdot\mathbf{r}) d^3\mathbf{k}$$
$$= \frac{\rho_0}{(2\pi)^{\frac{3}{2}} (\sigma^2 + 2Dt)^{\frac{3}{2}}} \exp\left(-\frac{r^2}{2\sigma^2 + 4Dt}\right).$$
(4.93)

We see that the fragrant gas expands from its initial radius  $\sigma$  (defined by the standard deviation of the Gaussian distribution) to  $\sqrt{\sigma^2 + 2Dt}$  after time t.

## 4.6 Random Walk

Consider a drunken man walking in a large empty field. For each step i, it takes time  $t_i$  to complete the walk. The position changes by  $\mathbf{r}_i$ , and the direction is randomly chosen. After n steps the distance  $R_n$  from the origin is

$$R_n^2 = \left|\sum_{i=1}^n \mathbf{r}_i\right|^2 = \sum_{i=1}^n |\mathbf{r}_i|^2 + \sum_{i \neq j} 2\mathbf{r}_i \cdot \mathbf{r}_j.$$
 (4.94)

The expectation value of  $R_n^2$  is

$$E\left(R_{n}^{2}\right) = nE\left(\left|\mathbf{r}\right|^{2}\right) = n\overline{r^{2}},\tag{4.95}$$

because  $\sum_{i \neq j} 2\mathbf{r}_i \cdot \mathbf{r}_j$  averages to zero. The time it takes to walk so far is  $t = \sum_i^n t_i$ , and its expectation value is  $nE(t) = n\overline{t}$ . Let us model the gas diffusion process by random walk. We call  $\sqrt{r^2}$  the mean-free path  $l_m$  and  $\overline{t}$  the mean-free time  $t_m$ . The mean-square range of diffusion as a function of time is

$$\overline{R(t)^2} = n l_m^2 = \frac{t l_m^2}{t_m}.$$
(4.96)

Since Eq. (4.93) is the density distribution of the gas at time t as a result of diffusion, if the probability distribution of the position of a gas molecule at t = 0 is

$$P(\mathbf{r},0) = \delta(\mathbf{r}) = \lim_{\sigma \to 0} \frac{1}{(2\pi)^{\frac{3}{2}} \sigma^3} \exp\left(-\frac{r^2}{2\sigma^2}\right),$$
(4.97)

the probability  $P(\mathbf{r}, t)$  of finding a gas molecule at time t and at  $|\mathbf{r}| = r$  is proportional to  $\exp[-r^2/(4Dt)]$ . The mean-square distance from the origin is

$$\overline{R(t)^2} = \frac{\int_0^\infty r^2 \exp\left(-\frac{r^2}{4Dt}\right) 4\pi r^2 dr}{\int_0^\infty \exp\left(-\frac{r^2}{4Dt}\right) 4\pi r^2 dr}$$
$$= 6Dt. \tag{4.98}$$

The integrals in the above equation can be evaluated by the formula in Eq. (1.247). Hence we have

$$D = \frac{l_m^2}{6t_m}.$$
 (4.99)

### 4.6. RANDOM WALK

It is tantalizing to identify

$$\frac{l_m}{t_m} = \overline{v},\tag{4.100}$$

where  $\overline{v}$  is the average velocity

$$\overline{v} = \int_0^\infty \left(\frac{m}{2\pi kT}\right)^{\frac{3}{2}} v \exp\left(-\frac{mv^2}{2kT}\right) 4\pi v^2 dv$$
$$= \sqrt{\frac{8kT}{\pi m}}.$$
(4.101)

Note that the evaluation of such integrals can be found in Eq. (1.388). However, because  $l_m$  is the root-mean-square displacement instead of the mean displacement, Eq. (4.100) is not exact. Bearing this in mind, we may write

$$D \approx \frac{l_m}{6} \sqrt{\frac{8kT}{\pi m}} = \frac{l_m}{3} \sqrt{\frac{2P}{\pi \rho_m}},\tag{4.102}$$

where P is the pressure and  $\rho_m$  is the mass density of the gas. By measuring the diffusion constant, one can estimate  $l_m$  from Eq. (4.102).

Let us use a hard sphere model to describe the gas particle and consider its cross section in collision. Although the physical cross section of a sphere is  $\pi a^2$ , where *a* is the radius of the sphere, the effective cross section in collision is larger. As a matter of fact, two spheres start to touch each other when their distance is 2*a*. Therefore the collisional cross section is  $4\pi a^2$  and the average volume a particle occupies is  $4\pi a^2 t_m v_r$ , where  $v_r$  is the average relative velocity between two colliding particles. The mathematical expression for  $v_r$  is

$$v_r = \int |\mathbf{v}_1 - \mathbf{v}_2| f(\mathbf{v}_1) f(\mathbf{v}_2) d^3 \mathbf{v}_1 d^3 \mathbf{v}_2, \qquad (4.103)$$

which can be calculated from the Maxwell distribution by changing variables:

$$\mathbf{v}_{d} = \frac{1}{\sqrt{2}} \left( \mathbf{v}_{1} - \mathbf{v}_{2} \right),$$
  
$$\mathbf{v}_{s} = \frac{1}{\sqrt{2}} \left( \mathbf{v}_{1} + \mathbf{v}_{2} \right).$$
 (4.104)

We have

$$v_r = \int |\mathbf{v}_1 - \mathbf{v}_2| f(\mathbf{v}_1) f(\mathbf{v}_2) d^3 \mathbf{v}_1 d^3 \mathbf{v}_2 = \sqrt{2} \int |\mathbf{v}_d| f(\mathbf{v}_s) f(\mathbf{v}_d) d^3 \mathbf{v}_d d^3 \mathbf{v}_s$$
  
=  $\sqrt{2} \overline{v}.$  (4.105)

Hence the average volume occupied by a particle is  $4\sqrt{2\pi}a^2t_m\overline{v} \approx 4\sqrt{2\pi}a^2l_m$ , and the number density of the gas is  $\rho_g \approx 1/(4\sqrt{2\pi}a^2l_m)$ . We can compare it with the number density of the same gas particle in the liquid or solid form. Assume in the liquid or solid form the number density  $\rho_c$  is close to that of the ideal close-packing of spheres, namely  $\rho_c = \sqrt{2}/(8a^3)$ . Let  $V_g$  be the volume per mole for the gas ( $\approx 22.4$  l), and  $V_c$  be the volume per mole for the liquid or solid form. These two numbers are not difficult to measure. We can obtain a by

$$\frac{\rho_g}{\rho_c} = \frac{V_c}{V_q} \approx \frac{a}{\pi l_m}.$$
(4.106)

The number of particles per mole, the Avogadro's number  $N_A$ , is then

$$N_A \approx \frac{V_g}{4\sqrt{2\pi}a^2 l_m}.\tag{4.107}$$

# 4.7 Boltzmann Distribution

In a typical macroscopic system, the number of equations that govern the motion of the constituent atoms or molecules can be as large as  $10^{23}$ . These equations are coupled to each others as a result of interaction between degrees of freedom. Even if such a large number of equations can be solved by some supercomputer in the future, there will be too much information, useful or not, in the solutions to be digested by a human being. In most cases, we are not so concerned with the individual dynamics of each degree of freedom. Instead, we are concerned with the average dynamics of the system. The key point is that each macroscopic state of matter corresponds to an extremely large number of microscopic states. Some macroscopic states are more probable than others because they correspond to a larger number of microscopic states with microscopic states, Boltzmann postulated that for an interactive system at equilibrium, the system has an equal probability in every microscopic state. This revolutionary idea led to a powerful method—statistical mechanics.

Let us denote  $p_i$  the probability of the *i*th microscopic state and  $T_{ij}$  the transition probability from state *j* to *i*. Since the equations of motion for the microscopic degrees of freedom are time-reversible, we may assume  $T_{ij} = T_{ji}$ . The rate of change of  $p_i$  can be written as

$$\frac{ap_i}{dt} = \sum_j T_{ij}p_j - \sum_j T_{ji}p_i = \sum_j T_{ij}(p_j - p_i).$$
(4.108)

### 4.7. BOLTZMANN DISTRIBUTION

Let us define a quantity s by

$$s \equiv -\sum_{i} p_i \ln p_i, \qquad (4.109)$$

then we have

$$\frac{ds}{dt} = -\sum_{i} \frac{dp_i}{dt} (1 + \ln p_i).$$
(4.110)

Substituting Eq. (4.108) in, we have

$$\frac{ds}{dt} = -\sum_{ij} T_{ij} (p_j - p_i) (1 + \ln p_i).$$
(4.111)

Since i, j are dummy indices, we may exchange them to get

$$\frac{ds}{dt} = -\sum_{ij} T_{ij}(p_i - p_j)(1 + \ln p_j) = -\sum_{ij} T_{ij}(p_j - p_i)(-1 - \ln p_j).$$
(4.112)

Adding these two equations, we have

$$\frac{ds}{dt} = -\frac{1}{2} \sum_{ij} T_{ij} (p_j - p_i) (\ln p_i - \ln p_j).$$
(4.113)

Since the right-hand side of Eq. (4.113) is always positive, we conclude that s always increases with time. Since  $p_i$  are constrained by the condition  $\sum_i p_i = 1$ , we can find the maximum of s by the method of Lagrange's multipliers. Namely

$$\frac{\partial s}{\partial p_i} + \lambda \frac{\partial}{\partial p_i} \left( \sum_j p_j - 1 \right) = -\ln p_i - 1 + \lambda = 0, \qquad (4.114)$$

where  $\lambda$  is the Lagrange's multiplier associated with the constraint  $\sum_i p_i = 1$ . Eq. (4.114) leads to the conclusion that as  $t \to \infty$ ,  $p_i = p_j$  for any i, j. Namely the probability of every microscopic state is the same.

We may look at  $I \equiv e^{-s}$  as the amount of information we have at hand. If we know the system is exactly in the *m*th state, we have the full information about the system. In this case  $p_m = 1$ ,  $p_i = 0$  for  $i \neq m$ , therefore s = 0, I =1. If every state has the same probability then we have the least information about the system. In this case  $p_i = 1/N$ ,  $s = \ln N$ , therefore I = 1/N, where N is the total number of microscopic states. Because we cannot keep track of all the state transitions, as time goes by information is lost. That is, s increases with time.

Let us consider a macroscopic system made of a large number of microscopic parts, each of which is characterized by its microscopic state. For simplicity, let us distinguish the microscopic states only by their energy  $E_i$ . Assume there are  $n_i$  microscopic systems, each of energy  $E_i$ . One has

$$\sum_{i} n_i = N, \tag{4.115}$$

$$\sum_{i} n_i E_i = E, \tag{4.116}$$

where N is the number of microscopic systems and E is the total energy. For each set  $\{n_i\}$  there are  $\Gamma(\{n_i\})$  ways of constructing the macroscopic system.

$$\Gamma(\{n_i\}) = \frac{N!}{\prod_i n_i!}.\tag{4.117}$$

We may refer to of each the  $\Gamma(\{n_i\})$  ways as a microscopic state of the macroscopic system. In Eq. (4.114) we have shown that as  $t \to \infty$  the probability of every microscopic state is the same, hence a set  $\{n_k\}$  is less probable than another set  $\{n_l\}$  if  $\Gamma(\{n_k\})$  is smaller than  $\Gamma(\{n_l\})$ . Consequently the most probable distribution of  $\{n_i\}$  is the one that maximizes  $\Gamma$  under the constraint of Eqs. (4.115) and (4.116). By the method of Lagrange multipliers

$$\frac{\partial}{\partial n_i} \left[ \ln \Gamma(\{n_i\}) + \alpha (N - \sum_i n_i) + \beta (E - \sum_i n_i E_i) \right] = 0.$$
 (4.118)

Using Stirling's approximation  $\ln N! \approx N \ln N - N$ ,

$$\ln \Gamma(\{n_i\}) \approx N \ln N - \sum_i n_i \ln n_i.$$
(4.119)

Eq. (4.118) becomes

$$-(\ln n_i + 1) - \alpha - \beta E_i = 0, \qquad (4.120)$$

hence  $n_i \propto \exp(-\beta E_i)$ , which means the probability of finding a microscopic system with energy  $E_i$  is proportional to  $\exp(-\beta E_i)$ .

Now consider two macroscopic systems, the total number of ways of constructing the two systems is  $\Gamma(\{n_i\}) = \Gamma_1(\{n_{1i}\})\Gamma_2(\{n_{2i}\})$ . If they are isolated, the individual distributions are determined by

$$\frac{\partial}{\partial n_{1i}} \left[ \ln \Gamma_1(\{n_{1i}\}) + \alpha_1 \left( N_1 - \sum_i n_{1i} \right) + \beta_1 \left( E_1 - \sum_i n_{1i} E_{1i} \right) \right] = 0$$
(4.121)

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and

$$\frac{\partial}{\partial n_{2i}} \left[ \ln \Gamma_2(\{n_{2i}\}) + \alpha_2 \left( N_2 - \sum_i n_{2i} \right) + \beta_2 \left( E_2 - \sum_i n_{2i} E_{2i} \right) \right] = 0$$

$$(4.122)$$

respectively. If the two systems are brought to thermal equilibrium, there is only one constraint of total energy,  $\sum_i n_{1i}E_{1i} + \sum_i n_{2i}E_{2i} = E$ , instead of two independent energy constraints  $\sum_i n_{1i}E_{1i} = E_1, \sum_i n_{2i}E_{2i} = E_2$ . Fewer constraints mean more possibility. Therefore we have  $\Gamma_{eq} \geq \Gamma_{iso}$ . Equality occurs only if  $\beta_1 = \beta_2$  initially. This means when a system approaches equilibrium,  $\ln \Gamma$  increases until the  $\beta$  of each of its parts becomes equal. This is a strong indication that  $\ln \Gamma$  is related to entropy and  $\beta$  is a measure of temperature.

Let us investigate the relation between  $\ln \Gamma$  and the internal energy of the system. The internal energy U of the system is  $U = \sum_i n_i E_i$ , and

$$dU = \sum_{i} E_i dn_i + \sum_{i} n_i dE_i.$$
(4.123)

On the right-hand side the first term is the change of thermal energy because  $dn_i$  changes the state distribution of the system. In contrast, the second term does not change the state distribution, instead it changes uniformly the energy of all the microscopic systems in the same state *i*. Such an energy change is produced by adiabatic macroscopic external forces. Therefore the second term is the work done by external forces. From

$$\ln \Gamma = N \ln N - \sum_{i} n_i \ln n_i, \qquad (4.124)$$

and

$$n_i = \frac{Ne^{-\beta E_i}}{Q}, \qquad (4.125)$$

$$Q = \sum_{i} e^{-\beta E_i}, \qquad (4.126)$$

we have

$$d\ln\Gamma = -\sum_{i} (\ln n_{i} + 1) dn_{i}$$
  
=  $-\sum_{i} (\ln N - \beta E_{i} - \ln Q + 1) dn_{i}.$  (4.127)

Because  $\ln N - \ln Q + 1$  is a constant and  $\sum_i dn_i = dN = 0$ , we have

$$d\ln\Gamma = \sum_{i} \beta E_{i} dn_{i}. \tag{4.128}$$

In other words,

$$\frac{d\ln\Gamma}{\beta} = d\left(\sum_{i} E_{i}n_{i}\right) - \sum_{i} n_{i}dE_{i} = dU + dW, \qquad (4.129)$$

where dW is the work done by the system to the outside world. Comparing with the first law of thermodynamics dU = dQ - dW, and noting the definition dQ = TdS, we have

$$S = k \ln \Gamma, \tag{4.130}$$

$$\beta = \frac{1}{kT}.$$
(4.131)

Eq. (4.130) relates the number of microscopic states  $\Gamma$  to the macroscopic quantity S, and Eq. (4.131) yields

$$n_i \propto \exp\left(-\frac{E_i}{kT}\right),$$
(4.132)

which is known as the **Boltzmann distribution**.

Using Eq. (4.119), and the fact  $\sum_i n_i = N$ , we have

$$\frac{S}{N} = -k \sum_{i} \frac{n_i}{N} \ln\left(\frac{n_i}{N}\right). \tag{4.133}$$

If we interpret  $n_i/N$  as the probability in the state *i*, according to Eq. (4.113), S/N always increases with time. We see that statistical mechanics provides a clear way to understand the second law of thermodynamics from a microscopic point of view.

By calculating  $\Gamma$  as a function of macroscopic variables, such as the energy E, the volume V etc., one can obtain the entropy function S(E, V). From S(E, V) one can obtain the equation of macroscopic state. This is how statistical mechanics works. As an example, let us derive the equation of state for the ideal gas. Envision N independent particles in a box of volume V. For each particle the number of possible states is proportional to V. Because the particles move independently, the number of microscopic states for the whole system is proportional to  $V^N$ . In addition, the particles can have different momenta subjected to the constraint

$$\sum_{i=1}^{3N} p_i^2 / (2m) = E.$$
(4.134)

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Considering the surface area of a 3N-dimensional sphere, the number of states with total energy E is proportional to  $\sqrt{E}^{3N-1}$ . Therefore one has

$$\Gamma(E,V) = CV^N \sqrt{E}^{3N-1}, \qquad (4.135)$$

where C is a proportional constant depending only on N and m and

$$S(E,V) = k \ln \Gamma(E,V) \approx kN \ln V + \frac{3}{2}kN \ln E + k \ln C(N).$$
 (4.136)

From the thermodynamic relation dE = TdS - PdV one has

$$dS = \frac{1}{T}dE + \frac{P}{T}dV, \qquad (4.137)$$

hence

$$\frac{P}{T} = \frac{\partial S}{\partial V} = kN/V, \qquad (4.138)$$

$$\frac{1}{T} = \frac{\partial S}{\partial E} = 3kN/(2E). \tag{4.139}$$

These are the equations of state for the ideal gas.

The entropy function is not always the most convenient to start with. For example, in studying a system which is in thermal contact with a large heat bath, it is more convenient to describe the system as a function of (T, V)than (E, V) because T is fixed by the temperature of the bath. Therefore one uses the Helmholtz free energy A = E - TS, in view of dA = -SdT - PdV. Since the system can exchange energy with the heat bath, its energy is not a fixed value as in an isolated system. Instead the energy follows a probability distribution, namely the Boltzmann distribution. The expectation value is

$$\overline{E} = \frac{\sum_{E_i} E_i \Gamma(N, V, E_i) e^{-E_i/kT}}{\sum_{E_i} \Gamma(N, V, E_i) e^{-E_i/kT}}.$$
(4.140)

Let us define the canonical partition function

$$Q(N,V,T) \equiv \sum_{E_i} \Gamma(N,V,E_i) e^{-E_i/kT}, \qquad (4.141)$$

one has

$$\overline{E} = \frac{-\partial \ln Q}{\partial \beta}.$$
(4.142)

On the other hand,

$$E = A - T\frac{\partial A}{\partial T} = -T^2 \frac{\partial (A/T)}{\partial T} = \frac{\partial (A/kT)}{\partial \beta}, \qquad (4.143)$$

therefore  $A = -kT \ln Q$ . By calculating Q from the microscopic states, one obtains the macroscopic quantity A.

## 4.8 Sedimentation and Brownian Motion

If you have watched a sedimentation pool, you must have found that heavy particles such as marbles and sands are all dropped to the bottom. But, for small particles the behavior is quite different. Not all of them drop to the bottom, nevertheless the concentration increases near the bottom. To obtain clear water, we must drain the pool from near the top, where the concentration of the particles are smallest. These particles are heavier than water, why don't they all drop to the bottom? The Boltzmann distribution provides the answer. Let the vertical distance from the bottom be z. The potential energy for a particle at z is mgz, where m is the effective mass of the particle. The effective mass is  $m_s - m_b$ , where  $m_s$  is the mass of the particle and  $m_b$  is the mass of the water of the same volume. From the Boltzmann distribution we have

$$\rho(z) = \rho(0) \exp\left(-\frac{mgz}{kT}\right), \qquad (4.144)$$

where  $\rho(z)$  is the concentration at z. For heavy particles,  $mgz \gg kT$ , the concentration is negligibly small for z > 0. In other words they all drop to the bottom. For particles of three times the water density, if the particle diameter is 10 nm, at 300 K the height at which the concentration drops to 1/e is 5 cm. By measuring the 1/e height of sedimentation, one can obtain the value of k, and then the Avogadro's number by  $N_A = R/k$ , where R is the gas constant.

The suspended particles are not hanging still in the water. They bounce around like random walk. This random motion can be observed under microscopes, and it is known as the Brownian motion. If the radius of the suspended particles is r and the viscosity of water is  $\eta$ , then according to Stokes law the particles fall down under gravity at a drift velocity  $mg/(6\pi r\eta)$ . The down drift flux  $\rho(z)mg/(6\pi r\eta)$  must be balanced by the diffusion caused by the concentration gradient. We have

$$D\frac{d\rho(z)}{dz} + \frac{mg}{6\pi r\eta}\rho(z) = 0.$$
(4.145)

The solution is

$$\rho(z) = \rho(0) \exp\left(-\frac{mgz}{6\pi r\eta D}\right). \tag{4.146}$$

Comparing with Eq. (4.144), we have

$$D = \frac{kT}{6\pi r\eta}.\tag{4.147}$$

By observing the random motion of a suspended particle under a microscope, one can obtain the mean-free path and mean free time and then the diffusion constant by Eq. (4.99). From the diffusion constant and Eq. (4.147), one can obtain the value of k, and then the Avogadro's number again by N = R/k.

## 4.9 Osmotic Pressure

Consider the particles in a suspension solution. If the particles are under the influence of an external conservative force  $F(\mathbf{r}) = -\nabla \phi(\mathbf{r})$ , then according to the Boltzmann distribution the concentration follows

$$\rho(\mathbf{r}) = \rho_0 \exp\left[\frac{-\phi(\mathbf{r})}{kT}\right]. \tag{4.148}$$

Since the particles' average velocity is zero, the net force applied to them must be zero. The external force per unit volume is  $-\rho(\mathbf{r})\nabla\phi(\mathbf{r})$ . This force must be balanced by a pressure difference that arises from the concentration difference. This is exactly the pressure difference that drives the diffusion. Let the pressure at  $\mathbf{r}$  be  $P(\mathbf{r})$ . For a thin-slab volume element of area Aand thickness dx, if the normal vector of the slab is in the same direction as  $\nabla P(\mathbf{r})$ , the force from the pressure difference on the two sides of the slab is  $-A\nabla Pdx$ . Therefore the force from the pressure difference per unit volume is  $-\nabla P(\mathbf{r})$ . The balance condition is

$$\rho(\mathbf{r})\nabla\phi(\mathbf{r}) + \nabla P(\mathbf{r}) = 0. \tag{4.149}$$

Taking the gradient of Eq. (4.148), we have

$$\nabla \rho(\mathbf{r}) = -\frac{\rho(\mathbf{r})}{kT} \nabla \phi(\mathbf{r}). \tag{4.150}$$

Comparing Eq. (4.149) and Eq. (4.150), we have

$$P(\mathbf{r}) = \rho(\mathbf{r})kT. \tag{4.151}$$

This is the extra pressure caused by the diffusion of the suspended particles, and is known as the **osmotic pressure**.

We may also understand the osmotic pressure from the point of view of entropy. When suspended particles are mixed into a solvent to form a solution, the suspended particles introduce a large number of microscopic states. This increases the entropy. If we assume that the concentration of the suspended particles is small, so that the particles move independently of each other, then

$$\Gamma_s = C(N)V^N f(E), \qquad (4.152)$$

where f(E) represents the total number of velocity combinations the suspended particles can have under the constraint that the total energy of them is E. Since the suspended particles form a subsystem that can exchange energy with the large system of the solvent, E is not a fixed number. Instead, the temperature is approximately fixed because the small energy exchange will not change the solvent temperature significantly. In this situation we should choose the Helmholtz free energy A(N,T,V) as the thermal dynamics variable to calculate. To obtain A(N,T,V), we should first evaluate the partition function Q(N,T,V).

$$Q(N,T,V) = \int C(N)V^N f(E) \exp\left(-\frac{E}{kT}\right) dE.$$
 (4.153)

Therefore

$$A(N,T,V) = -kT \ln Q = -kT \ln C(N) - kTN \ln V - kTD(T), \quad (4.154)$$

where

$$D(T) = \ln\left[\int f(E) \exp\left(-\frac{E}{kT}\right) dE\right].$$
(4.155)

From the relation

$$-P = \left(\frac{\partial A}{\partial V}\right)_T,\tag{4.156}$$

we have

$$-P = -kT\left(\frac{N}{V}\right). \tag{4.157}$$

In other words,

$$P = kT\rho, \tag{4.158}$$

where  $\rho$  is the concentration. This is exactly the same as Eq. (4.151). Note that we have only considered the pressure produced by the subsystem of the suspended particles, therefore Eq. (4.158) is the pressure difference between the suspension solution and the pure solvent. The pressure of the pure solvent can be obtained from  $\Gamma$  or Q of the solvent, which is not included in the calculation of this section.

It is known that plants gather water by the capillary effect. Since in most cases the leaves are surrounded by less moisture than the roots, water is transported from the roots to the leaves. However, because the capillary effect works in both directions, it does not explain why some plants, such as coconut and watermelon, are able to gather a large quantity of water in their fruits. It turns out that a little chemicals dissolved in water will help. Dissolving 30 g of fructose or 5 g of NaCl into 1 liter of water, you get a concentration of 0.17 mole of molecules or ions per liter. The osmotic pressure of this solution is about  $0.17 \times 22.4 = 3.9$  atm. Such a pressure is large enough to raise the solution to 40 meters high. Plants have developed semipermeable membranes to maintain an osmotic pressure that attracts water. In dry area, plants must maintain a high osmotic pressure to compete for water. If you grow such plants, you should be careful not to water them too much. Too much water will cause the cells to burst, and that kills the plant. The osmotic pressure also explains why watermelon grown in dryer sandy soil is sweeter.

### 4.10 Boiling Point

In Taiwan, tea tasting and mountain hiking are two popular recreational activities. If you boil water on a high mountain to prepare tea, you may notice that the boiling point is below 100°C. In contrast, if you dissolve some salt into the water, you may know that the boiling point rises. How do we understand these phenomena?

Since the boiling occurs in the open atmosphere, if the cover of the pot is not tightly sealed, the pressure is equal to the air pressure of the environment, which is held constant. Inside the pot the temperature also remains constant at the boiling point. As we have seen, in this case the best thermodynamic variable to choose is the Gibbs free energy G.

Because liquid water and water vapor are two different phases, the Gibbs free energy are two different functions of T and P. We have

$$dG_g = V_g dP - S_g dT,$$
  

$$dG_l = V_l dP - S_l dT,$$
(4.159)

where  $G_g$  is the free energy of the gas-phase water and  $G_l$  is that of the liquid-phase water. Since both V and S are proportional to the number of molecules, we may rewrite Eq. (4.159) as

$$dg_g = v_g dP - s_g dT,$$
  

$$dg_l = v_l dP - s_l dT,$$
(4.160)

where  $g_g$ ,  $v_g$ , and  $s_g$  are the specific Gibbs free energy (Gibbs free energy per mole), the specific volume (volume per mole), and the specific entropy (entropy per mole) respectively for the gas phase. Similarly,  $g_l$ ,  $v_l$ , and  $s_l$  are the same quantities for the liquid phase.

As we have shown in Section 4.3, at equilibrium the total change of G must be zero. Therefore at the boiling point the gain of G for the gas must be equal to the loss of G for the liquid if some water molecules are converted from the liquid phase to the gas phase. If m moles of water molecules are converted, the change of  $G_g$  is  $mg_g$ , and the change of  $G_l$  is  $-mg_l$ . The total change of G is zero means  $g_g = g_l$  at the boiling point. Since  $g_g$  and  $g_l$  are two different functions of T and P, in principle we can use the condition  $g_g = g_l$  to find T as an implicit function of P. Then for every P we have a corresponding T at which the water boils. In other words, in principle we can find the boiling temperature T as a function of  $g_g$  or  $g_l$ , can we still say something about the change of boiling temperature resulting from the change of pressure?

Empirically we know water boils at 1 atm, 100°C. We may extrapolate the implicit function T(P) near this known point. From

$$dg_g = v_g dP - s_g dT = dg_l = v_l dP - s_l dT.$$

$$(4.161)$$

we have

$$\frac{dP}{dT} = \frac{s_g - s_l}{v_q - v_l}.\tag{4.162}$$

Since the change of entropy  $s_l - s_g$  is done at constant T, we have  $q_l = T(s_g - s_l)$  and

$$\frac{dP}{dT} = \frac{q_l}{T(v_g - v_l)},\tag{4.163}$$

where  $q_l$  is the molar latent heat that must be supplied to vaporize the liquid. Eq. (4.163) is known as the **Clapeyron equation**.

Let us use the Clapeyron equation to calculate the boiling point at 2000 m above the sea level. The average mass of air per mole is 28.8 g. From the Boltzmann distribution, at 2000-m height the air pressure drops by 21%, assuming the temperature is 20°C. That is  $\Delta P = -2.1 \times 10^4$  Pa. Since the specific volume of liquid water is much smaller than that of the water vapor,

#### 4.10. BOILING POINT

we may ignore  $v_l$  in the Clapeyron equation in comparison with  $v_g$ . Then we can integrate the Clapeyron equation to get a relation between  $\Delta P$  and  $\Delta T$ , assuming the equation of state for the water vapor is the same as that of the ideal gas. Namely, one has

$$\frac{dP}{dT} = \frac{q_l P}{NkT^2}.\tag{4.164}$$

The equation can be integrated by separation of variables. That is

$$\Delta(\ln P) = -\frac{q_l}{Nk} \Delta\left(\frac{1}{T}\right). \tag{4.165}$$

The molar latent heat for water is 40860 J/mole. We have

$$\ln 0.79 = -\frac{40860}{6.02 \times 10^{23} \times 1.38 \times 10^{-23}} \left(\frac{1}{T} - \frac{1}{373}\right), \qquad (4.166)$$

which gives the boiling point  $T = 93.4^{\circ}$ C.

We can estimate the boiling point of a solution in a similar way. If we dissolve 5 g of NaCl in to 1 liter of water, we get 0.17 mole of ions in the solution. According to Raoult's law, the vapor pressure of the solution  $P_s$  will be reduced relative to the vapor pressure of pure water  $P_w$  according to the following equation.

$$\frac{P_s}{P_w} = \frac{\rho_l - \rho_i}{\rho_l},\tag{4.167}$$

where  $\rho_l$  is the number density of water and  $\rho_i$  is the number density of ions. The amount of vapor pressure difference one must compensate by increasing the temperature is therefore

$$\Delta P = P_w - P_s = \frac{P_w \rho_i}{\rho_l}.$$
(4.168)

Taking  $P_w = 1$  atm, we have  $\Delta P_v = 0.17 \times 0.018$  atm  $= 3.09 \times 10^2$  Pa. Using the Clapeyron equation again, we obtain  $\Delta T \approx 0.087^{\circ}$ C.

The vapor pressure difference  $\Delta P$  can also be derived without using Raoult's law. Consider the system shown in Fig. 4.6. The vapor is in equilibrium with both the solution and the pure water at the boiling temperature of the solution. At this temperature the vapor pressure of the pure water exceeds the boiling vapor pressure of the solution by

$$\Delta P = P_o \frac{\rho_v}{\rho_l},\tag{4.169}$$

where  $P_o$  is the osmotic pressure and  $\rho_v, \rho_l$  are the densities of the water vapor and the solution at the boiling point respectively. Using the relation  $P_w = \rho_v kT$  and  $P_o = \rho_i kT$ , we find that Eq. (4.169) is the same as Eq. (4.168).



Fig. 4.6: Vapor pressures of solutions. The osmotic pressure  $P_o$  is equal to  $P_A - P_B = \rho_l gh$ , and the difference in vapor pressure between the solution and the pure water is  $P_A - P_C = -\rho_v gh$ , where h is the height difference between the solution and the pure water.

## 4.11 Exercises

**Exercise 4.1.** The highest point of NTU campus is the Ling-Tou mountain at Xi-Tou experimental forest. The height is 2025 m. Assume the temperature of the atmosphere is fixed at 20°C. What is the ratio of oxygen concentration at this point to that at sea level?

**Exercise 4.2.** A thermally insulated box is divided into two compartments by a thin rigid wall. The volume of compartment A is 2 liters, and the volume of compartment B is 1 liter. We fill compartment A with 1 mole of He gas at 600 K and compartment B with 1 mole of Ne gas at 300 K. Then we drill a small hole on the wall between the two compartments so that the two gases can mix slowly with each other. After equilibrium is reached, how much is the change of entropy? In this exercise we assume both gases are ideal gas.

**Exercise 4.3.** The equation of state of a thermal dynamic system is PV = NkT. If we treat the internal energy U of the system as a function of volume V and temperature T, show that U is a function of T only. Namely,

$$\left(\frac{\partial U}{\partial V}\right)_T = 0. \tag{4.170}$$

#### 4.11. EXERCISES

Hint: Since we are using V and T as the independent variables, it is reasonable to start from the Helmholtz free energy

$$dA = -SdT - PdV, (4.171)$$

which yields

$$\left(\frac{\partial A}{\partial V}\right)_T = -P. \tag{4.172}$$

Since A = U - TS, we have

$$\left(\frac{\partial U}{\partial V}\right)_T - T\left(\frac{\partial S}{\partial V}\right)_T = -P. \tag{4.173}$$

Because S is not in the equation of state, we had better get rid of it, otherwise we would not know what to do with it. To do that, you need to derive the relation

$$\left(\frac{\partial S}{\partial V}\right)_T = \left(\frac{\partial P}{\partial T}\right)_V,\tag{4.174}$$

from dA = -SdT - PdV. Then you can use the equation of state to prove  $(\partial U/\partial V)_T = 0$ .

**Exercise 4.4.** If a 2-kg frozen chicken takes 10 hours to defrost, under the same condition how long does it take to defrost a 2-ton elephant? Although a chicken has a different body shape from an elephant, in this problem we assume both were curled up like a meat ball when they were frozen. We also assume the heat conductivity, specific heat, and mass density for both are the same. The time to defrost can be defined by that the temperature at the center reaches  $0.9T_0$ , where  $T_0$  is the absolute temperature of the environment.

**Exercise 4.5.** Dry ice can be made by suddenly opening the value of a high-pressure  $CO_2$  tank. The temperature of  $CO_2$  in the tank is 25°C. The process can be approximated by a simple model in which the  $CO_2$  gas goes through adiabatic expansion from pressure  $P = P_0$  to P = 1 atm. The ice point for  $CO_2$  is  $-78^{\circ}$ C. What is the minimum value of  $P_0$ ? For simplicity, we assume the heat capacity of  $CO_2$  is approximately 7k/2 per molecule at constant pressure, and 5k/2 per molecule at constant volume, where k is the Boltzmann constant.

**Exercise 4.6.** A thick round pipe buried under  $0^{\circ}$ C ground is used to transport hot water of 90°C. The inner radius of the pipe is 2 cm and the outer

radius is 5 cm. If the inner surface of the pipe is maintained at 90°C and the outer surface at 0°C, what is the temperature between the two surfaces as a function of r, where r is the distance from the center of the pipe? In this exercise we assume the specific heat of the pipe does not change with temperature. We also ignore thermal radiation.

**Exercise 4.7.** A factory extracts pure water from sea water at 300 K by using semipermeable membrane to filter out ions. The ion concentration of sea water is approximately 1 mole per liter. The factory extracts 1 liter of pure water from every 5 liters of sea water. How much minimum work must be done for each liter of pure water so produced?

**Exercise 4.8.** A high-speed centrifugal machine is used to separate  $U^{235}F_6$  gas from  $U^{238}F_6$  gas to make fuel for nuclear reactors. The machine is made of a tube 20 meters long lying horizontally on the *x-y* plane and rotating around the z-axis which passes through the mid-point of the tube. The tube is filled with a natural mixture of  $U^{235}F_6$  and  $U^{238}F_6$ . The speed of rotation is 3000 round per minute. The natural abundance of  $U^{235}$  is 0.72%, and that of  $U^{238}$  is 99.27%. After the two gases reach equilibrium, what is the ratio of number density between  $U^{235}F_6$  and  $U^{238}F_6$  at the two far ends of the tube? Assume the temperature of the gases is 300 K. The mass of Fluorine atom is 19 g/mole. In this exercise some numerical integrations are needed. If your hand-held calculator cannot do numerical integration, you may express the answer in terms of the following function:

$$F(x) = \int_0^x e^{t^2} dt.$$

Namely, assume the value of F(x) is known for all x.

**Exercise 4.9.** A high-pressure stewpot can greatly reduce the cooking time. One may view cooking as some kind of chemical reaction. From the order of the activation energy one may estimate that for every  $5^{\circ}$ C increase of temperature, the reaction rate is doubled. If a sealed high-pressure stewpot can maintain a pressure of 1.1 atm, by how much one can speed up the cooking? Namely, if the cooking takes 1 hour at 1 atm, how long will it take at 1.1 atm? In this exercise we assume the maximum temperature the stewpot can reach is the boiling point of water.

**Exercise 4.10.** In northern Taiwan, most people use electric heaters to keep their rooms warm during some cold days. Consider an insulated room sealed with 1-atm air. No heat or air can leak out of the room. The size of the room is  $10 \text{ m} \times 6 \text{ m} \times 4 \text{ m}$ . If the air in the room is an ideal gas with a heat

capacity per molecule at constant volume equal to 5k/2, how much energy it takes to heat up the room from 15°C to 20°C with an electric heater?

The energy-efficiency rating (EER) of an air-conditioner is defined by how many joules per second are removed for each watt of power it draws. Typical EER is 2.7 for small air-conditioners. If one uses an air-conditioner in the reverse direction to heat up the room, how much energy is needed to heat up the room from  $15^{\circ}$ C to  $20^{\circ}$ C? Although physically the EER will vary with both the indoor temperature and the outdoor temperature, for simplicity we assume the EER is a constant of 2.7.

If one uses an ideal Carnot engine running reversely to pump heat from outside into the room, where the temperature outside is also 15°C, how much work is needed to fulfill the same purpose?

**Exercise 4.11.** Consider two thermally insulated 100-liter tanks. One is filled with 100°C water and the other with 0°C water. If we use the two tanks to drive an ideal Carnot engine, what is the maximum work the engine can produce? The heat capacity of water is  $4.18 \text{ J/(K} \cdot \text{g})$  in the temperature range considered here.

**Exercise 4.12.** Consider a spherical water droplet of radius R surrounded by air of water-vapor concentration x in a large room. The air and the droplet are at the same temperature T. The density of the water droplet is  $\rho_w$ , and the density of the pure water vapor is  $\rho_v$ . The concentration is measured by the fraction of water molecules in the air. The water droplet will slowly evaporate as a result of the diffusion of water molecules. Since at the surface of the water droplet the liquid-phase water is in equilibrium with the gas-phase water, it is reasonable to assume that right above the surface of the water droplet the water-vapor concentration is  $x_0$ , which corresponds to the saturated vapor pressure at T, and far away from the droplet the water concentration is  $x (x < x_0)$  in the steady state. Then we have a steady-state concentration gradient of water molecules in the radial direction. This concentration gradient will drive the transport of water molecules by diffusion. The diffusion coefficient is D. What is the rate of change of the radius of the water droplet dR/dt as a function of  $x, x_0, \rho_w, \rho_v, R$ , and D? In this exercise we assume the evaporation rate is small so that the temperature of the droplet remains constant.

**Exercise 4.13.** The open-circuit voltage V of a battery is a function of

temperature T.

$$V = 12 + 0.05(T - T_0) - 0.0005(T - T_0)^2,$$

where V is measured in volts and  $T_0 = 25^{\circ}$ C. If the battery is kept at 18°C by thermal contact with a heat reservoir, for each Coulomb of electricity that flows through the battery, how much heat is absorbed by the battery from the reservoir? We assume the battery has no internal resistance.

**Exercise 4.14.** A gas is modeled as hard spheres undergoing random collisions. If the temperature is increased from T to 2T at the same pressure, by what factor the diffusion coefficient will change? If the pressure is increase from P to 2P at the same temperature, by what factor the diffusion coefficient will change?

**Exercise 4.15.** A person is confined in a sealed room. There is a round hole on the wall connected to the atmosphere through which oxygen can diffuse into the room. The hole is filled with porous material such that air convection through the hole is not possible. The thickness of the wall is 10 cm. In order for the person to remain comfortable, the concentration of the oxygen must not be lower than 80% of its normal concentration at 1 bar (100 kPa). Because a person consumes 30 g of oxygen per hour, the hole must be large enough to supply this amount of oxygen. If the oxygen molecule is modeled as a hard sphere of 0.3-nm diameter, what is the minimum area of the hole? In this problem we assume the temperature is 300 K and diffusion is the only mechanism oxygen can pass through the hole. We also note that oxygen occupies 20.94% of air by volume. To simplify the calculation we treat nitrogen and carbon dioxide molecules as hard spheres that have the same diameter and mass as the oxygen molecule, and assume that inside the room the concentration of oxygen is uniform.

**Exercise 4.16.** In a three-dimensional world, if gas diffusion is modeled by random walk, the diffusion coefficient D is related to the mean free path  $l_m$  by

$$D \approx \frac{l_m}{6} \sqrt{\frac{8kT}{\pi m}}$$

where T is the temperature and m is the mass of the gas molecule. How would this formula change in a two-dimensional world?

**Exercise 4.17.** A stack of poker cards can be considered as a macroscopic system which can have many different microscopic configurations. A stack of

52 cards is initially arranged sequentially from spade-A, spade-K, ... spade-3, spade-2, heart-A, heart-K, ... heart-3, heart-2, diamond-A, diamond-K, ... diamond-3, diamond-2, club-A, club-K, ... club-3, club-2. After shuffling it thoroughly how much does the entropy of this system increase? Note that you are required to give a numerical answer in the form of  $a.b \times 10^{\circ}$  J/K. To be fair to your poor classmates who do not own an advanced calculator that can do large factorial, you must use the Stirling formula to calculate the factorial.

**Exercise 4.18.** After a typhoon attack, the sedimentation pool of Taipei water department is full of dust. Assume the depth of the pool is 3 m, and the dust particles are spheres of 10-nm radius with a density equal to  $3.0\text{-g/cm}^3$ . Initially the number density of the dust in the pool is  $\rho_0$ , which is independent of the height h measured from the bottom of the pool. After some time the density becomes a decreasing function of h, because the particles fall to the bottom. How many days does it take for the density at h = 3 m to fall below  $\rho_0/10$ ? The temperature is 300 K and the viscosity of water is  $1.0 \times 10^{-3} \text{ N} \cdot \text{s/m}^2$ . If your answer is m days, you are only required to write a equation that determines m. The equation may contain an integral that cannot be integrated analytically. Note that the rectangular function  $\operatorname{recf}(x)$  is defined as

$$\operatorname{recf}(x) = \begin{cases} 1 & \text{for } x \text{ in } [-\frac{1}{2}, \frac{1}{2}] \\ 0 & \text{otherwise.} \end{cases}$$

The Fourier transform of recf(x) is

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \operatorname{recf}(x) e^{-ikx} dx = \frac{1}{\sqrt{2\pi}} \operatorname{sinc}(k/2) \equiv \frac{1}{\sqrt{2\pi}} \frac{\sin(k/2)}{k/2}.$$

For simplicity in notation, you may use the sinc function in the integral expression of your answer.

**Exercise 4.19.** The enthalpy change for the reaction  $\text{CO} + \frac{1}{2}\text{O}_2 \rightarrow \text{CO}_2$  is  $\Delta H = -283 \text{ kJ/mole}$  if the reactants are maintained at 1 bar (100 kPa), 25°C before the reaction, and the product is also maintained at the same condition after the reaction. If 0.5 mole of CO and 0.25 mole of O<sub>2</sub> react in a sealed box of volume 1 m<sup>3</sup>, and before the reaction the gas mixture is maintained at 1 bar (100 kPa), 25°C by filling the box with N<sub>2</sub> gas, how much will the temperature increase after the reaction? In this problem we assume CO, O<sub>2</sub>, N<sub>2</sub>, and CO<sub>2</sub> are all ideal gas, and in the temperature range considered here their heat capacities are all 5k/2. We also assume there is no reverse reaction and the N<sub>2</sub> gas does not participate in any reaction.
# Chapter 5

# Fluid Mechanics

# 5.1 Convective Derivative

A fluid is made of many particles each having its own position and velocity. As in the case of thermodynamics and statistical mechanics, there is no way we can track the motion of each particle, therefore we should use distribution functions to describe the average behavior of groups of particles. Because each group of particles are moving with time, and particle exchange between groups occurs frequently, it is difficult to keep track of the position, velocity, and number of particles in a group all the time. Instead, it is more convenient to keep track of the number of particles and the average velocity at fixed points in space. We may divide the three dimensional space into cells and label each cell by its location  $\mathbf{r}$ , then a way to describe the fluid is by the number density field  $\rho(\mathbf{r}, t)$  and velocity field  $\mathbf{u}(\mathbf{r}, t)$  at each location. In general the group of particles at a position does not have the same velocity, however, if the standard deviation of the velocity distribution is small compared with its average, we can use the average velocity as an approximation.

By noting that the flux vector  $\mathbf{J}$  is related to  $\rho$  and  $\mathbf{u}$  by

$$\mathbf{J} = \rho \mathbf{u},\tag{5.1}$$

we may take a close look at the continuity equation Eq. (4.84) by writing it

as

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \mathbf{u}) = -\nabla \rho \cdot \mathbf{u} - \rho \nabla \cdot \mathbf{u}.$$
(5.2)

Let us imagine a situation in which the flow field  $\mathbf{u}$  is a constant. In this case  $\nabla \cdot \mathbf{u} = 0$  and the particles have no chance to accumulate. Intuitively one may think if the particles do not accumulate, the density cannot change with time. Then, why is there still the possibility of density change as a function of time, as expressed by the rest of the equation

$$\frac{\partial \rho}{\partial t} + \nabla \rho \cdot \mathbf{u} = 0, \tag{5.3}$$

instead of simply

$$\frac{\partial \rho}{\partial t} = 0? \tag{5.4}$$

The answer is that in order to use this intuitive (and correct) argument, one must follow the motion of the group of particles in space, instead of looking at the density at a fixed point. If we follow the motion of a group of particles, the position of the group of particles changes with time, therefore the change of density with time for the group of particles is not simply  $\partial \rho / \partial t$ , but

$$\frac{d\rho(\mathbf{r}(t),t)}{dt} = \frac{\partial\rho}{\partial t} + \nabla\rho \cdot \frac{d\mathbf{r}}{dt},\tag{5.5}$$

where  $d\mathbf{r}/dt = \mathbf{u}$ . For example, let us imagine that a factory released a large quantity of pollutant gas through its chimney in a short period. The wind carries the pollutant to the east at a constant velocity. Even though the velocity is constant, a bird sitting on a tall tree on the path still experiences a density change of the pollutant. It first rises, then falls. In contrast, if the bird flies with the same velocity as the wind, it will experience a constant density of pollutant. Hence we can write either

$$\frac{d\rho}{dt} + \rho \nabla \cdot \mathbf{u} = 0, \qquad (5.6)$$

or

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0, \qquad (5.7)$$

with the understanding that

$$\frac{d\rho}{dt} = \frac{\partial\rho}{\partial t} + \nabla\rho \cdot \mathbf{u}.$$
(5.8)

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### 5.2. MOMENTUM CONSERVATION

They describe the same physical situation only from different points of view. The relation between  $d\rho/dt$  and  $\partial\rho/\partial t$  can be applied to other physical quantities too. In general,

$$\frac{d\mathbf{G}}{dt} = \frac{\partial \mathbf{G}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{G},\tag{5.9}$$

and  $d\mathbf{G}/dt$  written in the form of Eq. (5.9) is called the convective derivative of  $\mathbf{G}$ .

# 5.2 Momentum Conservation

Let us consider the conservation of momentum in the x-direction. Let  $f(\mathbf{r}, \mathbf{v})$  be the phase-space distribution function of the particles. We have

$$\int f(\mathbf{r}, \mathbf{v}) d^3 \mathbf{v} = \rho(\mathbf{r}), \qquad (5.10)$$

where  $\rho(\mathbf{r})$  is the number density at  $\mathbf{r}$ . The momentum density in the *x*-direction is

$$p_x(\mathbf{r}) = m \int v_x f(\mathbf{r}, \mathbf{v}) \, d^3 \mathbf{v} = m \rho(\mathbf{r}) \bar{v}_x(\mathbf{r}) = m \rho(\mathbf{r}) u_x(\mathbf{r}), \qquad (5.11)$$

where m is the mass of a single particle and  $u_x(\mathbf{r}) \equiv \bar{v}_x(\mathbf{r})$  is the x-component of the average velocity at **r**. Differentiating both sides, we have

$$\frac{\partial p_x}{\partial t} = \int \frac{\partial}{\partial t} \left[ m v_x f(\mathbf{r}, \mathbf{v}) \right] d^3 \mathbf{v}.$$
(5.12)

Replacing  $\rho$  in Eq. (5.2) by  $mv_x f(\mathbf{r}, \mathbf{v})$  and  $\mathbf{u}$  by  $\mathbf{v}$ , we have

$$\frac{\partial p_x}{\partial t} = \int -\nabla \cdot \left[ m v_x \mathbf{v} f(\mathbf{r}, \mathbf{v}) \right] d^3 \mathbf{v}.$$
(5.13)

Since  $\nabla$  is a differential operation with respect to spatial coordinates, it is independent of the integration over **v**. Under this condition we may move  $\nabla$  out of the integrand.

$$\frac{\partial p_x}{\partial t} = -\nabla \cdot \left( m \int v_x \mathbf{v} f(\mathbf{r}, \mathbf{v}) \, d^3 \mathbf{v} \right). \tag{5.14}$$

Under an external force field  $\mathbf{F}(\mathbf{r})$ , Eq. (5.14) becomes

$$\frac{\partial p_x}{\partial t} = -\nabla \cdot \left( m \int v_x \mathbf{v} f(\mathbf{r}, \mathbf{v}) \, d^3 \mathbf{v} \right) + m \rho F_x. \tag{5.15}$$

The first term on the right-hand side accounts for the net momentum flux that flows into the cell at  $\mathbf{r}$ , and the second term accounts for the momentum increase due to acceleration. If we define the stress tensor  $T_{ij}$  by

$$T_{ij} = m \int v_i v_j f(\mathbf{r}, \mathbf{v}) \, d^3 \mathbf{v} = m \rho \overline{v_i v_j}, \qquad (5.16)$$

where  $\overline{v_i v_j}$  denotes the average of  $v_i v_j$ , Eq. (5.15) can be written in the compact tensor form:

$$\frac{\partial p_i}{\partial t} = -\frac{\partial T_{ij}}{\partial x_i} + m\rho F_i, \qquad (5.17)$$

where repeated indices are summed automatically. We may decompose the velocity into the average velocity  $\mathbf{u}$  plus the random velocity  $\mathbf{v} - \mathbf{u}$ , then the stress tensor can be written as

$$T_{ij} = m\rho u_i u_j + m \int (v_i - u_i)(v_j - u_j) f(\mathbf{r}, \mathbf{v}) d^3 \mathbf{v}.$$
 (5.18)

The second term on the right-hand side averages to zero except for i = j. When i = j it is equal to  $m\rho(v_i - u_i)^2$ , which is 2/3 of the average kinetic energy seen by an observer moving with the fluid. By Eq. (4.62) we may write

$$T_{ij} = m\rho u_i u_j + P\delta_{ij},\tag{5.19}$$

where P is the pressure and  $\delta_{ij}$  is the Kronecker delta. We may expand both sides of Eq. (5.17) to obtain

$$m\rho\frac{\partial u_i}{\partial t} + mu_i\frac{\partial\rho}{\partial t} = -\frac{\partial P}{\partial x_i} - mu_i\frac{\partial(\rho u_j)}{\partial x_j} - m\rho u_j\frac{\partial u_i}{\partial x_j} + m\rho F_i.$$
 (5.20)

By the continuity equation, the second terms on both sides cancel each other. We have

$$m\rho \left[\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u}\right] = -\nabla P + m\rho \mathbf{F}.$$
(5.21)

We can use the identity  $(\mathbf{u} \cdot \nabla)\mathbf{u} = \nabla(u^2/2) - \mathbf{u} \times (\nabla \times \mathbf{u})$  to rewrite Eq. (5.21) into another form:

$$m\rho\left[\frac{\partial \mathbf{u}}{\partial t} + \nabla\left(\frac{u^2}{2}\right) - \mathbf{u} \times (\nabla \times \mathbf{u})\right] = -\nabla P + m\rho \mathbf{F}.$$
 (5.22)

### 5.2. MOMENTUM CONSERVATION

If **F** is a conservative force field, such as the gravitational field, we have  $\mathbf{F} = -\nabla\phi$ . For an irrotational steady-state flow of constant density, we have  $\nabla \times \mathbf{u} = 0$ ,  $\partial \mathbf{u}/\partial t = 0$ , and  $\nabla \rho = 0$ . Under these conditions we may integrate Eq. (5.22) and get

$$P + \frac{m\rho u^2}{2} + m\rho\phi = \text{constant.}$$
(5.23)

This is known as the **Bernoulli theorem**.

When the Bernoulli theorem is applied to air, it may not be quite practical to assume that the density is constant. After all, unlike water, air is compressible. In this case we need to consider the relation between the pressure and the density, which is determined by the equation of state in a thermodynamic system. Assume there is no heat conduction, the change of internal energy per mole is

$$d\epsilon = -Pd\left(\frac{N_A}{\rho}\right) = \frac{N_A P}{\rho^2} d\rho, \qquad (5.24)$$

where  $N_A$  is the Avogadro's number. In other words,

$$\nabla\left(\frac{\epsilon}{N_A} + \frac{P}{\rho}\right) = \frac{\nabla P}{\rho}.$$
(5.25)

Substituting it into Eq. (5.22), for a steady-state flow we have

$$\frac{\epsilon}{N_A} + \frac{P}{\rho} + \frac{mu^2}{2} + m\phi = \text{constant.}$$
(5.26)

In thermodynamics the enthalpy H is defined by H = U + PV. We see that  $\epsilon + PN_A/\rho$  is simply the enthalpy per mole. Therefore Eq. (5.26) can be interpreted as the conservation of energy in which the internal energy is replaced by the enthalpy. This is not difficult to understand, since in this case the volume of the fluid cell is not fixed, we need to add to the internal energy the work done by the pressure in squeezing the cell.

For ideal gases,  $\epsilon + PN_A/\rho$  is proportional to the temperature. Therefore when the flow is accelerated, the temperature drops. This can be seen in the moisture condensation near the tips of the wings or sails as the air flows fast around the tips, driven by the large pressure difference between the two sides.

### 5.3 Viscosity

When two adjacent cells flow at different velocities, due to friction the velocity difference has a tendency to diminish. The friction is caused by particle collisions at the boundary. On the average, collisions will cause some particles in the fast moving cell to slow down and some in the slow moving cell to speed up. Therefore, to the first order approximation there is a momentum transfer between the two cells proportional to the velocity difference. In deriving Eq. (5.21) we did not include such an effect known as viscosity.

Consider a cubic flow cell at (x, y, z) spanned by the three infinitesimal vectors  $\Delta x \mathbf{e}_1$ ,  $\Delta y \mathbf{e}_2$ , and  $\Delta z \mathbf{e}_3$ . In the x-direction, viscosity yields drag forces acting on the four surfaces of the flow cell parallel to the x-axis. The surface facing the y-direction is dragged by a force proportional to  $\partial u_x/\partial y$ , where the derivative  $\partial u_x/\partial y$  is evaluated at  $(x, y + \Delta y, z)$ , and the surface facing the -y-direction is dragged by a force proportional to  $-\partial u_x/\partial y$ , where the derivative  $\partial u_x/\partial y$  is evaluated at (x, y, z). Both forces are also proportional to the surface area. Let  $\mu$  be the proportional constant. The total force in the x-direction contributed from these two surfaces is

$$F_x^{(y)} = \mu \left[ \frac{\partial u_x}{\partial y} (x, y + \Delta y, z) - \frac{\partial u_x}{\partial y} (x, y, z) \right] \Delta x \Delta z$$
  

$$\approx \mu \frac{\partial^2 u_x}{\partial^2 y} \Delta x \Delta y \Delta z.$$
(5.27)

Similarly, the total drag force in the x-direction contributed from the two surfaces facing the z- and -z-directions is

$$F_x^{(z)} = \mu \left[ \frac{\partial u_x}{\partial z} (x, y, z + \Delta z) - \frac{\partial u_x}{\partial z} (x, y, z) \right] \Delta x \Delta y$$
  

$$\approx \mu \frac{\partial^2 u_x}{\partial^2 z} \Delta x \Delta y \Delta z.$$
(5.28)

Adding the forces acting at all the four surfaces, we see the force density contributed from viscosity is

$$f_x = \mu \left( \frac{\partial^2 u_x}{\partial^2 y} + \frac{\partial^2 u_x}{\partial^2 z} \right).$$
 (5.29)

Comparing Eq. (5.29) with Eq. (5.17), we find that terms in the form of  $\partial u_i/\partial x_j$  must be added to  $T_{ij}$  in order to take viscosity into account. Let  $T_{ij}^v$ 

#### 5.3. VISCOSITY

denotes the viscous part of the stress tensor that is to be added to  $T_{ij}$ . A possible choice of  $T_{ij}^{v}$  is

$$T_{ij}^{v} = -\mu \left[ \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) + \left( \frac{\partial u_i}{\partial x_j} - \frac{\partial u_j}{\partial x_i} \right) \right],$$
(5.30)

where  $T_{ij}^v$  is intentionally separated into two terms. The first term on the right-hand side is the symmetric part and the second term on the right-hand side is the asymmetric part. The asymmetric part is a component of  $\nabla \times \mathbf{u}$ , hence it represents pure rotation of the fluid at the spatial point  $\mathbf{r}$  under consideration. Since rotation of the fluid cannot change its linear momentum, the asymmetric part does not contribute to the viscous force. Therefore we have

$$T_{ij}^{\nu} = -\mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right).$$
(5.31)

We may further decompose  $T_{ij}^v$  into a traceless part and a scalar part. The traceless part represents the directional shearing of the flow at the spatial point **r** under consideration, whereas the scalar part represents the net outward flux of the fluid at the spatial point **r** under consideration. The traceless part of  $T_{ij}^v$  that can be constructed from  $\partial u_i/\partial x_j + \partial u_j/\partial x_i$  is

$$\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3}\delta_{ij}\nabla\cdot\mathbf{u}\right),\tag{5.32}$$

and the scalar part is just a term proportional to  $\nabla \cdot \mathbf{u}$ . Therefore the most general form of  $T_{ij}^v$  is

$$T_{ij}^{v} = -\mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \nabla \cdot \mathbf{u} \right) - \zeta \delta_{ij} \nabla \cdot \mathbf{u}, \qquad (5.33)$$

where  $\mu$  is the coefficient of viscosity and  $\zeta$  is the coefficient of bulk viscosity. To include  $T_{ij}^v$  in the equation of motion, we add the term  $-\partial(T_{ij}^v)/\partial x_j$  to Eq. (5.21).

$$-\frac{\partial T_{ij}^{v}}{\partial x_{j}} = \mu \frac{\partial}{\partial x_{j}} \left( \frac{\partial u_{i}}{\partial x_{j}} + \frac{\partial u_{j}}{\partial x_{i}} - \frac{2}{3} \delta_{ij} \nabla \cdot \mathbf{u} \right) + \zeta \delta_{ij} \frac{\partial}{\partial x_{j}} (\nabla \cdot \mathbf{u})$$
$$= \mu \left[ \nabla^{2} u_{i} + \frac{\partial}{\partial x_{i}} (\nabla \cdot \mathbf{u}) - \frac{2}{3} \frac{\partial}{\partial x_{i}} (\nabla \cdot \mathbf{u}) \right] + \zeta \frac{\partial}{\partial x_{i}} (\nabla \cdot \mathbf{u}).(5.34)$$

After that Eq. (5.21) becomes

$$m\rho\left[\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u}\cdot\nabla)\mathbf{u}\right] = -\nabla P + \mu\nabla^2\mathbf{u} + \left(\frac{\mu}{3} + \zeta\right)\nabla(\nabla\cdot\mathbf{u}) + m\rho\mathbf{F}.$$
 (5.35)

For the incompressible flow, we have  $\nabla \cdot \mathbf{u} = 0$ . The equation reduces to

$$m\rho \left[\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u}\right] = -\nabla P + \mu \nabla^2 \mathbf{u} + m\rho \mathbf{F}.$$
 (5.36)

This is known as the **Navier-Stokes equation**. It is different from Eq. (5.21) only by the term  $\mu \nabla^2 \mathbf{u}$ . Comparing with the diffusion equation Eq. (4.85), we see that  $\mu \nabla^2 \mathbf{u}$  is a diffusive term, which tends to equalize the flow velocity.

As an example of application, let us use the Navier-Stokes equation to solve the problem of flow in a round pipe. Because of viscosity, a finite pressure must be applied to make the liquid flow through the pipe. But the flow speed is not a constant. At the edge of the pipe the flow speed is zero, and at the center it is maximum. Let us assume the flow is in a steady state, and the flow velocity has only the z-component, which is a function of the radius. In the cylindrical coordinate system we have  $\mathbf{u} = [0, 0, u(r)]$ , and it is easy to see the left-hand side of Eq. (5.36) is zero. The pressure gradient cannot be a function of r, because there is no flow in the radial direction. It cannot be a function of z either, because u does not depend on z. Therefore it can only be a constant which is equal to  $-\Delta p/L$ , where  $\Delta p$  is the pressure difference between the two ends and L is the length of the pipe. Now we have

$$\nabla^2 u = -\frac{\Delta p}{\mu L}.\tag{5.37}$$

In the cylindrical coordinate system this is

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right)u = -\frac{\Delta p}{\mu L}.$$
(5.38)

Integrating with respect to r twice, we have

$$u(r) = -\frac{\Delta p}{\mu L} \frac{r^2}{4} + C \ln r + D, \qquad (5.39)$$

where C and D are to be determined by the boundary conditions. Because the flow is finite at the center, C = 0. At r = R, where R is the radius of the pipe, the flow is zero, therefore

$$u(r) = \frac{\Delta p}{\mu L} \frac{R^2 - r^2}{4}.$$
 (5.40)

Integrating the flux over r, we have

$$F = \frac{\Delta p}{\mu L} \int_0^R \frac{R^2 - r^2}{4} 2\pi r \, dr = \frac{\pi \Delta p R^4}{8\mu L}.$$
 (5.41)

This is known as the **Poiseuille's law**. The  $R^4$  dependence means the flux is very sensitive to the pipe radius. If the radius of the blood vessel is reduced to 90%, perhaps by plaques, the flow is reduced to 66%. That means the heart must produce 50% more pressure to keep the same flow. This is a dangerous situation if the blood vessel has weakened walls.

## 5.4 Sound Waves

In a fluid, sound wave can be treated as an oscillating perturbation of the steady state fluid. Neglecting viscosity, we may start from Eq. (5.21) and the continuity equation. We have five variables to solve. They are  $\rho$ , P, and **u**. But Eq. (5.21) and the continuity equation give only four equations. The last equation we need is the equation of state, which relates P to  $\rho$ . Consider the sound wave in an ideal gas, in which the equation of state is  $P = c\rho^{\gamma}$ , where  $\gamma = c_p/c_v$  and c is a constant. We have chosen the adiabatic equation of state instead of the isothermal equation of state ( $P = \rho kT$ ) because in the time scale of sound wave, the compression of an ideal gas under 1 atm and 300 K is effectively adiabatic. There is simply not enough time for the gas to reach thermal equilibrium. Let us assume the wave propagation is in the x-direction, and set  $\rho = \rho_0 + \Delta\rho$ ,  $u = u_0 + \Delta u$ , where  $\rho_0$  and  $u_0$  are constants and  $\Delta\rho$  and  $\Delta u$  are small perturbations. For an observer moving with the fluid,  $u_0 = 0$ . Neglecting second-order terms, the continuity equation becomes

$$\frac{\partial \Delta \rho}{\partial t} + \rho_0 \frac{\partial \Delta u}{\partial x} = 0, \qquad (5.42)$$

and Eq. (5.21) becomes

$$m\rho_0 \frac{\partial \Delta u}{\partial t} = -\frac{\gamma P_0}{\rho_0} \frac{\partial \Delta \rho}{\partial x}.$$
(5.43)

By eliminating  $\Delta u$ , the two equations can be combined into a wave equation

$$\frac{\partial^2 \Delta \rho}{\partial t^2} - \frac{\gamma P_0}{m \rho_0} \frac{\partial^2 \Delta \rho}{\partial x^2} = 0.$$
(5.44)

The velocity of the sound wave is

$$c_s = \sqrt{\frac{\gamma P_0}{m\rho_0}} = \sqrt{\frac{\gamma kT}{m}}.$$
(5.45)

## 5.5 Waves on Water Surface

Waves on water surface can be created by perturbations that change the height of the surface locally. Such perturbations may come from the wind, the wake of a passing ship, or even earth quakes. When the surface in a localized region is raised above its equilibrium height, gravity pulls the water back. At the same time, because the pressure under this region is higher than its neighboring regions, water also flows out underneath horizontally. By the time the water stops flowing, the surface has already dropped to below its equilibrium height, and then the reverse process occurs. This yields an oscillatory motion for the surface height.

Let us first write down the equations for a moving fluid near equilibrium. We keep only terms of first-order perturbation and neglect all the high-order terms. Assume the pressure is  $P + \Delta P$ , the horizontal velocity is  $u + \Delta u_x$ , the vertical velocity is  $\Delta u_z$ , and the mass density is  $\rho + \Delta \rho$ . The first-order perturbation terms  $\Delta P$ ,  $\Delta u_x$ ,  $\Delta u_z$ ,  $\Delta \rho$  are functions of x, z, t, and P, u,  $\rho$  are functions of z only. The equation of motion in the x-direction is

$$(\rho + \Delta \rho)\frac{d}{dt}(u + \Delta u_x) = -\frac{\partial}{\partial x}(P + \Delta P), \qquad (5.46)$$

and that in the z-direction is

$$(\rho + \Delta \rho)\frac{d\Delta u_z}{dt} = -\frac{\partial}{\partial z}(P + \Delta P) - g(\rho + \Delta \rho).$$
(5.47)

Since  $-\partial P/\partial z = g\rho$ , the above equation can be written as

$$(\rho + \Delta \rho) \frac{d\Delta u_z}{dt} = -\frac{\partial \Delta P}{\partial z} - g\Delta \rho.$$
(5.48)

Because water is nearly incompressible, it is reasonable to assume

$$\frac{d}{dt}(\rho + \Delta \rho) = 0. \tag{5.49}$$

From Eq. (5.6) we have

$$\nabla \cdot \mathbf{u} = 0. \tag{5.50}$$

Replacing d/dt by  $\partial/\partial t + \mathbf{u} \cdot \nabla$  and neglecting high-order terms, Eqs. (5.46)–(5.50) become

$$\rho\left(\frac{\partial\Delta u_x}{\partial t} + u\frac{\partial\Delta u_x}{\partial x} + \Delta u_z\frac{du}{dz}\right) = -\frac{\partial\Delta P}{\partial x},\tag{5.51}$$

### 5.5. WAVES ON WATER SURFACE

$$\rho\left(\frac{\partial\Delta u_z}{\partial t} + u\frac{\partial\Delta u_z}{\partial x}\right) = -\frac{\partial\Delta P}{\partial z} - g\Delta\rho,\tag{5.52}$$

$$\frac{\partial \Delta \rho}{\partial t} + u \frac{\partial \Delta \rho}{\partial x} + \Delta u_z \frac{d\rho}{dz} = 0, \qquad (5.53)$$

$$\frac{\partial \Delta u_x}{\partial x} + \frac{\partial \Delta u_z}{\partial z} = 0. \tag{5.54}$$

Since we are interested in perturbations having the form of a wave, let us assume the solutions for  $\Delta P$ ,  $\Delta u_x$ ,  $\Delta u_z$ ,  $\Delta \rho$  all have the form  $f(z)e^{i(kx-\omega t)}$ . Substituting it into Eqs. (5.51)–(5.54), we obtain

$$\rho \left[ -i(\omega - ku)\Delta u_x + \Delta u_z \frac{du}{dz} \right] = -ik\Delta P, \qquad (5.55)$$

$$-i\rho(\omega - ku)\Delta u_z = -\frac{\partial\Delta P}{\partial z} - g\Delta\rho, \qquad (5.56)$$

$$-i(\omega - ku)\Delta\rho + \Delta u_z \frac{d\rho}{dz} = 0, \qquad (5.57)$$

$$ik\Delta u_x + \frac{\partial\Delta u_z}{\partial z} = 0. \tag{5.58}$$

Substituting Eq. (5.58) into Eq. (5.55), we have

$$\frac{\rho}{k}(\omega - ku)\frac{\partial\Delta u_z}{\partial z} + \rho\Delta u_z\frac{du}{dz} = -ik\Delta P.$$
(5.59)

Substituting Eq. (5.57) into Eq. (5.56), we have

$$-i\rho(\omega - ku)\Delta u_z - ig\frac{\Delta u_z}{\omega - ku}\frac{d\rho}{dz} = -\frac{\partial\Delta P}{\partial z}.$$
(5.60)

Differentiating Eq. (5.59) and multiplying Eq. (5.60) by ik, we can eliminate  $\Delta P$  on the right-hand side of them and obtain

$$\frac{\partial}{\partial z} \left[ \frac{\rho}{k} (\omega - ku) \frac{\partial \Delta u_z}{\partial z} + \rho \Delta u_z \frac{du}{dz} \right]$$
  
=  $k\rho(\omega - ku)\Delta u_z + kg \frac{\Delta u_z}{\omega - ku} \frac{d\rho}{dz}.$  (5.61)

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To find out the boundary conditions for the equations above, let us consider not only the motion of the water, but also that of the air on top of the water. Now there are two layers of fluids to be considered. The interface is at z = 0. For z > 0 the air has a density  $\rho_1 + \Delta \rho_1$ , a pressure  $P_1 + \Delta P_1$ , and velocity components  $u_1 + \Delta u_{1x}$  and  $\Delta u_{1z}$ . Similarly, for -D < z < 0, where D is the depth of the water, the water has a density  $\rho_2 + \Delta \rho_2$ , a pressure  $P_2 + \Delta P_2$ , and velocity components  $u_2 + \Delta u_{2x}$  and  $\Delta u_{2z}$ .

Below and above the surface at z = 0, we may assume that the flow is uniform. Then we have du/dz = 0. If the densities of the fluids depend only weakly on z, we may ignore  $d\rho/dz$ . Under these conditions Eq. (5.61) is simplified to

$$\frac{\rho}{k}(\omega - ku) \left(\frac{\partial^2}{\partial z^2} - k^2\right) \Delta u_z = 0.$$
(5.62)

This implies

$$f(z) = Ae^{kz} + Be^{-kz}.$$
 (5.63)

For the air,  $\Delta u_{1z}$  must remain finite at  $z \to \infty$ , hence

$$\Delta u_{1z} = B_1 e^{-kz} e^{i(kx - \omega t)}.$$
 (5.64)

For the water we have  $\Delta u_z = 0$  at z = -D, hence

$$\Delta u_{2z} = A_2 \left( e^{kz} - e^{-2kD} e^{-kz} \right) e^{i(kx - \omega t)}.$$
 (5.65)

In addition to these boundary conditions, the deviation of a small patch of the air-water interface from its equilibrium position at z = 0, which we denote by  $\Delta z$ , must be the same for both sides. Let us assume  $\Delta z \propto e^{i(kx-\omega t)}$ . On the air side we have

$$\frac{d\Delta z}{dt} = \left(\frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla\right) \Delta z = -i(\omega - ku_1)\Delta z = \Delta u_{1z}.$$
(5.66)

On the water side we have

$$\frac{d\Delta z}{dt} = \left(\frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla\right) \Delta z = -i(\omega - ku_2) \Delta z = \Delta u_{2z}.$$
(5.67)

Therefore the consistency of the air-water interface implies

$$\frac{\Delta u_{1z}}{\omega - ku_1} = \frac{\Delta u_{2z}}{\omega - ku_2} \tag{5.68}$$

### 5.5. WAVES ON WATER SURFACE

at z = 0. With this relation we may rewrite Eqs. (5.66) and (5.67) as

$$\Delta u_{1z} = C(\omega - ku_1)e^{-kz}e^{i(kx-\omega t)}.$$
(5.69)

$$\Delta u_{2z} = C(\omega - ku_2) \left(\frac{e^{kz} - e^{-2kD}e^{-kz}}{1 - e^{-2kD}}\right) e^{i(kx - \omega t)}.$$
 (5.70)

To obtain the dispersion relation ( $\omega$  as a function of k), we may integrate Eq. (5.61) from  $z = 0^-$  to  $z = 0^+$  with the condition du/dz = 0.

$$\left[\frac{\rho}{k}(\omega - ku)\frac{\partial\Delta u_z}{\partial z} + \rho\Delta u_z\frac{du}{dz}\right]\Big|_{z=0^-}^{z=0^+}$$
$$= \int_{0^-}^{0^+} k\rho(\omega - ku)\Delta u_z\,dz + \left(\frac{\Delta u_z}{\omega - ku}\right)_{z=0}kg\rho\Big|_{z=0^-}^{z=0^+}.$$
 (5.71)

The second term on the left-hand side and the first term on the right-hand side are zero. The result is

$$\rho_1(\omega - ku_1)^2 + \rho_2 \coth(kD)(\omega - ku_2)^2 = kg(\rho_2 - \rho_1).$$
 (5.72)

Since the density of air is much smaller than the density of water, we may drop terms involving  $\rho_1$ . In the special case  $u_2 = 0$  we have

$$\omega^2 = kg \tanh(kD). \tag{5.73}$$

For a tidal wave the wavelength is much larger than the depth. Then we have  $kD \ll 1$ , and Eq. (5.73) becomes  $\omega = k\sqrt{gD}$ . The velocity of the tidal wave is  $\sqrt{gD}$ . Near the shore line where the depth is about 10 m, the wave travels at 10 m/s or 36 km/hr. At deep seas (D = 1000 m) the wave can travel at 360 km/hr, which is the speed of an airplane! That is why we have only a short warning time after a tsunami is triggered by an earth quake. The tidal wave propagates without dispersion until it approaches the shore line, where the depth gradient makes the rear part of the wave move faster than the front part. As a result, the wave can pile up many times higher than it is on the open sea. This is why tsunamis are rarely dangerous to ships on the sea, but can cause severe damage to the shore.

Eq. (5.73) also provide a clue on the speed of vessels that displace water to gain buoyancy. As the vessel moves forward with a velocity v, the bow pushes water aside and generate a trailing wave. The wave that has a phase velocity equal to v is excited most efficiently, because the excitation is synchronous

(resonant) to the motion of the vessel. If the wavelength  $\lambda$  is twice of the vessel length L, the stern of the vessel will sink into the trough of the wave generated by the bow. That will force the vessel to climb against the slope of the wave and encounter a large resistance. On the contrary, if  $\lambda = L$  the vessel will cruise at a level position with minimum resistance. Assume the vessel is cruising in deep water, we have  $kD \gg 1$  and Eq. (5.73) becomes

$$\omega^2 = kg, \tag{5.74}$$

which gives

$$\frac{\omega}{k} = \sqrt{\frac{\lambda g}{2\pi}}.\tag{5.75}$$

The conditions  $\lambda = L$  and  $v = \omega/k$  yield

$$v = \sqrt{\frac{Lg}{2\pi}}.$$
(5.76)

For a 100-m vessel this optimal speed is 45 km/hr (24.3 knots).

### 5.6 Kelvin-Helmholtz Instability

We know that waves on water surface can be created by wind. However, it is not obvious how the air that moves parallel to the water surface can cause waves. After all, the parallel wind does not apparently exert any force to disturb the surface. In order to understand this phenomenon, let us consider two layers of fluids. The upper layer is the wind, moving with a constant velocity  $u_1$  in the x-direction. The lower layer is the water, moving with a constant velocity  $u_2$  also in the x-direction. We shall see that if there is a small perturbation on the air-water interface at z = 0, under suitable conditions the perturbation will grow. This is known as the **Kelvin-Helmholtz instability**.

We may start from Eq. (5.72) with  $u_1 \neq u_2$  and  $D \rightarrow \infty$ .

$$\rho_1(\omega - ku_1)^2 + \rho_2(\omega - ku_2)^2 = kg(\rho_2 - \rho_1).$$
(5.77)

Solving for  $\omega$ , we have

$$\omega = k(\alpha_1 u_1 + \alpha_2 u_2) \pm \sqrt{-k^2 \alpha_1 \alpha_2 (u_1 - u_2)^2 + kg(\alpha_2 - \alpha_1)}, \qquad (5.78)$$

where

$$\alpha_1 = \frac{\rho_1}{\rho_1 + \rho_2}, \quad \alpha_2 = \frac{\rho_2}{\rho_1 + \rho_2}.$$
(5.79)

If  $\omega$  has an imaginary part,  $u_{1z}$  and  $u_{2z}$  which are proportional to  $e^{i(kx-\omega t)}$  will grow exponentially with time from an arbitrarily small initial perturbation. This occurs when

$$-k^2 \alpha_1 \alpha_2 (u_1 - u_2)^2 + kg(\alpha_2 - \alpha_1) < 0.$$
(5.80)

That is

$$k > \frac{g(\alpha_2 - \alpha_1)}{\alpha_1 \alpha_2 (u_1 - u_2)^2}.$$
(5.81)

Eq. (5.81) explains why low speed wind will only excite ripples of short wavelength. It is interesting to know that even if the two fluids are identical  $(\alpha_1 = \alpha_2)$ , the Kelvin-Helmholtz instability still exists. The instability can be suppressed by viscosity when the velocity difference is small. That is why adding soluble polymers to water circulation systems can increase pump efficiency by suppressing instabilities that cost energy.

## 5.7 The Reynolds number

In a system governed by the Navier-Stokes equation, instabilities that lead to turbulence may occur because the term  $(\mathbf{u} \cdot \nabla)\mathbf{u}$  is highly nonlinear. The instabilities can be suppressed by the diffusive term  $\mu \nabla^2 \mathbf{u}$  which tends to smooth out the spatial variation of  $\mathbf{u}$ . The crucial point is how large  $\mu$  is, comparing with other parameters of the system. In Section 4.5 we have seen that the range of action for diffusion within time t is on the order of  $\sqrt{Dt}$ . Hence for diffusion to be effective in smoothing out the spatial variation of density,  $\sqrt{Dt}$  must be comparable to the length scale  $l_0$  of the system. Let us write the Navier-Stokes equation in the following form,

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} = -\frac{\nabla P}{\rho_m} + \frac{\mu}{\rho_m} \nabla^2 \mathbf{u} + \mathbf{F}$$
(5.82)

where  $\rho_m$  is the mass density. By analogy, for viscosity to be effective in smoothing out the spatial variation of  $\mathbf{u}$ ,  $\sqrt{\mu t/\rho_m}$  must be comparable to  $l_0$ . If the velocity scale of the system is  $u_0$ , then the time scale of the system is

 $l_0/u_0$ . Thus it is reasonable to imagine that under the following condition, viscosity is likely to suppress instabilities.

$$\sqrt{\frac{\mu l_0}{\rho_m u_0}} \approx l_0. \tag{5.83}$$

In a dimensionless form, this condition is equivalent to

$$\frac{1}{R} \equiv \frac{\mu}{\rho_m u_0 l_0} \approx 1,\tag{5.84}$$

where R is known as the **Reynolds number**. Instabilities occur usually when R exceeds a few thousands.

### 5.8. EXERCISES

### 5.8 Exercises

**Exercise 5.1.** Consider a tube filled with an ideal gas and placed in an environment of 1 atm. One side of the tube is sealed, and the other side is a piston that can move freely. If the piston moves inwards the air in the tube is compressed. In this case the pressure will be larger than 1 atm, and a pressure difference is built up that works against the piston movement. On the contrary, if the piston moves outwards the air in the tube is diluted. In this case the pressure drops below 1 atm, and again a pressure difference is built up against the piston movement. If the range of the piston movement is small, this is an analogy of a spring. (From the view point of Taylor expansion, as long as the derivative of the restoring force with respect to the displacement is not zero, any small oscillation can be treated as simple harmonic oscillation.) Assume the mass of the piston is 1 kg, and the cross section is  $10 \text{ cm}^2$ . At equilibrium the distance between the piston and the sealed end is 1 m, and the air temperature is 25 °C. What is the resonance frequency of this air-spring? Hint: the thermal conductivity of air is poor, therefore in the time scale of the piston movement, the gas in the tube should be treated as adiabatic expansion or compression.

**Exercise 5.2.** A round concentric pipe is used to transport water. Water flows between the inner tube and the outer tube under pressure. The radius of the outer surface of the inner tube is  $r_1$  and the radius of the inner surface of the outer tube is  $r_2$ . Derive a formula that describes the water flux as a function of the pressure difference  $\Delta P$  between the two ends of the pipe,  $r_1$  and  $r_2$ , and the viscosity of water  $\mu$ .

**Exercise 5.3.** A cart on a railway track carries a water tank. The tank is drained by a horizontal pipe shown in Fig. 5.1. As the water is being drained, Peter thinks the cart will move to the left, because due to the viscosity of water, the pipe will be dragged by the water which is moving to the left. But Paul does not agree. He thinks the right end of the pipe is under a higher pressure than the left end. After all, and the water flow is driven by this pressure difference. Because of the pressure difference, the cart will move to the right. Who is correct? Does the cart continue to move after the tank becomes empty? Can you calculate the speed of the cart as a function of time? The mass of the cart is M, the initial height of the water in the tank is h, the diameter of the tank is D, the radius of the pipe is R, the length of the pipe is L, and the viscosity is  $\mu$ . We assume  $R \ll D$  so that the flow speed in the tank is negligible comparing with that in the pipe.



Fig. 5.1: Draining a tank.



Fig. 5.2: A balloon attached to an accelerating boxcar by a thread.

**Exercise 5.4.** A uniform solid plastic ball of density  $0.5 \text{ g/cm}^3$  is floating on the surface of a water tank. Assume water is incompressible. If the atmosphere pressure is increased at a constant temperature, the volume of the ball submerged in the water (1) increases, (2) decreases, (3) does not change. Choose your answer and explain why.

**Exercise 5.5.** A sealed boxcar is gliding down a slope with acceleration  $a = g \sin \theta$  as shown in Fig. 5.2, where g is the free-fall acceleration at the surface of the Earth and  $\theta$  is the angle of the slope. A balloon filled with helium is attached to the floor by a thin thread. What is the angle  $\phi$  between the thread and the normal vector of the floor? You may not need the following data. But we provide them anyway in case you complain. The density of the air is 1.143 g/l. The density of helium in the balloon is 0.18 g/l. The volume of the balloon is 10 l, and the weight of the balloon when empty is 4 g.

**Exercise 5.6.** An hourglass is made by welding the tips of two cone-shaped glass bottle together. The full angle of the cone is  $30^{\circ}$  and the height of each cone is 10 cm. The neck connecting the two bottles has an inner diameter



Fig. 5.3: Mechanical coupling by viscous fluid.

of 2 mm. The lower bottle is filled with tiny teflon balls whose diameter is much smaller than 2 mm. Now we flip the hourglass. How long does it take for 7/8 of the teflon balls to flow into the lower bottle? In this problem we assume the teflon balls collectively behave like an incompressible fluid, and the gap between the balls allows air to pass from the lower bottle to the upper bottle. We also assume the teflon balls are slippery enough so that the surface of the "fluid" remains flat all the time.

**Exercise 5.7.** Consider a shaft of radius r positioned at the center of a rotating tube of length l as shown in Fig. 5.3. The inner radius of the tube is R, and the angular velocity of the tube is  $\omega$ . A viscous fluid of viscosity  $\mu$  is sealed in the space between the shaft and the tube. To prevent the shaft from rotating together with the tube, how much toque must be applied to the shaft? In this exercise we ignore the viscous force from the end caps of the tube.

**Exercise 5.8.** It is well-known that the gravitational force from the Moon is the major cause of the tidal wave observed twice a day. However, because the Earth is spinning and the tidal wave can only propagate with a finite speed, the tidal wave is not synchronized with the motion of the Moon. Assume the Moon moves circularly in the equatorial plane of the Earth, and assume there is no land on the surface of the Earth to interfere with the tidal-wave propagation. If the wave length of the tidal wave is much larger than the depth of the sea, how deep the sea must be for the tidal wave to synchronize with the motion of the Moon? In this exercise we assume the curvature of the Earth's surface is negligibly small.

# Chapter 6

# Electrostatics

# 6.1 Gauss' Law

From Coulomb's law, the electric field at  ${\bf r}$  produced by a charge density distribution  $\rho({\bf r}')$  is

$$\mathbf{E}(\mathbf{r}) = \frac{1}{4\pi\epsilon_0} \int \rho(\mathbf{r}') \frac{\mathbf{r} - \mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|^3} d^3 \mathbf{r}', \qquad (6.1)$$

and the force acted on a charge density distribution by an external electric field is

$$\mathbf{F} = \int \rho(\mathbf{r}) \mathbf{E}(\mathbf{r}) \, d^3 \mathbf{r}. \tag{6.2}$$

Since

$$\nabla \frac{1}{|\mathbf{r} - \mathbf{r}'|} = -\frac{\mathbf{r} - \mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|^3},\tag{6.3}$$

Eq. (6.1) can also be written as

$$\mathbf{E}(\mathbf{r}) = -\frac{1}{4\pi\epsilon_0} \nabla \int \frac{\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d^3 \mathbf{r}' = -\nabla \phi(\mathbf{r}), \qquad (6.4)$$

where

$$\phi(\mathbf{r}) = \frac{1}{4\pi\epsilon_0} \int \frac{\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d^3 \mathbf{r}'$$
(6.5)

is the electric potential. Mathematically Eq. (6.1) or (6.5) are not convenient to use because they involve integration all over the space. Moreover, if the charge distribution changes with time, because the electric field cannot change instantly with the motion of the charges, the change of the electric field will be delayed by  $|\mathbf{r} - \mathbf{r}'|/c$ . Namely,

$$\mathbf{E}(\mathbf{r},t) = \frac{1}{4\pi\epsilon_0} \int \rho(\mathbf{r}',t') \frac{\mathbf{r} - \mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|^3} d^3 \mathbf{r}', \tag{6.6}$$

where  $t' = t - |\mathbf{r} - \mathbf{r}'|/c$ . This further complicates the calculation. It turns out that the  $1/r^2$  dependence on the Coulomb force allows us to write a much simpler mathematical equation for the electric field, which is known as the **Gauss' law**.

Let us start by calculating the divergence of the electric field  $\mathbf{E}_p$  produced by a single point charge q. From Eq. (1.343), it can be readily seen that

$$\nabla \cdot \frac{\mathbf{r}}{|\mathbf{r}|^3} = 0, \tag{6.7}$$

everywhere except at  $\mathbf{r} = 0$ , where the equation is undefined, therefore  $\nabla \cdot \mathbf{E}_p = 0$  except at  $\mathbf{r} = 0$ . Consider the surface integral

$$\int_{S} \mathbf{E}_{p} \cdot d\mathbf{a},$$

where S is an arbitrary surface enclosing the charge. Imagine cutting the volume enclosed by S into two parts  $V_1$  and  $V_2$ . The first part  $V_1$  contains the charge, and the second part  $V_2$  does not. The surface S is also divided correspondingly into two surfaces  $S_1$  and  $S_2$ . Let us denote H the interface surface between  $V_1$  and  $V_2$ , then  $S_1 + H$  encloses  $V_1$  and  $S_2 + H$  encloses  $V_2$ . We have

$$\int_{S} \mathbf{E}_{p} \cdot d\mathbf{a} = \int_{S_{1}+H} \mathbf{E}_{p} \cdot d\mathbf{a} + \int_{S_{2}+H} \mathbf{E}_{p} \cdot d\mathbf{a}, \qquad (6.8)$$

because the surface integral at H cancels. Because  $\nabla \cdot \mathbf{E}_p = 0$  everywhere in  $V_2$ , by Gauss' theorem Eq. (1.322) the second term on the right-hand side of Eq. (6.8) is zero. Hence we have

$$\int_{S} \mathbf{E}_{p} \cdot d\mathbf{a} = \int_{S_{1}+H} \mathbf{E}_{p} \cdot d\mathbf{a}, \tag{6.9}$$

This means we can deform the surface S successively to a small sphere around the charge without changing the surface integral. Namely

$$\int_{S} \mathbf{E}_{p} \cdot d\mathbf{a} = \int_{\sigma} \mathbf{E}_{p} \cdot d\mathbf{a}, \qquad (6.10)$$

### 6.1. GAUSS' LAW

where  $\sigma$  represents a sphere of radius r in which the charge sits at the center. But

$$\int_{\sigma} \mathbf{E}_p \cdot d\mathbf{a} = \frac{q}{\epsilon_0},\tag{6.11}$$

hence

$$\int_{S} \mathbf{E}_{p} \cdot d\mathbf{a} = \frac{q}{\epsilon_{0}},\tag{6.12}$$

for any surface enclosing the charge.

Now consider a group of charges enclosed by S. Since the field **E** produced by a group of charges is the superposition of that produced by each individual charge, we have

$$\int_{S} \mathbf{E} \cdot d\mathbf{a} = \frac{1}{\epsilon_0} \int_{V} \rho(\mathbf{r}) d^3 \mathbf{r}.$$
(6.13)

This is the integral form of the Gauss' law. Using Gauss' theorem, we have

$$\int_{V} \nabla \cdot \mathbf{E} \, d^{3}\mathbf{r} = \int_{S} \mathbf{E} \cdot d\mathbf{a} = \frac{1}{\epsilon_{0}} \int_{V} \rho(\mathbf{r}) \, d^{3}\mathbf{r}.$$
(6.14)

Since V can be an arbitrarily small region, we have

$$\nabla \cdot \mathbf{E} = \frac{\rho}{\epsilon_0}.\tag{6.15}$$

This is the differential form of the Gauss' law. In terms of the electric potential, Gauss' law is written as

$$-\nabla^2 \phi = \frac{\rho}{\epsilon_0}.\tag{6.16}$$

Using Gauss' law, we can prove the shell theorems easily. Let us consider a sphere of uniform charge density. The radius of the sphere is R, and the total charge on the sphere is q. Let us choose the center of the sphere to be the origin. By symmetry at position  $\mathbf{r}$  the field is in the direction of  $\mathbf{r}$  and only a function of r. If r > R,

$$\int_{S} \mathbf{E} \cdot d\mathbf{a} = E(r) 4\pi r^{2} = \frac{q}{\epsilon_{0}},$$
(6.17)

where S is a sphere centered at the origin with radius r. In other words

$$E(r) = \frac{1}{4\pi\epsilon_0} \frac{q}{r^2}.$$
(6.18)

This is the same as the case in which all the charge is put at the origin. In contrast, if r < R there is no charge enclosed in the surface, hence E(r) = 0.

We can use Gauss' law to calculate the electric field produced by charge distributions that have high symmetries. For example, for charges uniformly distributed on a infinite long line along the z-axis, by symmetry the electric field is in the horizontal radial direction and is a function of r only. Let us choose the surface of integration to be that of a cylinder along the z-axis, with radius r and length L. Gauss' law yields

$$E(r)2\pi rL = \frac{\rho_l L}{\epsilon_0},\tag{6.19}$$

where  $\rho_l$  is the line charge density. Hence

$$E(r) = \frac{\rho_l}{2\pi\epsilon_0 r}.$$
(6.20)

Similarly, one can prove that the electric field produced by charges on a infinitely extended sheet is a constant. Again, by symmetry the electric field is normal to the sheet and is only a function of the distance d to the sheet. By choosing the surface of integration to be that of a rectangular box enclosing a rectangular area A of the sheet, Gauss' law yields

$$E(d)2A = \frac{\rho_s A}{\epsilon_0},\tag{6.21}$$

where  $\rho_s$  is the line charge density. Therefore

$$E(d) = \frac{\rho_s}{2\epsilon_0},\tag{6.22}$$

which is a constant.

## 6.2 Electric Dipole

The simplest charge distribution beyond a single point charge or an uniform distribution is the electric dipole. An electric dipole is formed by two charges of opposite signs separated by a small distance. The electric field produced by an electric dipole at the origin is

$$\mathbf{E}(\mathbf{r}) = -\frac{q}{4\pi\epsilon_0} \nabla \left[ \frac{1}{|\mathbf{r} - \mathbf{d}/2|} - \frac{1}{|\mathbf{r} + \mathbf{d}/2|} \right].$$
 (6.23)

### 6.2. Electric Dipole

Consider the Taylor expansion of  $1/|\mathbf{r} - \mathbf{r}'|$  around  $\mathbf{r}$  for the case  $|\mathbf{r}'| \ll |\mathbf{r}|$ .

$$\frac{1}{|\mathbf{r} - \mathbf{r}'|} = \frac{1}{r} + \nabla \left(\frac{1}{r}\right) \cdot (-\mathbf{r}') + \dots$$
$$= \frac{1}{r} + \frac{\mathbf{r} \cdot \mathbf{r}'}{r^3} + \dots$$
(6.24)

At a distance r much larger than d, the first term of the Taylor expansion of Eq. (6.23) is

$$\mathbf{E}(\mathbf{r}) = -\frac{1}{4\pi\epsilon_0} \nabla \left( \mathbf{p} \cdot \frac{\mathbf{r}}{r^3} \right), \tag{6.25}$$

where  $\mathbf{p} = q\mathbf{d}$  is called the electric dipole moment. For a charge distribution centered around the origin, the definition of the dipole moment can be generalized to

$$\mathbf{p} \equiv \int \mathbf{r}' \rho(\mathbf{r}') \, d^3 \mathbf{r}'. \tag{6.26}$$

Applying Eq. (6.24) to Eq. (6.5), we have

$$\phi(\mathbf{r}) = \frac{1}{4\pi\epsilon_0} \left[ \frac{1}{r} \int \rho(\mathbf{r}') d^3 \mathbf{r}' + \frac{\mathbf{r}}{r^3} \cdot \int \mathbf{r}' \rho(\mathbf{r}') d^3 \mathbf{r}' + \dots \right]$$
$$= \frac{1}{4\pi\epsilon_0} \left( \frac{q}{r} + \mathbf{p} \cdot \frac{\mathbf{r}}{r^3} + \dots \right).$$
(6.27)

The first term on the right-hand side is the monopole potential, and the second term is the dipole potential, which agrees with Eq. (6.25). For **p** in the z-direction, Eqs. (6.25) and (1.339) gives

$$\mathbf{E}(\mathbf{r}) = -\frac{1}{4\pi\epsilon_0} \left( \frac{\partial}{\partial r} \hat{\mathbf{r}} + \frac{1}{r} \frac{\partial}{\partial \theta} \hat{\theta} \right) \left( \frac{p\cos\theta}{r^2} \right), \tag{6.28}$$

hence

$$E_{r}(\mathbf{r}) = \frac{1}{4\pi\epsilon_{0}} \frac{2p\cos\theta}{r^{3}},$$
  

$$E_{\theta}(\mathbf{r}) = \frac{1}{4\pi\epsilon_{0}} \frac{p\sin\theta}{r^{3}},$$
  

$$E_{\phi}(\mathbf{r}) = 0.$$
(6.29)

Consider a static charge distribution centered around the origin in an external field. If the length scale of variation of the external field is much

larger than the size of the charge distribution, the force experienced by the charge distribution is

$$F_i = \int \rho(\mathbf{r}) E_i(\mathbf{r}) \, d^3 \mathbf{r} \approx \int \rho(\mathbf{r}) \left[ E_i(0) + \frac{\partial E_i}{\partial r_j} r_j \right] \, d^3 \mathbf{r}.$$
(6.30)

If the net charge is zero, the term involving  $E_i(0)$  is zero, and the term involving  $\partial E_i/\partial r_j$  is the dipole force.

$$F_i = \frac{\partial E_i}{\partial r_j} p_j,\tag{6.31}$$

or

$$\mathbf{F} = (\mathbf{p} \cdot \nabla) \mathbf{E}. \tag{6.32}$$

Using the vector identity

$$\nabla(\mathbf{a} \cdot \mathbf{b}) = (\mathbf{a} \cdot \nabla)\mathbf{b} + (\mathbf{b} \cdot \nabla)\mathbf{a} + \mathbf{a} \times (\nabla \times \mathbf{b}) + \mathbf{b} \times (\nabla \times \mathbf{a})$$
(6.33)

and noting that **p** is a constant vector and  $\nabla \times \mathbf{E} = -\nabla \times \nabla \phi = 0$ , we have

$$\mathbf{F} = \nabla(\mathbf{p} \cdot \mathbf{E}). \tag{6.34}$$

The potential energy stored in the dipole is

$$U = -\int \mathbf{F} \cdot d\mathbf{s} = -\int \nabla (\mathbf{p} \cdot \mathbf{E}) \cdot d\mathbf{s} = -\mathbf{p} \cdot \mathbf{E}.$$
 (6.35)

The torque experienced by the charge distribution is

$$\boldsymbol{\tau} = \int \rho(\mathbf{r})\mathbf{r} \times \mathbf{E}(\mathbf{r}) \, d^3 \mathbf{r} \approx \int \rho(\mathbf{r})\mathbf{r} \times \mathbf{E}(0) \, d^3 \mathbf{r} = \mathbf{p} \times \mathbf{E}.$$
(6.36)

### 6.3 Electric Polarization

Some molecules have a permanent dipole moment. They are called polar molecules. Under an external field polar molecules will rotate until the dipole moment is parallel to the field. For nonpolar molecules, the charge distribution can be deformed by the external field, such that the positive charge moves in the direction of the field and the negative charge moves in the opposite direction. If the medium does not conduct electricity, the movement will not continue, because after all the electrons cannot leave the atoms. But still,

### 6.3. Electric Polarization

the slight deformation will create a dipole moment again parallel to the field. Such dipoles are called induced dipoles. For a nonconducting medium let us define the electric polarization  $\mathbf{P}$  to be the dipole moment per unit volume. From Eq. (6.25) it is seen that the electric polarization also contributes to the electric potential. Namely,

$$\phi(\mathbf{r}) = \frac{1}{4\pi\epsilon_0} \int \left[ \frac{\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} + \mathbf{P}(\mathbf{r}') \cdot \frac{\mathbf{r} - \mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|^3} \right] d^3\mathbf{r}'$$
$$= \frac{1}{4\pi\epsilon_0} \int \left[ \frac{\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} + \mathbf{P}(\mathbf{r}') \cdot \nabla' \frac{1}{|\mathbf{r} - \mathbf{r}'|} \right] d^3\mathbf{r}'.$$
(6.37)

Assuming  $\mathbf{P} = 0$  at the boundary in the infinity, integration by parts gives

$$\phi(\mathbf{r}) = \frac{1}{4\pi\epsilon_0} \int \left[ \frac{\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} - \frac{\nabla' \cdot \mathbf{P}(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \right] d^3\mathbf{r}'.$$
(6.38)

This is the potential produced by the charge distribution  $\rho - \nabla \cdot \mathbf{P}$ . Therefore, in a polarizable medium Gauss' law becomes

$$\nabla \cdot \mathbf{E} = \frac{1}{\epsilon_0} \left( \rho - \nabla \cdot \mathbf{P} \right). \tag{6.39}$$

The electric displacement  $\mathbf{D}$  is defined by

$$\mathbf{D} = \epsilon_0 \mathbf{E} + \mathbf{P}.\tag{6.40}$$

We have

$$\nabla \cdot \mathbf{D} = \rho. \tag{6.41}$$

In the linear regime the induced dipole moment is proportional to the external field, hence we may define  $\chi_e$  such that

$$\mathbf{P} = \epsilon_0 \chi_e \mathbf{E},\tag{6.42}$$

where  $\chi_e$  is called the electric susceptibility. In this case **D** is proportional to **E**. The electric permittivity  $\epsilon$  is defined by the following relation

$$\mathbf{D} = \epsilon \mathbf{E},\tag{6.43}$$

where

$$\kappa_e \equiv \frac{\epsilon}{\epsilon_0} = 1 + \chi_e \tag{6.44}$$

is called the dielectric constant or the relative electric permittivity. Substituting Eq. (6.43) into Eq. (6.41), one obtains

$$\nabla \cdot \mathbf{E} = \frac{\rho}{\kappa_e \epsilon_0},\tag{6.45}$$

or equivalently

$$\int_{S} \mathbf{E} \cdot d\mathbf{a} = \frac{1}{\epsilon} \int_{V} \rho(\mathbf{r}) d^{3}\mathbf{r} = \frac{q}{\kappa_{e}\epsilon_{0}}.$$
(6.46)

### 6.4 Capacitors

A capacitor is usually made of two narrowly spaced metal films, with a thin layer of dielectric material sandwiched in between. Charges of opposite signs can be stored temporally on the two films without neutralizing each other. Due to the attractive force between the charges on the two films and the repulsive force between charges on the same film, the larger the film and the thinner the layer between them, the easier charges can be stored.

Let us model a capacitor by two infinitely large parallel plates with a small gap between them. One surface is uniformly charged to +q and the other to -q. On both sides of the capacitor, because the electric field produced by a uniformly charged sheet is a constant, the field produced by two uniformly charged sheets of opposite sign is zero. Hence E = 0 everywhere except between the gap. To evaluate E between the gap, let us choose a rectangular box that encloses a rectangular area A of only one sheet. Then the only surface on which E is nonzero is the surface between the gap. Gauss' law yields

$$EA = \frac{\rho_s A}{\epsilon_0},\tag{6.47}$$

hence between the gap E is a constant. The voltage difference between the plates is simply V = Ed, and the charge is simply  $q = \rho_s A$ . The capacitance C is defined by

$$C = \frac{q}{V},\tag{6.48}$$

hence

$$C = \frac{\epsilon_0 A}{d}.\tag{6.49}$$

#### 6.4. CAPACITORS

Next we consider a capacitor made of two concentric cylinders with a dielectric medium filling between them. The outer cylinder is charged to +q and the inner cylinder is charged to -q. Again the capacitance C is defined by C = q/V where V is the difference of the electrical potential between the two cylinders. By cylindrical symmetry, the electric field has only the radial component. At radius r, we have

$$E_r(r)2\pi rL = \frac{q}{\kappa_e \epsilon_0},\tag{6.50}$$

where L is the length of the cylinders. The potential difference is

$$V = \int_{R_1}^{R_2} E_r(r) \, dr = \frac{q}{2\pi L \kappa_e \epsilon_0} \ln\left(\frac{R_2}{R_1}\right), \tag{6.51}$$

where  $R_1$  and  $R_2$  are the radii of the inner and outer cylinders respectively. Hence

$$C = \frac{2\pi L \kappa_e \epsilon_0}{\ln(R_2/R_1)}.$$
(6.52)

In the limit  $R_2 - R_1 = d$ ,  $d \ll R_1$ ,

$$C = \frac{2\pi L\kappa_e \epsilon_0}{\ln\left(1 + d/R_1\right)} \approx \frac{A\kappa_e \epsilon_0}{d},\tag{6.53}$$

where  $A = 2\pi R_1 L$  is the area of the conducting plate. This is the capacitance of two parallel plates. Note that the capacitance is proportional to  $\kappa_e$ , hence filling the gap with media of large dielectric constants is a common practice in manufacturing capacitors.

When a small amount of charge  $\Delta q$  leaves the capacitor, it carries away a small amount of energy equal to  $V\Delta q$ . The total amount of energy that can be carried away from a capacitor of charge Q is

$$E = \int_{0}^{Q} V(q) dq = \int_{0}^{Q} \frac{Q-q}{C} dq$$
  
=  $\frac{Q^{2}}{2C} = \frac{CV^{2}}{2} = \frac{QV}{2}.$  (6.54)

### 6.5 Exercises

**Exercise 6.1.** 12 resistive wires are employed to construct the frame of a cube. The resistance of each wire is R. If we connect one corner of the cube to the ground and its diagonal corner to a voltage source of voltage V, what is the current that flows out of the voltage source?

**Exercise 6.2.** Write down the electric potential produced by a charge +q at (d, 0, 0) and a charge -q at (-d, 0, 0). Show that the potential is zero on the *y*-*z* plane.

**Exercise 6.3.** An infinitely large plane conductor is placed at the y-z plane. A charged particle carrying charge +q is placed on the x-axis with a distance d from the y-z plane. The charges on the conductor are attracted by the charged particle, therefore they gather around the x-axis. Find the induced surface charge density as a function of the distance from the origin. Note that if you know the electric field normal to the conductor, you can calculate the surface charge density by Gauss' law. Hint: On a conductor the electric potential is a constant. Therefore the induced charge density must arrange itself together with the charged particle at (d, 0, 0) to make the electric potential a constant. Because the conductor plane extends to infinity where the potential is zero, the constant potential must be zero. Therefore the situation is similar to that of Exercise 6.2.

**Exercise 6.4.** Replace the infinitely large plane conductor in Exercise 6.3 by a conducting sphere of radius R at the origin, where R < d. The sphere is connected to the ground so that its potential is zero. Calculate the induced surface charge density on the sphere. Hint: You may try to replace the sphere by a negative charge -q' at (d', 0, 0) to make the electric potential at the sphere equal to zero.

**Exercise 6.5.** Consider the circuit shown in Fig. 6.1. Each capacitor has a capacitance of 1  $\mu$ F, and  $R \gg 1$  k $\Omega$ . In the beginning switches  $S_1$ - $S_6$  are opened, are closed and  $S_7$ - $S_9$  are open. At certain time switches  $S_1$ - $S_6$  are opened, and immediately after that switches  $S_7$ - $S_9$  are closed. What is the output voltage? If we close  $S_{10}$  now, how long does it take for the output voltage to drop to 1/e of its maximum value? A simplified version of the same circuit is shown in Fig. 6.2. Explain in words why the output pulse is practically the same as that in Fig. 6.1 if  $R \gg 1$  k $\Omega$ . (If you can explain by calculation, it will even be better. But explaining in words is already acceptable.)



Fig. 6.1: Maxbank high-voltage pulse generator.



Fig. 6.2: Maxbank high-voltage pulse generator, a simplified version.

**Exercise 6.6.** Two spherical electrodes of radius R separated by a distance d are buried deeply into a conducting material that extends to infinity in all directions. Assume  $R \ll d$ . The conductivity of the material is  $\sigma$ . One electrode is connected to a voltage source of +V and the other electrode is connected to a voltage source of -V. What is the total current that flows between the two electrodes? Use this method to measure the conductivity of distilled water, and compare it with the value on textbooks.

**Exercise 6.7.** A capacitor is made of two parallel conducting plates. Between the plates is a plastic sheet with a dielectric constant  $\kappa_e > 1$ . If the capacitor is charged by a battery and then disconnected, show that by removing the plastic sheet, the energy stored in the capacitor is increased. Where does the extra energy come from? In contrast, if the capacitor remains connected to the battery after it is charged, show that by removing the plastic sheet, the energy stored in the capacitor is decreased. Where does the energy go?

**Exercise 6.8.** In a conductor charges can move freely to form a steady-state distribution  $\rho_s(\mathbf{r})$ . At t = 0 if we set up a charge distribution  $\rho(\mathbf{r}, 0)$  which is different from  $\rho_s(\mathbf{r})$ , the charge distribution will evolve into  $\rho_s(\mathbf{r})$  after a

while. Show that

$$\rho(\mathbf{r},t) = \rho_s(\mathbf{r}) + [\rho(\mathbf{r},0) - \rho_s(\mathbf{r})]e^{-\lambda t}.$$

where  $\lambda$  is related to the conductivity  $\sigma$  of the conductor. What is  $\lambda$ ? In this exercise we assume the current associated with the change of charge distribution is small enough such that the effect of inductance is negligible.

**Exercise 6.9.** In experimental physics it is important to confine the motion of ions in a small space in order to make the interaction time long enough. Show that it is impossible to make an ion trap by using only static electric field.

# Chapter 7

# Magnetostatics

# 7.1 Ampere's Law

In 1819 Oersted observed that magnetic flux can be produced by electric currents. This was an important discovery, because it established the relation between electricity and magnetism, which appeared as two different phenomena before. By the experimental works of Biot and Savart, and later that of Ampere, it was established that the magnetic-flux density **B** produced by a current density distribution **J** can be written as

$$\mathbf{B}(\mathbf{r}) = \frac{\mu_0}{4\pi} \int \mathbf{J}(\mathbf{r}') \times \frac{\mathbf{r} - \mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|^3} d^3 \mathbf{r}', \tag{7.1}$$

and the force acted on a current density distribution by an external magnetic-flux density is

$$\mathbf{F} = \int \mathbf{J}(\mathbf{r}) \times \mathbf{B}(\mathbf{r}) \, d^3 \mathbf{r}.$$
(7.2)

Since

$$\nabla \frac{1}{|\mathbf{r} - \mathbf{r}'|} = -\frac{\mathbf{r} - \mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|^3},\tag{7.3}$$

from the vector identity

$$\nabla \times (\psi \mathbf{a}) = \nabla \psi \times \mathbf{a} + \psi \nabla \times \mathbf{a}, \tag{7.4}$$

Eq. (7.1) can be transformed into

$$\mathbf{B}(\mathbf{r}) = \nabla \times \frac{\mu_0}{4\pi} \int \frac{\mathbf{J}(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d^3 \mathbf{r}' - \frac{\mu_0}{4\pi} \int \frac{\nabla \times \mathbf{J}(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d^3 \mathbf{r}'.$$
 (7.5)

The second term on the right-hand side is zero because  $\mathbf{J}(\mathbf{r}')$  does not depend on  $\mathbf{r}$ . It then follows that

$$\nabla \cdot \mathbf{B} = 0, \tag{7.6}$$

because  $\nabla \cdot (\nabla \times \mathbf{F}) = 0$  for any vector field  $\mathbf{F}$ . Eq. (7.6) is consistent with the fact that no magnetic charge has ever been found.

Similar to the transformation from Eq. (6.1) to Eq. (6.15), Eq. (7.1) can be reduced to a much simpler form. By taking the curl of Eq. (7.1) and using the vector identity

$$\nabla \times (\mathbf{a} \times \mathbf{b}) = \mathbf{a}(\nabla \cdot \mathbf{b}) - \mathbf{b}(\nabla \cdot \mathbf{a}) + (\mathbf{b} \cdot \nabla)\mathbf{a} - (\mathbf{a} \cdot \nabla)\mathbf{b}, \quad (7.7)$$

we have

$$\nabla \times \mathbf{B}(\mathbf{r}) = \frac{\mu_0}{4\pi} \int \mathbf{J}(\mathbf{r}') \nabla \cdot \frac{\mathbf{r} - \mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|^3} d^3 \mathbf{r}' - \frac{\mu_0}{4\pi} \int [\mathbf{J}(\mathbf{r}') \cdot \nabla] \frac{\mathbf{r} - \mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|^3} d^3 \mathbf{r}'.$$
(7.8)

For the first term on the right-hand side of Eq. (7.8), since

$$\nabla \cdot \frac{\mathbf{r} - \mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|^3} = 0 \tag{7.9}$$

except at  $\mathbf{r} = \mathbf{r}'$ , we may reduce the integration region to a small sphere  $\sigma$  around  $\mathbf{r}$  without changing value of the integral.

$$\int \mathbf{J}(\mathbf{r}')\nabla \cdot \frac{\mathbf{r} - \mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|^3} d^3 \mathbf{r}' = \int_{\sigma} \mathbf{J}(\mathbf{r}')\nabla \cdot \frac{\mathbf{r} - \mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|^3} d^3 \mathbf{r}'.$$
 (7.10)

In the limit where the radius of  $\sigma$  approaches zero, we have

$$\int_{\sigma} \mathbf{J}(\mathbf{r}') \nabla \cdot \frac{\mathbf{r} - \mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|^3} d^3 \mathbf{r}' = \mathbf{J}(\mathbf{r}) \int_{\sigma} \nabla \cdot \frac{\mathbf{r} - \mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|^3} d^3 \mathbf{r}' = 4\pi \mathbf{J}(\mathbf{r}), \quad (7.11)$$

where we obtain the second equality by Gauss' theorem. For the second term on the right-hand side of Eq. (7.8), we note that

$$-\int \left[\mathbf{J}(\mathbf{r}') \cdot \nabla\right] \frac{\mathbf{r} - \mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|^3} d^3 \mathbf{r}'$$
  
=  $\nabla \int \left[\mathbf{J}(\mathbf{r}') \cdot \nabla\right] \frac{1}{|\mathbf{r} - \mathbf{r}'|} d^3 \mathbf{r}'$   
=  $\nabla \int \mathbf{J}(\mathbf{r}') \cdot \nabla \frac{1}{|\mathbf{r} - \mathbf{r}'|} d^3 \mathbf{r}'.$  (7.12)

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### 7.1. Ampere's Law

Because

$$\nabla \frac{1}{|\mathbf{r} - \mathbf{r}'|} = -\nabla' \frac{1}{|\mathbf{r} - \mathbf{r}'|},\tag{7.13}$$

where  $\nabla'$  means differentiation with respect to  $\mathbf{r}'$ , we have

$$\nabla \int \mathbf{J}(\mathbf{r}') \cdot \nabla \frac{1}{|\mathbf{r} - \mathbf{r}'|} d^{3}\mathbf{r}'$$

$$= \nabla \int \mathbf{J}(\mathbf{r}') \cdot (-\nabla') \frac{1}{|\mathbf{r} - \mathbf{r}'|} d^{3}\mathbf{r}'$$

$$= \nabla \int \left[ -\nabla' \cdot \frac{\mathbf{J}(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} + \frac{\nabla' \cdot \mathbf{J}(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \right] d^{3}\mathbf{r}'$$

$$= \nabla \left[ -\int_{S} \frac{\mathbf{J}(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \cdot d\mathbf{a} + \int \frac{\nabla' \cdot \mathbf{J}(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d^{3}\mathbf{r}' \right]. \quad (7.14)$$

Assuming that there is no current at the boundary surface in the infinity, the first term on the right-hand side is zero. By the continuity equation  $\nabla' \cdot \mathbf{J} = -\partial \rho / \partial t$ , we have  $\nabla' \cdot \mathbf{J} = 0$  in the static case. Hence the second term on the right-hand side is also zero. Back to Eq. (7.8), we have

$$\nabla \times \mathbf{B} = \mu_0 \mathbf{J}.\tag{7.15}$$

This is known as **Ampere's law**. Its integral form is, according to Stokes's theorem,

$$\oint \mathbf{B} \cdot d\mathbf{l} = \mu_0 \int_S \mathbf{J} \cdot d\mathbf{a}.$$
(7.16)

One may use Ampere's law to calculate the magnetic flux density produced by current distributions of high symmetry. Let us consider the magnetic flux density produced by a current I on a infinitely long wire along the z-axis. At a distance r from the wire, by Eq. (7.1) we see that **B** is perpendicular to both the wire and **r**. Hence **B** has only the azimuthal component. Choosing the loop of integration to be a circle around the wire, Ampere's law yields

$$B_{\theta}2\pi r = \mu_0 I, \tag{7.17}$$

hence

$$B_{\theta} = \frac{\mu_0 I}{2\pi r}.\tag{7.18}$$

Similarly, let us consider the magnetic flux density produced by a infinitely large sheet of current distribution. Assuming the sheet is on the y-zplane with the current in the y-direction, and the observation point is at (d, y, z). Since the current distribution is independent of y and z, the magnetic flux density at (d, y, z) is the same as that at (d, 0, 0). By Eq. (7.1), **B** at (d, 0, 0) must be perpendicular to both the y-axis and the position vector  $d\hat{\mathbf{x}}$ , hence has only the z-component. Eq. (7.1) also tells us that  $B_z(-d, 0, 0) = -B_z(d, 0, 0)$ . We may choose the loop of integration to be a rectangular path in the z-x plane defined by the four corners (d, 0, -L/2), (d, 0, L/2), (-d, 0, L/2), and (-d, 0, -L/2). Ampere's law yields

$$B_z(d)2L = \mu_0 J_s L, (7.19)$$

where  $J_s$  is the surface current density. Therefore the magnetic flux density produced by a infinitely large sheet of current distribution is a constant  $\mu_0 J_s/2$ .

### 7.2 Lorentz Force

Since a current is nothing but a stream of moving charges, Eq. (7.2) gives the force experienced by a group of moving charges in a magnetic flux density.

$$\mathbf{F} = \int \mathbf{J}(\mathbf{r}) \times \mathbf{B}(\mathbf{r}) d^{3}\mathbf{r}$$
  
=  $\int \rho(\mathbf{r}) \mathbf{v}(\mathbf{r}) \times \mathbf{B}(\mathbf{r}) d^{3}\mathbf{r}$   
=  $\sum_{i} q_{i} \mathbf{v}_{i} \times \mathbf{B}_{i},$  (7.20)

where  $q_i$  and  $\mathbf{v}_i$  are the charge and velocity of the *i*th particle respectively, and  $\mathbf{B}_i$  is the **B**-field at the location of the *i*th particle. Combining with the force produced by the electric field, a moving charge experiences a force

$$\mathbf{F} = q(\mathbf{E} + \mathbf{v} \times \mathbf{B}). \tag{7.21}$$

This is known as the **Lorentz Force**.

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# 7.3 Force between Current Loops

Consider the force between two current loops. According to Eqs. (7.1) and (7.2), the force is

$$\mathbf{F} = \int \mathbf{J}_{1}(\mathbf{r}) \times \left[ \frac{\mu_{0}}{4\pi} \int \mathbf{J}_{2}(\mathbf{r}') \times \frac{\mathbf{r} - \mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|^{3}} d^{3}\mathbf{r}' \right] d^{3}\mathbf{r}$$
$$= \frac{\mu_{0}}{4\pi} I_{1} I_{2} \oint \oint d\mathbf{s} \times \left( d\mathbf{s}' \times \frac{\mathbf{r} - \mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|^{3}} \right), \qquad (7.22)$$

where we have used the relation

$$Id\mathbf{s} = \mathbf{J} \, d^3 \mathbf{r}.\tag{7.23}$$

By the vector identity Eq. (1.357), Eq. (7.22) can be reduced to

$$\mathbf{F} = \frac{\mu_0}{4\pi} I_1 I_2 \left[ \oint \oint d\mathbf{s} \cdot \frac{\mathbf{r} - \mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|^3} \, d\mathbf{s}' - \oint \oint d\mathbf{s} \cdot d\mathbf{s}' \frac{\mathbf{r} - \mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|^3} \right].$$
(7.24)

Since

$$\frac{\mathbf{r} - \mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|^3} = -\nabla \frac{1}{|\mathbf{r} - \mathbf{r}'|},\tag{7.25}$$

the first term on the right-hand side of Eq. (7.24) is zero. Hence

$$\mathbf{F} = -\frac{\mu_0}{4\pi} I_1 I_2 \oint \oint d\mathbf{s} \cdot d\mathbf{s}' \frac{\mathbf{r} - \mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|^3}.$$
 (7.26)

# 7.4 Vector Potential

The vector potential  $\mathbf{A}$  of the magnetic-flux density is defined by

$$\mathbf{B} = \nabla \times \mathbf{A}.\tag{7.27}$$

This definition automatically satisfies the equation  $\nabla \cdot \mathbf{B} = 0$ . But how do we know there is such a vector field satisfying Eq. (7.27)? Eq. (7.27) can be explicitly written as

$$\frac{\partial A_z}{\partial y} - \frac{\partial A_y}{\partial z} = B_x,$$

$$\frac{\partial A_x}{\partial z} - \frac{\partial A_z}{\partial x} = B_y,$$

$$\frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y} = B_z.$$
(7.28)

These are the three equations for the three components of **A**. However, since  $\nabla \cdot \mathbf{B} = 0$  these three equations are not independent. It is easy to see that if **A** satisfies the equation

$$\nabla \times \mathbf{A} = \mathbf{B},\tag{7.29}$$

 $\mathbf{A}' = \mathbf{A} + \nabla \phi$  also satisfies the same equation, because  $\nabla \times \nabla \phi = 0$  for any  $\phi$ . Therefore we must impose another condition to make the solution unique. A convenient condition to fix the solution is  $\nabla \cdot \mathbf{A} = 0$ . By adding the condition  $\nabla \cdot \mathbf{A} = 0$ , we have enough equations to determine  $\mathbf{A}$ . If  $\nabla \cdot \mathbf{A} \neq 0$ , we can choose  $\phi$  such that

$$\nabla^2 \phi = -\nabla \cdot \mathbf{A}.\tag{7.30}$$

Then we have  $\nabla \cdot \mathbf{A}' = \nabla \cdot \mathbf{A} + \nabla^2 \phi = 0$ . Since Eq. (7.30) is the same as that for the electric potential Eq. (6.16), by Eq. (6.5) we see the appropriate  $\phi$  to choose is

$$\phi(\mathbf{r}) = \frac{1}{4\pi} \int \frac{\nabla' \cdot \mathbf{A}(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d^3 \mathbf{r}'.$$
(7.31)

To write out  $\mathbf{A}$  explicitly, let us take the curl of Eq. (7.27). By the vector identity

$$\nabla \times (\nabla \times \mathbf{A}) = \nabla (\nabla \cdot \mathbf{A}) - \nabla^2 \mathbf{A}, \qquad (7.32)$$

we have

$$\nabla^2 \mathbf{A} = -\nabla \times \mathbf{B}.\tag{7.33}$$

For each component of  $\mathbf{A}$ , the equation is the same as that for the electric potential Eq. (6.16), hence by Eq. (6.5) we have

$$\mathbf{A}(\mathbf{r}) = \frac{1}{4\pi} \int \frac{\nabla' \times \mathbf{B}(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d^3 \mathbf{r}'.$$
(7.34)

The vector potential given by Eq. (7.34) satisfies  $\nabla \cdot \mathbf{A} = 0$ , because

$$\nabla \cdot \mathbf{A}(\mathbf{r}) = \frac{1}{4\pi} \int [\nabla' \times \mathbf{B}(\mathbf{r}')] \cdot \nabla \frac{1}{|\mathbf{r} - \mathbf{r}'|} d^3 \mathbf{r}'$$

$$= \frac{1}{4\pi} \int [\nabla' \times \mathbf{B}(\mathbf{r}')] \cdot (-\nabla') \frac{1}{|\mathbf{r} - \mathbf{r}'|} d^3 \mathbf{r}'$$

$$= -\frac{1}{4\pi} \int \nabla' \cdot \left[ \frac{\nabla' \times \mathbf{B}(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \right] d^3 \mathbf{r}' + \frac{1}{4\pi} \int \frac{\nabla' \cdot [\nabla' \times \mathbf{B}(\mathbf{r}')]}{|\mathbf{r} - \mathbf{r}'|} d^3 \mathbf{r}'$$

$$= -\frac{1}{4\pi} \int_S \frac{\nabla' \times \mathbf{B}(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \cdot d\mathbf{a} + \frac{1}{4\pi} \int \frac{\nabla' \cdot [\nabla' \times \mathbf{B}(\mathbf{r}')]}{|\mathbf{r} - \mathbf{r}'|} d^3 \mathbf{r}'$$

$$= -\frac{\mu_0}{4\pi} \int_S \frac{\mathbf{J}(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \cdot d\mathbf{a} + \frac{\mu_0}{4\pi} \int \frac{\nabla' \cdot [\mathbf{J}(\mathbf{r}')]}{|\mathbf{r} - \mathbf{r}'|} d^3 \mathbf{r}'. \quad (7.35)$$

### 7.5. MAGNETIC DIPOLE

Assuming that there is no current at the boundary surface in the infinity, the first term on the right-hand side is zero. In the static case we have  $\partial \rho / \partial t = 0$ . By the continuity equation it implies  $\nabla \cdot \mathbf{J} = 0$ . Hence the second term on the right-hand side is also zero. Since  $\nabla' \times \mathbf{B}(\mathbf{r}') = \mu_0 \mathbf{J}(\mathbf{r}')$ , Eq. (7.34) can be written as

$$\mathbf{A}(\mathbf{r}) = \frac{\mu_0}{4\pi} \int \frac{\mathbf{J}(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d^3 \mathbf{r}'.$$
(7.36)

This is the same result we have already derived in Eq. (7.5). The symmetry between Eq. (6.5) and (7.36) reveals that using **A** to replace **B** in calculation has the same advantage as using  $\phi$  to replace **E**, as we shall see in the subsequent sections.

## 7.5 Magnetic Dipole

Since an isolated magnetic charge has never been found, the simplest magnetic structure is a magnetic dipole. A magnetic dipole can be defined by the magnetic-flux density generated by a small current loop. Similar to the Taylor expansion of  $\phi$  in Eq. (6.27), we may expand **A** in the following way:

$$A_i(\mathbf{r}) = \frac{\mu_0}{4\pi} \left[ \frac{1}{r} \int J_i(\mathbf{r}') \, d^3 \mathbf{r}' + \frac{\mathbf{r}}{r^3} \cdot \int \mathbf{r}' J_i(\mathbf{r}') \, d^3 \mathbf{r}' + \dots \right]. \tag{7.37}$$

By the vector identity

$$r_i \frac{\partial J_k}{\partial x_k} = \frac{\partial}{\partial x_k} (x_i J_k) - \frac{\partial x_i}{\partial x_k} J_k = \frac{\partial}{\partial x_k} (x_i J_k) - J_i, \qquad (7.38)$$

which reads

$$r_i \nabla \cdot \mathbf{J} = \nabla \cdot (r_i \mathbf{J}) - J_i, \tag{7.39}$$

and the fact  $\nabla \cdot \mathbf{J} = 0$ , we have

$$\nabla \cdot (r_i \mathbf{J}) = J_i. \tag{7.40}$$

Hence

$$\int J_i d^3 \mathbf{r} = \int \nabla \cdot (r_i \mathbf{J}) d^3 \mathbf{r} = \int_S r_i \mathbf{J} \cdot d\mathbf{a}, \qquad (7.41)$$

where in the last step we have used Gauss' theorem. For a localized current distribution, we may assume that  $\mathbf{J}$  vanishes at some boundary surface. Then

the first term on the right-hand side of Eq. (7.37) is zero. The second term on the right-hand side of Eq. (7.37) can be reduced by the vector identity

$$(\mathbf{r} \cdot \mathbf{r}')\mathbf{J} = (\mathbf{r} \cdot \mathbf{J})\mathbf{r}' - \mathbf{r} \times (\mathbf{r}' \times \mathbf{J}).$$
(7.42)

We shall first prove

$$\int (\mathbf{r} \cdot \mathbf{r}') \mathbf{J}(\mathbf{r}') d^3 \mathbf{r}' = -\int [\mathbf{r} \cdot \mathbf{J}(\mathbf{r}')] \mathbf{r}' d^3 \mathbf{r}'.$$
(7.43)

From Eq. (7.40) one has

$$\int r'_k \nabla' \cdot [r'_i \mathbf{J}(\mathbf{r}')] d^3 \mathbf{r}' = \int r'_k J_i(\mathbf{r}') d^3 \mathbf{r}'.$$
(7.44)

Using the identity

$$\nabla \cdot (\psi \mathbf{a}) = (\mathbf{a} \cdot \nabla)\psi + \psi \nabla \cdot \mathbf{a}$$
(7.45)

we have

$$\int r'_{k} \nabla' \cdot [r'_{i} \mathbf{J}(\mathbf{r}')] d^{3}\mathbf{r}' = \int \nabla' \cdot [r'_{k} r'_{i} \mathbf{J}(\mathbf{r}')] d^{3}\mathbf{r}' - \int r'_{i} \mathbf{J}(\mathbf{r}') \cdot (\nabla' r'_{k}) d^{3}\mathbf{r}'$$

$$= \int_{S} r'_{k} r'_{i} \mathbf{J}(\mathbf{r}') \cdot d\mathbf{a}' - \int r'_{i} \mathbf{J}(\mathbf{r}') \cdot (\delta_{lk} \mathbf{e}_{l}) d^{3}\mathbf{r}'$$

$$= \int_{S} r'_{k} r'_{i} \mathbf{J}(\mathbf{r}') \cdot d\mathbf{a}' - \int r'_{i} J_{k}(\mathbf{r}') d^{3}\mathbf{r}'. \quad (7.46)$$

For a localized current distribution, we may assuming  $\mathbf{J} = 0$  at some boundary surface. Then the first term on the right-hand side vanishes, and from Eq. (7.40) we have

$$-\int r'_i J_k(\mathbf{r}') \, d^3 \mathbf{r}' = \int r'_k J_i(\mathbf{r}') \, d^3 \mathbf{r}'.$$
(7.47)

Multiplying both sides by  $r_i$  and summing over i, we have

$$-\int r_i r'_i J_k(\mathbf{r}') \, d^3 \mathbf{r}' = \int r_i J_i(\mathbf{r}') r'_k \, d^3 \mathbf{r}', \qquad (7.48)$$

where the repeated index is by definition summed over. This is exactly Eq. (7.43). Integrating Eq. (7.42) and substituting Eq. (7.43) into it, we obtain

$$\int (\mathbf{r} \cdot \mathbf{r}') \mathbf{J}(\mathbf{r}') d^3 \mathbf{r}' = -\mathbf{r} \times \frac{1}{2} \int \mathbf{r}' \times \mathbf{J}(\mathbf{r}') d^3 \mathbf{r}'.$$
(7.49)

With this identity, Eq. (7.37) is reduced to

$$\mathbf{A}(\mathbf{r}) = -\frac{\mu_0}{4\pi r^3} \mathbf{r} \times \frac{1}{2} \int \mathbf{r}' \times \mathbf{J}(\mathbf{r}') \, d^3 \mathbf{r}'.$$
(7.50)

### 7.5. MAGNETIC DIPOLE

The magnetic moment is defined as

$$\mathbf{m} = \frac{1}{2} \int \mathbf{r}' \times \mathbf{J}(\mathbf{r}') \, d^3 \mathbf{r}', \qquad (7.51)$$

and

$$\mathbf{A} = \frac{\mu_0}{4\pi} \frac{\mathbf{m} \times \mathbf{r}}{r^3}.\tag{7.52}$$

For  $\mathbf{m}$  in the *z*-direction,

$$\mathbf{A} = \frac{\mu_0}{4\pi} \frac{m\sin\theta}{r^2} \hat{\boldsymbol{\phi}}.$$
 (7.53)

 $\mathbf{B} = \nabla \times \mathbf{A}$  and Eq. (1.350) gives

$$B_{r} = \frac{\mu_{0}}{4\pi} \frac{1}{r^{2} \sin \theta} \frac{\partial}{\partial \theta} \left[ r \sin \theta \left( \frac{m \sin \theta}{r^{2}} \right) \right] = \frac{\mu_{0}}{4\pi} \frac{2m \cos \theta}{r^{3}},$$
  

$$B_{\theta} = -\frac{\mu_{0}}{4\pi} \frac{1}{r \sin \theta} \frac{\partial}{\partial r} \left[ r \sin \theta \left( \frac{m \sin \theta}{r^{2}} \right) \right] = \frac{\mu_{0}}{4\pi} \frac{m \sin \theta}{r^{3}}.$$
 (7.54)

The field pattern is exactly the same as in Eq. (6.29), hence justifying Eq. (7.51) as the definition of magnetic dipole moment.

If a current I flows in a closed loop whose line element is  $d\mathbf{l}$ , Eq. (7.51) becomes

$$\mathbf{m} = \frac{I}{2} \int \mathbf{r} \times d\mathbf{l}. \tag{7.55}$$

If the loop is in a plane,

$$\int \mathbf{r} \times d\mathbf{l} = 2\mathbf{a},\tag{7.56}$$

where  $a = |\mathbf{a}|$  is the area enclosed by the loop, and the direction of  $\mathbf{a}$  is normal to the plane. Hence we have

$$\mathbf{m} = I\mathbf{a}.\tag{7.57}$$

If we replace  $\mathbf{J}(\mathbf{r}')$  by  $\rho(\mathbf{r}')\mathbf{v}(\mathbf{r}')$  in Eq. (7.51) and note that  $\mathbf{r}' \times \mathbf{v}(\mathbf{r}')$  is simply the angular momentum  $\mathbf{L}$  divided by the mass m of the charges, we have

$$\mathbf{m} = \frac{q}{2m} \mathbf{L}.\tag{7.58}$$

Because the magnetic-flux density produced by a tiny magnet has the same pattern as Eq. (7.54), Eq. (7.58) suggests that magnetism originates from the angular momentum of electrons in atoms.

To find out the force and torque acted on a magnetic dipole, let us consider the following function

$$U_m(\mathbf{r}) = -\int \mathbf{J}(\mathbf{r}' - \mathbf{r}) \cdot \mathbf{A}(\mathbf{r}') d^3 \mathbf{r}'.$$
(7.59)

Taking the gradient of both sides and using

$$\nabla(\mathbf{a} \cdot \mathbf{b}) = (\mathbf{a} \cdot \nabla)\mathbf{b} + (\mathbf{b} \cdot \nabla)\mathbf{a} + \mathbf{a} \times (\nabla \times \mathbf{b}) + \mathbf{b} \times (\nabla \times \mathbf{a}), \quad (7.60)$$

we have

$$\nabla U_m(\mathbf{r}) = -\int \left\{ [\mathbf{A}(\mathbf{r}') \cdot \nabla] \mathbf{J}(\mathbf{r}' - \mathbf{r}) + \mathbf{A}(\mathbf{r}') \times [\nabla \times \mathbf{J}(\mathbf{r}' - \mathbf{r})] \right\} d^3 \mathbf{r}'.$$
(7.61)

Because **J** is a function of  $\mathbf{r}' - \mathbf{r}$ , we can replace  $\nabla$  by  $-\nabla'$  which operates on functions of  $\mathbf{r}'$ .

$$\nabla U_m(\mathbf{r}) = \int \left\{ [\mathbf{A}(\mathbf{r}') \cdot \nabla'] \mathbf{J}(\mathbf{r}' - \mathbf{r}) + \mathbf{A}(\mathbf{r}') \times [\nabla' \times \mathbf{J}(\mathbf{r}' - \mathbf{r})] \right\} d^3 \mathbf{r}'.$$
(7.62)

Using Eq. (7.60) again, we have

$$\nabla U_m(\mathbf{r}) = \int \nabla' [\mathbf{J}(\mathbf{r}' - \mathbf{r}) \cdot \mathbf{A}(\mathbf{r}')] d^3 \mathbf{r}'$$
  
- 
$$\int \left\{ [\mathbf{J}(\mathbf{r}' - \mathbf{r}) \cdot \nabla'] \mathbf{A}(\mathbf{r}') + \mathbf{J}(\mathbf{r}' - \mathbf{r}) \times [\nabla' \times \mathbf{A}(\mathbf{r}')] \right\} d^3 \mathbf{r}'. \quad (7.63)$$

Let us examine the x'-component of the first term on the right-hand side.

$$\int \frac{\partial}{\partial x'} [\mathbf{J}(\mathbf{r}' - \mathbf{r}) \cdot \mathbf{A}(\mathbf{r}')] dx' dy' dz' = \int [\mathbf{J}(\mathbf{r}' - \mathbf{r}) \cdot \mathbf{A}(\mathbf{r}')] dy' dz' \Big|_{x' = -\infty}^{x' = \infty} . (7.64)$$

Assuming  $\mathbf{J} = 0$  at the boundary surface in the infinity, this term vanishes. The same is true for the other two components. Hence the first term on the right-hand side of Eq. (7.63) is zero. Using

$$\nabla \cdot (\psi \mathbf{a}) = (\mathbf{a} \cdot \nabla)\psi + \psi \nabla \cdot \mathbf{a}$$
(7.65)

the second term on the right-hand side of Eq. (7.63) becomes

$$\int [\mathbf{J}(\mathbf{r}' - \mathbf{r}) \cdot \nabla'] A_i(\mathbf{r}') d^3 \mathbf{r}'$$
  
= 
$$\int \nabla' \cdot [\mathbf{J}(\mathbf{r}' - \mathbf{r}) A_i(\mathbf{r}')] - A_i(\mathbf{r}') [\nabla' \cdot \mathbf{J}(\mathbf{r}' - \mathbf{r})] d^3 \mathbf{r}'. \quad (7.66)$$

### 7.5. MAGNETIC DIPOLE

The first term on the right-hand side can be reduced to a surface integral. Assuming  $\mathbf{J} = 0$  at the boundary surface in the infinity, this term is zero. The second term on the right-hand side is also zero because for static current density distributions,  $\nabla \cdot \mathbf{J} = 0$ . Therefore we have

$$\nabla U_m(\mathbf{r}) = -\int \mathbf{J}(\mathbf{r}' - \mathbf{r}) \times [\nabla' \times \mathbf{A}(\mathbf{r}')] d^3 \mathbf{r}'$$
$$= -\int \mathbf{J}(\mathbf{r}' - \mathbf{r}) \times \mathbf{B}(\mathbf{r}') d^3 \mathbf{r}'.$$
(7.67)

From Eq. (7.2), we see that  $-\nabla U_m(\mathbf{r})$  is the force experienced by the current density distribution  $\mathbf{J}(\mathbf{r'} - \mathbf{r})$ . Hence in Eq. (7.59)

$$U_m(\mathbf{r}) = -\int \mathbf{J}(\mathbf{r}' - \mathbf{r}) \cdot \mathbf{A}(\mathbf{r}') d^3 \mathbf{r}'$$
(7.68)

is the potential energy of a current density distribution  $\mathbf{J}(\mathbf{r}' - \mathbf{r})$  in a fixed external field  $\mathbf{A}(\mathbf{r}')$ .

Next, we expand **A** in Eq. (7.59) to show the contribution of the magnetic dipole in  $U_m(0)$ .

$$U_m(0) = -\int J_i(\mathbf{r}') A_i(\mathbf{r}') d^3 \mathbf{r}'$$
  
=  $-\int [A_i(0) + \mathbf{r}' \cdot \nabla A_i(0)] J_i(\mathbf{r}') d^3 \mathbf{r}'.$  (7.69)

By the vector identity

$$r_i \nabla \cdot \mathbf{J} = \nabla \cdot (r_i \mathbf{J}) - J_i \tag{7.70}$$

and the fact  $\nabla \cdot \mathbf{J} = 0$ , we have

$$\nabla \cdot (r_i \mathbf{J}) = J_i, \tag{7.71}$$

hence

$$\int J_i d^3 \mathbf{r} = \int \nabla \cdot (r_i \mathbf{J}) d^3 \mathbf{r} = \int_S r_i \mathbf{J} \cdot d\mathbf{a}, \qquad (7.72)$$

where in the last step we have used Gauss' theorem. Assuming there is no current at the boundary surface in the infinity, it is seen the first term on the right-hand side of Eq. (7.69) vanishes. In the tensor notation we have

$$\mathbf{a} \times \mathbf{b} = a_i b_j \epsilon_{ijk},\tag{7.73}$$

where  $\epsilon_{ijk} = 1$  if the order of permutation for  $\{ijk\}$  is even,  $\epsilon_{ijk} = -1$  if the order of permutation is odd, and  $\epsilon_{ijk} = 0$  if any two indices are the same. Define  $A_i^i \equiv \partial A_i / \partial r_j$ , in the tensor notation Eq. (7.69) becomes

$$U_m(0) = -\int r'_j A^i_j J_i \, d^3 \mathbf{r}'.$$
(7.74)

Using the identity  $\epsilon_{ijk}\epsilon_{lmk} = \delta_{il}\delta_{jm} - \delta_{im}\delta_{jl}$  in Eq. (1.355), Eq. (7.47) can be written as

$$\int r'_l J_m d^3 \mathbf{r}' = \frac{1}{2} \int (r'_l J_m - r'_m J_l) d^3 \mathbf{r}'$$
$$= \frac{1}{2} \int r'_i J_j (\delta_{il} \delta_{jm} - \delta_{im} \delta_{jl}) d^3 \mathbf{r}'$$
$$= \frac{1}{2} \int r'_i J_j \epsilon_{ijk} \epsilon_{lmk} d^3 \mathbf{r}'.$$
(7.75)

Multiplying both sides by  $A_l^{\alpha}$ , we have

$$\int A_l^{\alpha} r_l' J_m \, d^3 \mathbf{r}' = \frac{1}{2} \int r_i' J_j \epsilon_{ijk} A_l^{\alpha} \epsilon_{lmk} \, d^3 \mathbf{r}'. \tag{7.76}$$

Eq. (7.51) is equivalent to

$$\frac{1}{2} \int r'_i J_j \epsilon_{ijk} \, d^3 \mathbf{r}' = m_k, \tag{7.77}$$

where  $m_k$  is the kth component of **m**, hence we have

$$\int A_l^{\alpha} r_l' J_m \, d^3 \mathbf{r}' = m_k A_l^{\alpha} \epsilon_{lmk}. \tag{7.78}$$

Multiplying both sides by  $\delta_{m\alpha}$ , it becomes

$$\int A_l^{\alpha} r_l' J_{\alpha} \, d^3 \mathbf{r}' = m_k A_l^{\alpha} \epsilon_{l\alpha k}. \tag{7.79}$$

Noting that the left hand side is  $\int A_l^{\alpha} r_l' J_{\alpha} d^3 \mathbf{r}' = -U_m(0)$  and on the righthand side  $A_l^{\alpha} \epsilon_{l\alpha k}$  is simply the *k*th component of  $\nabla \times \mathbf{A} = \mathbf{B}$ . That is,

$$U_m = -m_k B_k = -\mathbf{m} \cdot \mathbf{B}. \tag{7.80}$$

The force acted on the current distribution is therefore

$$\mathbf{F} = \nabla(\mathbf{m} \cdot \mathbf{B}). \tag{7.81}$$

To find out the torque au acted on a magnetic dipole, we note that

$$\boldsymbol{\tau} \approx \int \mathbf{r}' \times [\mathbf{J}(\mathbf{r}') \times \mathbf{B}(0)] d^3 \mathbf{r}'$$
  
= 
$$\int [\mathbf{r}' \cdot \mathbf{B}(0)] \mathbf{J}(\mathbf{r}') d^3 \mathbf{r}' - \int [\mathbf{r}' \cdot \mathbf{J}(\mathbf{r}')] \mathbf{B}(0) d^3 \mathbf{r}'. \quad (7.82)$$

### 7.6. MAGNETIZATION

By the same method we derive Eq. (7.49), namely replacing  $\mathbf{r}$  by  $\mathbf{B}(0)$ , we can show that

$$\int [\mathbf{B}(0) \cdot \mathbf{r}'] \mathbf{J}(\mathbf{r}') d^3 \mathbf{r}' = -\mathbf{B}(0) \times \frac{1}{2} \int \mathbf{r}' \times \mathbf{J}(\mathbf{r}') d^3 \mathbf{r}'$$
$$= \mathbf{m} \times \mathbf{B}(0), \qquad (7.83)$$

while by Eq. (7.47)

$$\int [\mathbf{r}' \cdot \mathbf{J}(\mathbf{r}')] \mathbf{B}(0) d^3 \mathbf{r}' = \mathbf{B}(0) \int \mathbf{r}' \cdot \mathbf{J}(\mathbf{r}') d^3 \mathbf{r}' = 0.$$
(7.84)

Therefore

$$\boldsymbol{\tau} = \mathbf{m} \times \mathbf{B}.\tag{7.85}$$

## 7.6 Magnetization

Some materials are made of atoms or molecules with a permanent magnetic dipole moment. Under an external field the atoms or molecules may rotate to make their magnetic moment parallel to the field. Even without rotation, the current distribution can be deformed by the external field, as a result the magnetic moment changes. Let us define the magnetization  $\mathbf{M}$  to be the magnetic dipole moment per unit volume. From Eqs. (7.50) and (7.51) it is seen that the magnetization also contributes to the vector potential. Namely,

$$\mathbf{A}(\mathbf{r}) = \frac{\mu_0}{4\pi} \int \left[ \frac{\mathbf{J}(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} + \frac{\mathbf{M}(\mathbf{r}') \times (\mathbf{r} - \mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|^3} \right] d^3\mathbf{r}'.$$
 (7.86)

The magnetization term can be written as

$$\int \frac{\mathbf{M}(\mathbf{r}') \times (\mathbf{r} - \mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|^3} d^3 \mathbf{r}' = \int \mathbf{M}(\mathbf{r}') \times \left(\nabla' \frac{1}{|\mathbf{r} - \mathbf{r}'|}\right) d^3 \mathbf{r}'$$
$$= \int \frac{\nabla' \times \mathbf{M}(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d^3 \mathbf{r}' - \int \nabla' \times \frac{\mathbf{M}(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d^3 \mathbf{r}', \tag{7.87}$$

where we have used the vector identity  $\nabla \times (\psi \mathbf{a}) = \nabla \psi \times \mathbf{a} + \psi \nabla \times \mathbf{a}$ . The second term on the right-hand side can be reduced to surface integral by Stokes' theorem. Let us consider its z-component by defining a new vector

$$\mathbf{N}(\mathbf{r}') = \frac{M_x(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \hat{\mathbf{x}} + \frac{M_y(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \hat{\mathbf{y}}.$$
(7.88)

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$$\left(\int \nabla' \times \frac{\mathbf{M}(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d^3 \mathbf{r}'\right)_z = \int [\nabla' \times \mathbf{N}(\mathbf{r}')] \cdot \hat{\mathbf{z}} dx dy dz$$
$$= \int \left(\oint \mathbf{N}(\mathbf{r}') \cdot d\mathbf{l}\right) dz, \qquad (7.89)$$

where the line integral is over a loop at infinity on the x-y plane. Assuming  $\mathbf{M} = 0$  in the infinity, this term vanishes. From Eq. (7.34) we have

$$\nabla \times \mathbf{B} = \mu_0 \mathbf{J} + \mu_0 \nabla \times \mathbf{M}. \tag{7.90}$$

The magnetization thus plays the role of an effective current density

$$\mathbf{J}_M = \nabla \times \mathbf{M}.\tag{7.91}$$

The macroscopic field  $\mathbf{H}$  called the magnetic field is defined by

$$\mathbf{H} = \frac{\mathbf{B}}{\mu_0} - \mathbf{M}.\tag{7.92}$$

Then we have

$$\nabla \times \mathbf{H} = \mathbf{J}.\tag{7.93}$$

For some materials  $\mathbf{M}$  is proportional to  $\mathbf{H}$ , then we have

$$\mathbf{M} = \chi_m \mathbf{H},\tag{7.94}$$

where  $\chi_m$  is the magnetic susceptibility. In this case

$$\mathbf{B} = \mu_0(\chi_m + 1)\mathbf{H} = \kappa_m \mu_0 \mathbf{H} = \mu \mathbf{H}, \tag{7.95}$$

where  $\kappa_m$  is called the relative permeability and  $\mu$  the absolute permeability.

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## 7.7 Exercises

**Exercise 7.1.** Two charged particles carrying charges +q and -q are separated by a distance d in the y-direction. They are also moving in the x-direction with the same velocity v. The mutual attraction force between them is F when v = 0. At what v the mutual attraction between them is reduced to F/2?

**Exercise 7.2.** A solid metal cylinder rotating with angular velocity  $\omega$  about its axis is put in a uniform magnetic field *B* parallel to its axis. The Lorentz force and the centrifugal force push electrons to create a charge distribution. What is the charge distribution? If the charge distribution you obtained can be positive or negative everywhere, how would you explain the law of charge conservation? Hint: Since the charge cannot leave the cylinder, it may accumulate on the surface.

# Chapter 8

# Electrodynamics

# 8.1 Faraday's Law

In 1831 Faraday discovered that an electric current can be induced in a closed wire loop by changing the magnetic flux that goes through the loop. This important discovery can be written in the following mathematical form:

$$\mathcal{E} = -\frac{d}{dt} \int \mathbf{B} \cdot d\mathbf{a},\tag{8.1}$$

where  $\mathcal{E}$  is called the electromotive force, and the integration on the righthand side covers the surface enclosed by the wire loop. Faraday observed that the relation between  $\mathcal{E}$  and the induced current I simply follows the Ohm's law:

$$\mathcal{E} = IR,\tag{8.2}$$

where R is the resistance of the wire. Hence  $\mathcal{E}$  can be interpreted as the result of an induced electric field that drives the current. The direction of the electromotive force is such that the magnetic flux produced by the induced current is opposite to the change of the magnetic flux. In other words, the induced current works against the change of the magnetic flux. This is known as **Lenz' law**.

Maxwell recognized that Eq. (8.1) is more general than it appears. Because it does not require a wire to define the electric field, and in fact an electric field can be defined even in vacuum, Maxwell rewrote Eq. (8.1) in the following form which is independent of the presence of a wire.

$$\oint \mathbf{E} \cdot d\mathbf{s} = -\frac{d}{dt} \int \mathbf{B} \cdot d\mathbf{a}.$$
(8.3)

This is an important step in the development of electrodynamics, because it reveals directly that an electric field can be induced by a changing magnetic flux, even in vacuum. For the case of a static loop, by using the Stoke's theorem Eq. (8.3) can be written in the differential form

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}.$$
(8.4)

But what about a moving wire loop? In Faraday's experiments the changing magnetic flux may arise from a wire loop moving in a static magnetic flux density distribution. How should we describe such cases by Eq. (8.3)? It turns out that as a wire moves relative to a magnetic flux density, a charge q in the wire will also experience a force proportional to  $q\mathbf{v} \times \mathbf{B}$ , in additional to the electric force  $q\mathbf{E}$ , as shown in Eq. (7.21). Consider a closed loop moving at velocity  $\mathbf{v}$ . If the loop has a fixed shape, then every point on the loop labeled by the position vector  $\mathbf{r}$  must move at the same velocity. In this case  $\mathbf{v}$  is independent of  $\mathbf{r}$ . We may apply the convective derivative to the right-hand side of Eq. (8.1).

$$\frac{d\mathbf{B}}{dt} = \frac{\partial \mathbf{B}}{\partial t} + (\mathbf{v} \cdot \nabla)\mathbf{B} = \frac{\partial \mathbf{B}}{\partial t} + \nabla \times (\mathbf{B} \times \mathbf{v}) + \mathbf{v}(\nabla \cdot \mathbf{B}).$$
(8.5)

Substituting into Eq. (8.3), for a static **B**-field we have

$$\oint \mathbf{E} \cdot d\mathbf{s} = -\int \nabla \times (\mathbf{B} \times \mathbf{v}) \cdot d\mathbf{a}.$$
(8.6)

Using the Stoke's theorem, we have

$$\oint \mathbf{E} \cdot d\mathbf{s} = \int (\mathbf{v} \times \mathbf{B}) \cdot d\mathbf{s}. \tag{8.7}$$

This establishes the fact that in the case of a moving wire loop, the electromotive force is nothing but the Lorentz force. Because  $\mathbf{v} \times d\mathbf{s}$  is the area swept by the line element  $d\mathbf{s}$  per unit time, we have

$$\oint (\mathbf{v} \times \mathbf{B}) \cdot d\mathbf{s} = \oint \mathbf{B} \cdot (d\mathbf{s} \times \mathbf{v}) = -\int \mathbf{B} \cdot \frac{\partial (d\mathbf{a})}{\partial t}.$$
(8.8)

#### 8.2. MAXWELL EQUATIONS

Substituting back into Eq. (8.7), we have

$$\oint \mathbf{E} \cdot d\mathbf{s} = -\int \mathbf{B} \cdot \frac{\partial (d\mathbf{a})}{\partial t}.$$
(8.9)

For a loop of fixed shape the area enclosed by the loop does not change, hence we have

$$\int \frac{\partial (d\mathbf{a})}{\partial t} = \frac{\partial}{\partial t} \int d\mathbf{a} = 0.$$
(8.10)

If **B** is uniform, the right-hand side of Eq. (8.9) vanishes. However, if **B** is not uniform, the right-hand side of Eq. (8.9) does not vanish because each point of integration is weighted by a different **B**. This is the electromotive force induced by a loop moving in a static **B** field. The change of flux arises from the change of the surface of integration.

# 8.2 Maxwell Equations

Let us summarize the four laws we have learned that govern the electromagnetic interactions.

Gauss' law:

$$\nabla \cdot \mathbf{D} = \rho. \tag{8.11}$$

Ampere's law:

$$\nabla \times \mathbf{H} = \mathbf{J}.\tag{8.12}$$

Faraday's law:

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}.$$
(8.13)

and because no magnetic charge has ever been found, we have

$$\nabla \cdot \mathbf{B} = 0. \tag{8.14}$$

Among these laws, Ampere's law is valid only for static cases. By applying  $\nabla \cdot$  on both sides of Eq. (8.12), it leads to  $\nabla \cdot \mathbf{J} = 0$ . This cannot be right for the general case because the conservation of charge requires that  $\nabla \cdot \mathbf{J} + \partial \rho / \partial t = 0$ . Therefore Maxwell modified Eq. (8.12) to make it consistent with the continuity equation. The modification is done by adding  $\mathbf{J}_D = \partial \mathbf{D} / \partial t$  on the

right-hand side of Eq. (8.12), where  $\mathbf{J}_D \equiv \partial \mathbf{D} / \partial t$  is called the displacement current. This is known as the **Ampere-Maxwell law:** 

$$\nabla \times \mathbf{H} = \mathbf{J} + \frac{\partial \mathbf{D}}{\partial t}.$$
(8.15)

These equations are now called the **Maxwell equations** collectively.

The need to introduce  $\mathbf{J}_D$  in Ampere's law can also be seen in Eq. (7.8). By Eq. (7.14), the second term on the right-hand side of Eq. (7.8) is

$$\nabla \int \frac{\mu_0}{4\pi} \frac{\nabla' \cdot \mathbf{J}(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d^3 \mathbf{r}'$$

$$= \frac{\mu_0}{4\pi} \nabla \int \left[ -\frac{\partial \rho(\mathbf{r}')}{\partial t} \right] \frac{1}{|\mathbf{r} - \mathbf{r}'|} d^3 \mathbf{r}'$$

$$= \frac{\mu_0}{4\pi} \frac{\partial}{\partial t} \int \rho(\mathbf{r}') \frac{\mathbf{r} - \mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|^3} d^3 \mathbf{r}'$$

$$= \mu_0 \epsilon_0 \frac{\partial \mathbf{E}}{\partial t}.$$
(8.16)

Therefore Eq. (7.15) should be

$$\nabla \times \mathbf{B} = \mu_0 \mathbf{J} + \mu_0 \epsilon_0 \frac{\partial \mathbf{E}}{\partial t}.$$
(8.17)

In a polarizable and magnetizable medium it becomes Eq. (8.15).

Substituting  $\mathbf{B} = \nabla \times \mathbf{A}$  into Faraday's law, we have

$$\nabla \times \left( \mathbf{E} + \frac{\partial \mathbf{A}}{\partial t} \right) = 0. \tag{8.18}$$

This allows us to define a scalar potential  $\phi$  by

$$-\nabla\phi = \mathbf{E} + \frac{\partial \mathbf{A}}{\partial t},\tag{8.19}$$

or

$$\mathbf{E} = -\nabla\phi - \frac{\partial \mathbf{A}}{\partial t}.\tag{8.20}$$

The vacuum forms of Eqs. (8.11) and (8.15) are

$$\nabla \cdot \mathbf{E} = \frac{\rho}{\epsilon_0}, \tag{8.21}$$

$$\nabla \times \mathbf{B} = \mu_0 \left( \mathbf{J} + \epsilon_0 \frac{\partial \mathbf{E}}{\partial t} \right). \tag{8.22}$$

### 8.2. MAXWELL EQUATIONS

Substituting Eq. (8.20) into Eq. (8.21), we obtain

$$\nabla^2 \phi + \frac{\partial}{\partial t} (\nabla \cdot \mathbf{A}) = -\frac{\rho}{\epsilon_0}.$$
(8.23)

Substituting  $\mathbf{B} = \nabla \times \mathbf{A}$  and Eq. (8.20) into Eq. (8.22), we obtain

$$\nabla(\nabla \cdot \mathbf{A}) - \nabla^2 \mathbf{A} = \mu_0 \mathbf{J} - \nabla \left( \mu_0 \epsilon_0 \frac{\partial \phi}{\partial t} \right) - \mu_0 \epsilon_0 \frac{\partial^2 \mathbf{A}}{\partial t^2}, \quad (8.24)$$

where  $\nabla \times \nabla \times \mathbf{A} = \nabla (\nabla \cdot \mathbf{A}) - \nabla^2 \mathbf{A}$ . That is,

$$\nabla^{2}\mathbf{A} - \mu_{0}\epsilon_{0}\frac{\partial^{2}\mathbf{A}}{\partial t^{2}} - \nabla\left(\mu_{0}\epsilon_{0}\frac{\partial\phi}{\partial t} + \nabla\cdot\mathbf{A}\right) = -\mu_{0}\mathbf{J}.$$
(8.25)

We have already mentioned that the equation  $\mathbf{B} = \nabla \times \mathbf{A}$  is not sufficient to determine  $\mathbf{A}$  uniquely. The three components of the equation are not independent because  $\nabla \cdot \mathbf{B} = 0$ . This allows us to impose an additional condition on  $\mathbf{A}$ . For static cases we used to choose  $\nabla \cdot \mathbf{A} = 0$ , but now if we choose

$$\mu_0 \epsilon_0 \frac{\partial \phi}{\partial t} + \nabla \cdot \mathbf{A} = 0, \qquad (8.26)$$

Eqs. (8.23) and (8.25) can be simplified to the following form:

$$\nabla^2 \phi - \mu_0 \epsilon_0 \frac{\partial^2 \phi}{\partial t^2} = -\frac{\rho}{\epsilon_0}.$$
(8.27)

$$\nabla^2 \mathbf{A} - \mu_0 \epsilon_0 \frac{\partial^2 \mathbf{A}}{\partial t^2} = -\mu_0 \mathbf{J}.$$
(8.28)

Eqs. (8.26), (8.27), and (8.28) are equivalent to the Maxwell equations.

In a medium whose polarization and magnetization response linearly to the electromagnetic field, Eqs. (8.11) and (8.12) become

$$\nabla \cdot \mathbf{E} = \frac{\rho}{\epsilon}, \tag{8.29}$$

$$\nabla \times \mathbf{B} = \mu \left( \mathbf{J} + \epsilon \frac{\partial \mathbf{E}}{\partial t} \right),$$
 (8.30)

and Eqs. (8.26), (8.27), and (8.28) become

$$\mu \epsilon \frac{\partial \phi}{\partial t} + \nabla \cdot \mathbf{A} = 0, \qquad (8.31)$$

$$\nabla^2 \phi - \mu \epsilon \frac{\partial^2 \phi}{\partial t^2} = -\frac{\rho}{\epsilon},\tag{8.32}$$

$$\nabla^2 \mathbf{A} - \mu \epsilon \frac{\partial^2 \mathbf{A}}{\partial t^2} = -\mu \mathbf{J}.$$
(8.33)

### 8.3 Electromagnetic Waves

Before Maxwell, **E** and **B** are thought of as mathematical instruments for calculating the interactions between charges and currents. It is more convenient to calculate first **E** and **B** from the charge and current sources then use them to calculate the force experienced by a test charge or current. But Eqs. (8.27) and (8.28) reveal that even if there is no charge and current, **E** and **B** can exist in the form of electromagnetic waves. Of course, one can argue that the existence of the wave equation does not guarantee its solution, because after all, there must be an initial disturbance of charges or currents at some place to produce the wave, just like a pendulum will not oscillate by itself; there must be someone to give it an initial push. Such kinds of debate in point of view can become philosophical. In the end, it is hard to deny the advantage of treating **E** and **B** as real physical quantities. This is because in terms of source charges and currents, the interaction is distributed. Namely, as we shall see in Section 8.5, the force between a test charge q and a charge distribution  $\rho(\mathbf{r}', t')$  is

$$\mathbf{F}(\mathbf{r},t) = \frac{q}{4\pi\epsilon_0} \int \rho(\mathbf{r}',t') \frac{\mathbf{r} - \mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|^3} d^3\mathbf{r}', \qquad (8.34)$$

where  $t' = t - |\mathbf{r} - \mathbf{r}'|/c$  and c is the speed of propagation for the electromagnetic disturbance, and the force between a current I of length dl and a current distribution  $\mathbf{J}(\mathbf{r}', t')$  is

$$d\mathbf{F}(\mathbf{r},t) = \frac{\mu_0 I d\mathbf{l}}{4\pi} \times \int \mathbf{J}(\mathbf{r}',t') \times \frac{\mathbf{r} - \mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|^3} d^3 \mathbf{r}'.$$
 (8.35)

In contrast, in terms of  $\mathbf{E}$  and  $\mathbf{B}$ , the interaction is simply the Lorentz force equation

$$\mathcal{F}(\mathbf{r},t) = \rho \mathbf{E}(\mathbf{r},t) + \mathbf{J} \times \mathbf{B}(\mathbf{r},t), \qquad (8.36)$$

where  $\mathcal{F}(\mathbf{r}, t)$  is the force per unit volume. The interaction is local, meaning that only physical quantities at  $\mathbf{r}$  is involved. This is why it is advantageous to treat electromagnetic fields as real physical quantities such that we do not always need to know where the sources are and what they are doing. As a matter of fact, no one has ever looked at a charge as a banana in one's hand; we know the existence of charges only through their interaction with other charges. Therefore, in physics the interaction between various physical quantities is the only thing we are sure about. In this point of view electromagnetic fields are physically as real as charges and currents.

#### 8.3. Electromagnetic Waves

When there is no charge or current, Eqs. (8.32) and (8.33) become the wave equations. They show that even when locally there is no source of the electromagnetic field, the electromagnetic field can still exist as waves. The prediction of the existence of electromagnetic waves is a great triumph of the Maxwell equations. It turns out that  $1/\sqrt{\mu_0\epsilon_0}$ , the phase velocity of the electromagnetic wave, is the same as the speed of light. Hence Maxwell equations also suggested that light is a kind of electromagnetic waves.

The existence of electromagnetic waves can also be seen directly from the Maxwell equations without going through the scalar and vector potentials. By taking the curl of both sides of Eq. (8.13), we have

$$\nabla \times (\nabla \times \mathbf{E}) = -\frac{\partial}{\partial t} \nabla \times \mathbf{B}.$$
(8.37)

Using  $\mu \mathbf{H} = \mathbf{B}$  and Eq. (8.15) to replace  $\nabla \times \mathbf{B}$ , we have

$$\nabla \times (\nabla \times \mathbf{E}) = \nabla (\nabla \cdot \mathbf{E}) - \nabla^2 \mathbf{E} = -\mu \frac{\partial}{\partial t} \left( \mathbf{J} + \frac{\partial \mathbf{D}}{\partial t} \right).$$
(8.38)

Using  $\epsilon \mathbf{E} = \mathbf{D}$  and Eq. (8.11)

$$\nabla^{2}\mathbf{E} - \mu\epsilon \frac{\partial^{2}\mathbf{E}}{\partial t^{2}} = \frac{1}{\epsilon}\nabla\rho + \mu \frac{\partial \mathbf{J}}{\partial t}.$$
(8.39)

Similarly, taking the curl of both sides of Eq. (8.15) and using  $\epsilon \mathbf{E} = \mathbf{D}$ ,  $\mu \mathbf{H} = \mathbf{B}$ , we have

$$\nabla \times (\nabla \times \mathbf{B}) = \mu \nabla \times \mathbf{J} + \mu \epsilon \frac{\partial}{\partial t} \nabla \times \mathbf{E}.$$
 (8.40)

Using Eq. (8.13) to replace  $\nabla \times \mathbf{E}$ , we have

$$\nabla \times (\nabla \times \mathbf{B}) = \nabla (\nabla \cdot \mathbf{B}) - \nabla^2 \mathbf{B} = \mu \nabla \times \mathbf{J} - \mu \epsilon \frac{\partial^2 \mathbf{B}}{\partial t^2}, \quad (8.41)$$

or

$$\nabla^2 \mathbf{B} - \mu \epsilon \frac{\partial^2 \mathbf{B}}{\partial t^2} = -\mu \nabla \times \mathbf{J}.$$
(8.42)

When there is no charge or current, **E** and **B** can still exist as waves with phase velocity  $v = 1/\sqrt{\mu\epsilon}$  in media and  $v = 1/\sqrt{\mu_0\epsilon_0} = c$  in vacuum.

### 8.4 Radiation by Charge Acceleration

Let us look into the solutions of Eqs. (8.27) and (8.28). The equations are of the form

$$\nabla^2 \phi(\mathbf{r}, t) - \frac{1}{c^2} \frac{\partial^2 \phi(\mathbf{r}, t)}{\partial t^2} = -f(\mathbf{r}, t).$$
(8.43)

By expanding  $\phi(\mathbf{r}, t)$  and  $f(\mathbf{r}, t)$  into a superposition of modes with time dependent amplitudes,

$$\phi(\mathbf{r},t) = \sum_{\mathbf{k}} a(\mathbf{k},t) u_{\mathbf{k}}(\mathbf{r}), \qquad (8.44)$$

$$f(\mathbf{r},t) = \sum_{\mathbf{k}} g(\mathbf{k},t) u_{\mathbf{k}}(\mathbf{r}), \qquad (8.45)$$

we have

$$\sum_{\mathbf{k}} \left[ \nabla^2 u_{\mathbf{k}}(\mathbf{r}) a(\mathbf{k}, t) - \frac{1}{c^2} u_{\mathbf{k}}(\mathbf{r}) \ddot{a}(\mathbf{k}, t) \right] = -\sum_{\mathbf{k}} u_{\mathbf{k}}(\mathbf{r}) g(\mathbf{k}, t).$$
(8.46)

For simplicity, let us choose  $u_{\mathbf{k}}(\mathbf{r})$  to be the Fourier components  $\exp(i\mathbf{k} \cdot \mathbf{r})$ . Then we have

$$\sum_{\mathbf{k}} \left[ -k^2 u_{\mathbf{k}}(\mathbf{r}) a(\mathbf{k}, t) - \frac{1}{c^2} u_{\mathbf{k}}(\mathbf{r}) \ddot{a}(\mathbf{k}, t) \right] = -\sum_{\mathbf{k}} u_{\mathbf{k}}(\mathbf{r}) g(\mathbf{k}, t).$$
(8.47)

Because  $\exp(i\mathbf{k} \cdot \mathbf{r})$  forms a complete orthonormal basis, we have

$$k^{2}a(\mathbf{k},t) + \frac{1}{c^{2}}\ddot{a}(\mathbf{k},t) = g(\mathbf{k},t).$$
 (8.48)

For each  $\mathbf{k}$ , this is the equation of a driven harmonic oscillator. In reality any harmonic oscillator must have a damping factor, no matter how small it is. Similarly we can add a damping term to Eq. (8.48) even though it is negligibly small. The reason we keep it here is that it helps in the following calculation. With the damping term added Eq. (8.48) becomes

$$k^{2}a(\mathbf{k},t) + \frac{\gamma}{c^{2}}\dot{a}(\mathbf{k},t) + \frac{1}{c^{2}}\ddot{a}(\mathbf{k},t) = g(\mathbf{k},t), \qquad (8.49)$$

where  $\gamma$  is a positive constant. For each **k** this is the same equation as that of a driven harmonic oscillator, which has been solved in Eq. (3.11). Therefore we may write out the solution directly. In the case  $\gamma \to 0$  we have

$$a(\mathbf{k},t) = \frac{c}{k} \int_{t>t'} \sin[ck(t-t')]g(\mathbf{k},t') \, dt'.$$
(8.50)

### 8.5. Retarded Potentials

In the above analysis, we see that electromagnetic waves are driven by time-varying charges and currents. If the electromagnetic radiation is produced by currents in a charge neutral environment such as a metal wire, we have  $\rho = 0$ . In this case we see **J** must be a function of time in order to produce radiation ( $\omega \neq 0$ ). In other words, electromagnetic waves are produced by accelerating charges.

# 8.5 Retarded Potentials

According to Eq. (1.346), in the spherically symmetric case Eq. (8.27) becomes

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left[r^2\frac{\partial\phi(r,t)}{\partial r}\right] - \frac{1}{c^2}\frac{\partial^2\phi(r,t)}{\partial t^2} = -\frac{\rho(r,t)}{\epsilon_0}.$$
(8.51)

Let us change the variable to  $u(r,t) \equiv r\phi(r,t)$ , we have

$$\frac{1}{r} \left[ \frac{\partial^2 u(r,t)}{\partial r^2} - \frac{1}{c^2} \frac{\partial^2 u(r,t)}{\partial t^2} \right] = -\frac{\rho(r,t)}{\epsilon_0}.$$
(8.52)

For a point charge at  $\mathbf{r} = 0$ , we have

$$\left[\frac{\partial^2 u(r,t)}{\partial r^2} - \frac{1}{c^2} \frac{\partial^2 u(r,t)}{\partial t^2}\right] = 0, \qquad (8.53)$$

except for  $\mathbf{r} = 0$ . The solution is

$$u(r,t) = \sum_{k} a_k(t) e^{ikr},$$
 (8.54)

where  $a_k(t)$  satisfies the equation for the harmonic oscillator.

$$\ddot{a}_k(t) + c^2 k^2 a_k(t) = 0. ag{8.55}$$

Define  $\omega \equiv ck$ , we have

$$u(r,t) = \sum_{k} c_k e^{i(kr - \omega t)} + d_k e^{i(kr + \omega t)}.$$
(8.56)

At this point let us focus our attention only on the outgoing wave, then we choose only the first term

$$u(r,t) = \sum_{k} c_k e^{i(kr-\omega t)}.$$
(8.57)

Hence

$$\phi(r,t) = \sum_{k} c_k \frac{e^{i(kr-\omega t)}}{r}.$$
(8.58)

This is the outgoing-wave solution of Eq. (8.51) for  $\mathbf{r} \neq 0$  when the only source of  $\phi$  is a point charge at  $\mathbf{r} = 0$ . Let us expand  $\rho(r, t)$  into a Fourier series,

$$-\frac{\rho(r,t)}{\epsilon_0} = -\frac{1}{\epsilon_0} \sum_{\omega} \tilde{\rho}(r,\omega) e^{-i\omega t}$$
(8.59)

and substitute it and Eq. (8.58) back into Eq. (8.51). We have

$$\sum_{k} c_{k} e^{-i\omega t} \left[ \nabla^{2} \left( \frac{e^{ikr}}{r} \right) + k^{2} \frac{e^{ikr}}{r} \right] = -\frac{1}{\epsilon_{0}} \sum_{\omega} \tilde{\rho}(r,\omega) e^{-i\omega t}.$$
(8.60)

Since  $\omega = ck$ , we may replace  $\sum_k$  in Eq. (8.60) by  $\sum_{\omega}$ . Comparing coefficients, we have

$$c_k \left[ \nabla^2 \left( \frac{e^{ikr}}{r} \right) + k^2 \frac{e^{ikr}}{r} \right] = -\frac{1}{\epsilon_0} \tilde{\rho}(r, \omega).$$
(8.61)

Since  $\tilde{\rho}(r, \omega) = 0$  except at  $\mathbf{r} = 0$ , we may integrate the above equation over a small sphere  $\sigma$  with radius  $r_{\sigma}$  around the origin.

$$c_k \int_{\sigma} \left[ \nabla^2 \left( \frac{e^{ikr}}{r} \right) + k^2 \frac{e^{ikr}}{r} \right] d^3 \mathbf{r} = -\frac{1}{\epsilon_0} \int_{\sigma} \tilde{\rho}(r,\omega) d^3 \mathbf{r}.$$
(8.62)

The second term on the left-hand side approaches zero as  $r_\sigma \to 0$  because

$$\begin{aligned} \int_{\sigma} \frac{e^{ikr}}{r} d^{3}\mathbf{r} &| \leq \int_{\sigma} \frac{1}{r} d^{3}\mathbf{r} \\ &= \int_{0}^{r_{\sigma}} 4\pi r dr \\ &= 2\pi r_{\sigma}^{2}. \end{aligned}$$
(8.63)

The first term can be reduced to a surface integral by Gauss' theorem.

$$c_{k} \int_{\sigma} \nabla^{2} \left( \frac{e^{ikr}}{r} \right) d^{3}\mathbf{r}$$

$$= c_{k} \int_{\sigma} \nabla \cdot \left[ ik \frac{e^{ikr}}{r} \hat{\mathbf{r}} + e^{ikr} \nabla \left( \frac{1}{r} \right) \right] d^{3}\mathbf{r}$$

$$= c_{k} \int_{s_{\sigma}} \left[ ik \frac{e^{ikr}}{r} \hat{\mathbf{r}} + e^{ikr} \nabla \left( \frac{1}{r} \right) \right] \cdot d\mathbf{a}, \qquad (8.64)$$

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### 8.5. Retarded Potentials

where  $s_{\sigma}$  is the surface of  $\sigma$ . The first term on the right-hand side approaches zero as  $r_{\sigma} \to 0$ , because

$$\left| \int_{s_{\sigma}} \frac{e^{ikr}}{r} \hat{\mathbf{r}} \cdot d\mathbf{a} \right| \le \frac{1}{r_{\sigma}} 4\pi r_{\sigma}^2 \tag{8.65}$$

The second term is equal to  $-4\pi c_k$  as  $r_{\sigma} \to 0$ , because

$$\lim_{r_{\sigma} \to 0} e^{ikr_{\sigma}} \to 1, \tag{8.66}$$

and

$$\lim_{r_{\sigma}\to 0} \int_{s_{\sigma}} \nabla\left(\frac{1}{r}\right) \cdot d\mathbf{a} = \lim_{r_{\sigma}\to 0} \int_{s_{\sigma}} \left(\frac{-\hat{\mathbf{r}}}{r^2}\right) \cdot d\mathbf{a} = -4\pi.$$
(8.67)

Hence

$$c_k = \frac{1}{4\pi\epsilon_0} \int_{\sigma} \tilde{\rho}(r',\omega) \, d^3 \mathbf{r}'. \tag{8.68}$$

Putting  $c_k$  back into Eq. (8.58), we have

$$\begin{split} \phi(r,t) &= \frac{1}{4\pi\epsilon_0} \sum_k \frac{e^{i(kr-\omega t)}}{r} \int_{\sigma} \tilde{\rho}(r',\omega) \, d^3 \mathbf{r}' \\ &= \frac{1}{4\pi\epsilon_0} \frac{1}{r} \int_{\sigma} \sum_k \tilde{\rho}(r',\omega) e^{-i(\omega t-kr)} \, d^3 \mathbf{r}' \\ &= \frac{1}{4\pi\epsilon_0} \frac{1}{r} \int_{\sigma} \sum_{\omega} \tilde{\rho}(r',\omega) e^{-i\omega(t-r/c)} \, d^3 \mathbf{r}' \\ &= \frac{1}{4\pi\epsilon_0} \int_{\sigma} \frac{\rho(r',t')}{r} \, d^3 \mathbf{r}', \end{split}$$
(8.69)

where t' = t - r/c. Eq. (8.69) describes the scalar potential produced by a time-varying charge density at the origin. If there is charge density in other locations, by superposition of  $\phi$  we have

$$\phi(\mathbf{r},t) = \frac{1}{4\pi\epsilon_0} \int \frac{\rho(\mathbf{r}',t')}{|\mathbf{r}-\mathbf{r}'|} d^3\mathbf{r}'.$$
(8.70)

This is called the retarded scalar potential. It describes the scalar potential at  $(\mathbf{r}, t)$  produced by a time-varying charge density at  $(\mathbf{r}', t')$  with  $t' = t - |\mathbf{r} - \mathbf{r}'|/c$ .

Similarly, we have the retarded vector potential

$$\mathbf{A}(\mathbf{r},t) = \frac{\mu_0}{4\pi} \int \frac{\mathbf{J}(\mathbf{r}',t')}{|\mathbf{r}-\mathbf{r}'|} d^3 \mathbf{r}'$$
(8.71)

which describes the vector potential at  $(\mathbf{r}, t)$  produced by a time-varying current density at  $(\mathbf{r}', t')$  with  $t' = t - |\mathbf{r} - \mathbf{r}'|/c$ .

### 8.6 Energy Density of Electromagnetic Fields

For a static charge distribution in a static external electric field, the potential energy is

$$U_E = \int \rho(\mathbf{r})\phi(\mathbf{r}) \, d^3\mathbf{r}. \tag{8.72}$$

Let us write  $\rho(\mathbf{r}) = \alpha n(\mathbf{r})$ , where  $\alpha$  is a scalar proportional constant. If  $\phi(\mathbf{r})$  is established by the charge distribution itself, then  $\phi(\mathbf{r})$  is also proportional to  $\alpha$ , namely  $\phi(\mathbf{r}) = \alpha \psi(\mathbf{r})$ . The potential energy stored in the charge distribution is the energy spent in building up the distribution as we let  $\alpha$  increase from 0 to its final value.

$$U_E = \int_0^\alpha \alpha d\alpha \int n(\mathbf{r})\psi(\mathbf{r}) \, d^3\mathbf{r} = \frac{1}{2} \int \rho(\mathbf{r})\phi(\mathbf{r}) \, d^3\mathbf{r}.$$
 (8.73)

Using the identity  $\nabla \cdot (\psi \mathbf{a}) = \psi \nabla \cdot \mathbf{a} + \mathbf{a} \cdot \nabla \psi$ , we may write Eq. (8.73) in a different form:

$$U_{E} = \frac{1}{2} \int \rho(\mathbf{r})\phi(\mathbf{r}) d^{3}\mathbf{r}$$
  

$$= \frac{1}{2} \int [\nabla \cdot \mathbf{D}(\mathbf{r})]\phi(\mathbf{r}) d^{3}\mathbf{r}$$
  

$$= \frac{1}{2} \int \nabla \cdot [\phi(\mathbf{r})\mathbf{D}(\mathbf{r})] d^{3}\mathbf{r} - \frac{1}{2} \int \mathbf{D}(\mathbf{r}) \cdot [\nabla \phi(\mathbf{r})] d^{3}\mathbf{r}$$
  

$$= \frac{1}{2} \int_{S} \phi(\mathbf{r})\mathbf{D}(\mathbf{r}) \cdot d\mathbf{a} - \frac{1}{2} \int \mathbf{D}(\mathbf{r}) \cdot [\nabla \phi(\mathbf{r})] d^{3}\mathbf{r}$$
  

$$= \frac{1}{2} \int \mathbf{D}(\mathbf{r}) \cdot \mathbf{E}(\mathbf{r}) d^{3}\mathbf{r}, \qquad (8.74)$$

where we assume the surface integral of  $\phi(\mathbf{r})\mathbf{D}(\mathbf{r})$  at infinity vanishes. The equivalence between Eq. (8.73) and Eq. (8.74) suggests that we may look at the electric potential energy from two different points of view, one as the energy stored in the charges in a potential field according to Eq. (8.73), the other as the energy stored in the field itself according to Eq. (8.74). Using the equation  $\nabla \cdot \mathbf{E} = \rho/\epsilon_0$ , we may switch between these two points of view freely. If we allow the charges to move by themselves, the movement will reduce the potential energy, and the difference will be converted to the kinetic energy of the charges. Conversely, if the kinetic energy of the charges is decreased, it is converted into potential energy described by Eq. (8.73), which can also be viewed as the energy stored in the electric fields according to Eq. (8.74).

### 8.6. Energy Density of Electromagnetic Fields

For a static current distribution in a static magnetic field, the situation is different. In Eqs. (7.59) and (7.67) we have shown that if the force experienced by a static current distribution in a static magnetic field is considered, the potential energy is

$$U_m = -\int \mathbf{J}(\mathbf{r}) \cdot \mathbf{A}(\mathbf{r}) \, d^3 \mathbf{r}.$$
(8.75)

However, since  $\mathbf{v} \times \mathbf{B}$  is perpendicular to  $\mathbf{v}$ , the magnetic field cannot change the kinetic energy of the charges. Where does this potential energy come from then? It turns out that Eq. (8.75) does not account for the total change of energy, because it requires an external battery to maintain the static current distribution. As a current is moved across a magnetic field, the Lorentz force will generate an equivalent electromotive force as shown in Eq. (8.7). If the electromotive force is anti-parallel to the current density, the external battery must do extra work against this electromotive force. If the electromotive force is parallel to the current density, the external battery can save work by using the electromotive force as part of the driving force. Therefore, the extra power delivered by the battery for a current density  $\mathbf{J}(\mathbf{r}' - \mathbf{r})$  is

$$P^{(I)}(\mathbf{r}) = -\int \mathbf{E}^{(I)}(\mathbf{r}') \cdot \mathbf{J}(\mathbf{r}' - \mathbf{r}) d^{3}\mathbf{r}'$$
  
$$= -\int [\mathbf{v} \times \mathbf{B}(\mathbf{r}')] \cdot \mathbf{J}(\mathbf{r}' - \mathbf{r}) d^{3}\mathbf{r}'$$
  
$$= \int [\mathbf{J}(\mathbf{r}' - \mathbf{r}) \times \mathbf{B}(\mathbf{r}')] \cdot \mathbf{v} d^{3}\mathbf{r}', \qquad (8.76)$$

where  $\mathbf{v}$  is the velocity of the parallel-moving current density and  $\mathbf{E}^{(I)}(\mathbf{r}')$  is the electric field induced by the Faraday's law. The energy delivered within a time dt by the battery is therefore

$$P^{(I)}(\mathbf{r}) dt = d\mathbf{r} \cdot \int \mathbf{J}(\mathbf{r}' - \mathbf{r}) \times \mathbf{B}(\mathbf{r}') d^3 \mathbf{r}', \qquad (8.77)$$

where  $\mathbf{r}$  is the parallel displacement of the current density distribution. In other words, the energy  $U_b$  stored in the external battery has changed by

$$dU_b = -d\mathbf{r} \cdot \int \mathbf{J}(\mathbf{r}' - \mathbf{r}) \times \mathbf{B}(\mathbf{r}') d^3 \mathbf{r}', \qquad (8.78)$$

That is

$$\nabla U_b(\mathbf{r}) = -\int \mathbf{J}(\mathbf{r}' - \mathbf{r}) \times \mathbf{B}(\mathbf{r}') d^3 \mathbf{r}', \qquad (8.79)$$

Comparing with Eq. (7.67), we see  $U_m = U_b$ . The mechanical potential energy  $U_m$  is simply the energy stored in the external battery.

Let us investigate how much energy is needed to build up a static magnetic field. In this case we do not parallel-move the current density distribution. Instead, we increase the magnetic field while keeping the current density distribution fixed. The total power supplied by the external battery that maintains the current density distribution is

$$P = -\int \mathbf{E}(\mathbf{r}) \cdot \mathbf{J}(\mathbf{r}) d^{3}\mathbf{r}$$
  
= 
$$\int \left[\nabla \phi + \frac{\partial \mathbf{A}}{\partial t}\right] \cdot \mathbf{J} d^{3}\mathbf{r}$$
  
= 
$$\int \left[\nabla \cdot (\phi \mathbf{J}) - \phi \nabla \cdot \mathbf{J} + \frac{\partial \mathbf{A}}{\partial t} \cdot \mathbf{J}\right] d^{3}\mathbf{r}.$$
 (8.80)

Assuming there is no current on the boundary surface in the infinity, the first term on the right-hand side is zero. The second term on the right-hand side is also zero because  $\nabla \cdot \mathbf{J} = 0$ . Therefore

$$P = \int \mathbf{J} \cdot \frac{\partial \mathbf{A}}{\partial t} d^3 \mathbf{r}.$$
 (8.81)

The total energy supplied by the battery to build up  $\mathbf{A}(\mathbf{r})$  while maintaining  $\mathbf{J}(\mathbf{r})$  fixed is

$$U_B = \int \mathbf{J}(\mathbf{r}) \cdot \mathbf{A}(\mathbf{r}) \, d^3 \mathbf{r}. \tag{8.82}$$

To see more clearly the physical meaning of Eq. (8.82), let us rewrite Eq. (8.76) in the following way.

$$P^{(I)}(\mathbf{r}) = \int \mathbf{v} \cdot [\mathbf{J}(\mathbf{r}' - \mathbf{r}) \times \mathbf{B}(\mathbf{r}')] d^{3}\mathbf{r}'$$
  

$$= -\int \mathbf{B}(\mathbf{r}') \cdot [\mathbf{J}(\mathbf{r}' - \mathbf{r}) \times \mathbf{v}] d^{3}\mathbf{r}'$$
  

$$= -\int \nabla' \times \mathbf{A}(\mathbf{r}') \cdot [\mathbf{J}(\mathbf{r}' - \mathbf{r}) \times \mathbf{v}] d^{3}\mathbf{r}'$$
  

$$= \int \nabla' \cdot \{[\mathbf{J}(\mathbf{r}' - \mathbf{r}) \times \mathbf{v}] \times \mathbf{A}(\mathbf{r}')\} d^{3}\mathbf{r}'$$
  

$$-\int \nabla' \times [\mathbf{J}(\mathbf{r}' - \mathbf{r}) \times \mathbf{v}] \cdot \mathbf{A}(\mathbf{r}') d^{3}\mathbf{r}'$$
  

$$= \int_{S} \{[\mathbf{J}(\mathbf{r}' - \mathbf{r}) \times \mathbf{v}] \times \mathbf{A}(\mathbf{r}')\} \cdot d\mathbf{a}'$$
  

$$+ \int \nabla \times [\mathbf{J}(\mathbf{r}' - \mathbf{r}) \times \mathbf{v}] \cdot \mathbf{A}(\mathbf{r}') d^{3}\mathbf{r}'. \quad (8.83)$$

In the derivation we have used the facts that  $\mathbf{v}$  does not depend on  $\mathbf{r}$  or  $\mathbf{r}'$  and  $\nabla'$  operated on  $\mathbf{J}(\mathbf{r}'-\mathbf{r})$  is equal to  $-\nabla$  operated on  $\mathbf{J}(\mathbf{r}'-\mathbf{r})$ . Assuming there

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is no current on the boundary surface in the infinity, the surface integration in Eq. (8.83) is zero. Using the identity

$$\nabla \times (\mathbf{J} \times \mathbf{v}) = -\mathbf{v}(\nabla \cdot \mathbf{J}) + (\mathbf{v} \cdot \nabla)\mathbf{J}, \qquad (8.84)$$

and noting that  $\nabla \cdot \mathbf{J} = 0$ , we obtain

$$P^{(I)}(\mathbf{r}) = \int [(\mathbf{v} \cdot \nabla) \mathbf{J}(\mathbf{r}' - \mathbf{r})] \cdot \mathbf{A}(\mathbf{r}') d^3 \mathbf{r}'. \qquad (8.85)$$

Because

$$\frac{d\mathbf{J}(\mathbf{r}'-\mathbf{r})}{dt} = \frac{\partial \mathbf{J}}{\partial t} + (\mathbf{v} \cdot \nabla)\mathbf{J}(\mathbf{r}'-\mathbf{r})$$
(8.86)

and  $\partial \mathbf{J}/\partial t = 0$ , Eq. (8.85) can be reduced to

$$P^{(I)}(\mathbf{r}) = \int \frac{d\mathbf{J}(\mathbf{r}' - \mathbf{r})}{dt} \cdot \mathbf{A}(\mathbf{r}') d^3 \mathbf{r}'.$$
(8.87)

That is

$$P^{(\mathrm{I})} = \int \frac{d\mathbf{J}(\mathbf{r}')}{dt} \cdot \mathbf{A}(\mathbf{r}') d^3 \mathbf{r}'.$$
(8.88)

Combining Eqs. (8.81), (8.82), and (8.88), we see

$$\frac{dU_B}{dt} = \int \left[ \frac{d\mathbf{J}(\mathbf{r})}{dt} \cdot \mathbf{A}(\mathbf{r}) + \mathbf{J}(\mathbf{r}) \cdot \frac{\partial \mathbf{A}(\mathbf{r})}{\partial t} \right] d^3\mathbf{r}$$
$$= P^{(I)} + P.$$
(8.89)

Therefore  $U_B$  is the total energy supplied by the batteries to build up the combination of  $\mathbf{J}(\mathbf{r})$  and  $\mathbf{A}(\mathbf{r})$ . This energy can be thought of as the energy stored in the configuration specified by  $\mathbf{J}(\mathbf{r})$  and  $\mathbf{A}(\mathbf{r})$ .

Let us write  $\mathbf{J}(\mathbf{r}) = \beta \mathbf{j}(\mathbf{r})$ , where  $\beta$  is a scalar proportional constant. If  $\mathbf{A}(\mathbf{r})$  is established by the current distribution itself, then  $\mathbf{A}(\mathbf{r})$  is also proportional to  $\beta$ , namely  $\mathbf{A}(\mathbf{r}) = \beta \mathbf{a}(\mathbf{r})$ . The potential energy stored in the current distribution is the energy spent in building up the distribution as we let  $\beta$  increase from 0 to its final value.

$$U_B = \int_0^\beta \beta d\beta \int \mathbf{j}(\mathbf{r}) \cdot \mathbf{a}(\mathbf{r}) \, d^3 \mathbf{r} = \frac{1}{2} \int \mathbf{J}(\mathbf{r}) \cdot \mathbf{A}(\mathbf{r}) \, d^3 \mathbf{r}.$$
(8.90)

### CHAPTER 8. ELECTRODYNAMICS

Using  $\nabla \cdot (\mathbf{a} \times \mathbf{b}) = \mathbf{b} \cdot (\nabla \times \mathbf{a}) - \mathbf{a} \cdot (\nabla \times \mathbf{b})$  and Gauss' theorem, we have

$$U_{B} = \frac{1}{2} \int \mathbf{J}(\mathbf{r}) \cdot \mathbf{A}(\mathbf{r}) d^{3}\mathbf{r}$$
  

$$= \frac{1}{2} \int [\nabla \times \mathbf{H}(\mathbf{r})] \cdot \mathbf{A}(\mathbf{r}) d^{3}\mathbf{r}$$
  

$$= \frac{1}{2} \int \nabla \cdot [\mathbf{H}(\mathbf{r}) \times \mathbf{A}(\mathbf{r})] d^{3}\mathbf{r} + \frac{1}{2} \int \mathbf{H}(\mathbf{r}) \cdot [\nabla \times \mathbf{A}(\mathbf{r})] d^{3}\mathbf{r}$$
  

$$= \frac{1}{2} \int_{S} [\mathbf{H}(\mathbf{r}) \times \mathbf{A}(\mathbf{r})] \cdot d\mathbf{a} + \frac{1}{2} \int \mathbf{H}(\mathbf{r}) \cdot [\nabla \times \mathbf{A}(\mathbf{r})] d^{3}\mathbf{r}$$
  

$$= \frac{1}{2} \int \mathbf{H}(\mathbf{r}) \cdot \mathbf{B}(\mathbf{r}) d^{3}\mathbf{r}, \qquad (8.91)$$

where we assume the surface integral of  $\mathbf{H}(\mathbf{r}) \times \mathbf{A}(\mathbf{r})$  vanishes at infinity.

Let us consider now the energy density of time-varying electromagnetic fields. The increase rate of the mechanical energy of a system of charged particles can be written as

$$P_m = \sum_{i} \mathbf{F}_i \cdot \mathbf{v}_i = \sum_{i} q_i \left[ \mathbf{E}(\mathbf{r}_i) + \mathbf{v}_i \times \mathbf{B}(\mathbf{r}_i) \right] \cdot \mathbf{v}_i$$
$$= \int \mathbf{E}(\mathbf{r}) \cdot \mathbf{J}(\mathbf{r}) d^3 \mathbf{r}.$$
(8.92)

Replacing  $\mathbf{J}$  by using the Ampere-Maxwell law,

$$P_m = \int \left[ \mathbf{E} \cdot (\nabla \times \mathbf{H}) - \mathbf{E} \cdot \frac{\partial \mathbf{D}}{\partial t} \right] d^3 \mathbf{r}.$$
 (8.93)

Using the vector identity

$$\nabla \cdot (\mathbf{a} \times \mathbf{b}) = \mathbf{b} \cdot (\nabla \times \mathbf{a}) - \mathbf{a} \cdot (\nabla \times \mathbf{b})$$
(8.94)

and Faraday's law, we have

$$P_{m} = -\int \left[ \nabla \cdot (\mathbf{E} \times \mathbf{H}) - \mathbf{H} \cdot (\nabla \times \mathbf{E}) + \mathbf{E} \cdot \frac{\partial \mathbf{D}}{\partial t} \right] d^{3}\mathbf{r}$$
$$= -\int \left[ \nabla \cdot (\mathbf{E} \times \mathbf{H}) + \mathbf{H} \cdot \frac{\partial \mathbf{B}}{\partial t} + \mathbf{E} \cdot \frac{\partial \mathbf{D}}{\partial t} \right] d^{3}\mathbf{r}.$$
(8.95)

Define

$$U \equiv \frac{1}{2} (\mathbf{E} \cdot \mathbf{D} + \mathbf{B} \cdot \mathbf{H}), \qquad (8.96)$$

and

$$\mathbf{S} \equiv \mathbf{E} \times \mathbf{H}.\tag{8.97}$$

For media with linear polarization and magnetization, we have

$$-\mathbf{E} \cdot \mathbf{J} = \frac{\partial U}{\partial t} + \nabla \cdot \mathbf{S}.$$
(8.98)

This is known as the **Poynting's theorem**, and **S** is called the Poynting vector. Since the decrease of the mechanical energy must be equal to the increase of the electromagnetic energy, Poynting's theorem suggests that U is the energy density of the electromagnetic field, and **S** is the energy flux density.

# 8.7 Inductors and Transformers

Consider the interaction of two circuits fixed in space through Faraday's law. The electromotive forces in the circuits are induced by the total magnetic fluxes that go through the surfaces enclosed by the circuits. For each circuit, electromotive force arises from two contributions. One is the magnetic flux generated by the current in the circuit itself, and the other is the magnetic flux produced by the other circuit.

$$\mathcal{E}_1 = -\frac{d}{dt} \int (\mathbf{B}_1 + \mathbf{B}_2) \cdot d\mathbf{a}_1, \qquad (8.99)$$

where  $\mathcal{E}_1$  is the electromotive force induced in circuit 1,  $d\mathbf{a}_1$  is the surface element of the surface enclosed by circuit 1, and  $\mathbf{B}_1$  and  $\mathbf{B}_2$  are the magnetic flux densities generated by circuit 1 and circuit 2 respectively. Using Eq. (7.27), we have

$$\mathcal{E}_1 = -\frac{d}{dt} \int \nabla \times (\mathbf{A}_1 + \mathbf{A}_2) \cdot d\mathbf{a}_1.$$
(8.100)

Applying the Stokes theorem, we have

$$\mathcal{E}_1 = -\frac{d}{dt} \oint (\mathbf{A}_1 + \mathbf{A}_2) \cdot d\mathbf{s}_1.$$
(8.101)

Substituting Eq. (7.36) in for the vector potentials, we have

$$\mathcal{E}_{1} = -\frac{\mu_{0}}{4\pi} \frac{d}{dt} \oint \left( \int \frac{\mathbf{J}_{1}(\mathbf{r}_{1}')}{|\mathbf{r}_{1} - \mathbf{r}_{1}'|} d^{3}\mathbf{r}_{1}' + \int \frac{\mathbf{J}_{2}(\mathbf{r}_{2})}{|\mathbf{r}_{1} - \mathbf{r}_{2}|} d^{3}\mathbf{r}_{2} \right) \cdot d\mathbf{s}_{1}.$$
(8.102)

Note that  $\mathbf{J}_1(\mathbf{r}'_1) d^3 \mathbf{r}'_1 = I_1 d\mathbf{s}'_1$  and  $\mathbf{J}_2(\mathbf{r}_2) d^3 \mathbf{r}_2 = I_2 d\mathbf{s}_2$ . The replacement leads to

$$\mathcal{E}_1 = -\frac{\mu_0}{4\pi} \left( \frac{dI_1}{dt} \oint \oint \frac{d\mathbf{s}_1' \cdot d\mathbf{s}_1}{|\mathbf{r}_1 - \mathbf{r}_1'|} + \frac{dI_2}{dt} \oint \oint \frac{d\mathbf{s}_2 \cdot d\mathbf{s}_1}{|\mathbf{r}_1 - \mathbf{r}_2|} \right).$$
(8.103)

The self-inductance of circuit 1 is defined by

$$L_{11} = \frac{\mu_0}{4\pi} \oint \oint \frac{d\mathbf{s}_1' \cdot d\mathbf{s}_1}{|\mathbf{r}_1 - \mathbf{r}_1'|},\tag{8.104}$$

and the mutual inductance between circuit 1 and circuit 2 is defined by

$$L_{12} = \frac{\mu_0}{4\pi} \oint \oint \frac{d\mathbf{s}_2 \cdot d\mathbf{s}_1}{|\mathbf{r}_1 - \mathbf{r}_2|},\tag{8.105}$$

In terms of self-inductance and mutual inductance, Eq. (8.103) can be written as

$$\mathcal{E}_1 = -L_{11} \frac{dI_1}{dt} - L_{12} \frac{dI_2}{dt}.$$
(8.106)

An inductor is a wire loop with a significant self-inductance. According to Lenz' law, the induced current works against the change of the magnetic flux, therefore an inductor has a tendency of resisting the change of current that flows through it. In contrast to a capacitor, which stores energy in the electric field, an inductor can be thought as a device that stores energy in the magnetic field. Let us "charge up" an inductor by turning on the current gradually from 0 to I. As the current is increased, an electric field builds up against the flow of the current. Between t and  $t + \Delta t$ , the work done by the external device that drives the current is simply

$$\Delta w = \Delta q \oint \mathbf{E} \cdot (-d\mathbf{l})$$
$$= I \Delta t \left( L \frac{dI}{dt} \right). \tag{8.107}$$

The minus sign in the first equality means the charge is transported against the **E** field. In other words, the motion of the charge is in the opposite direction of the line element  $d\mathbf{l}$ . In the limit of  $\Delta t \to 0$ ,

$$dw = LI \, dI. \tag{8.108}$$

Hence the energy stored in an inductor L is

$$w = \int LI \, dI = \frac{LI^2}{2}.$$
 (8.109)

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We may also obtain the same result directly from Eq. (8.90). By replacing  $\mathbf{J}d^{3}\mathbf{r}$  with  $Id\mathbf{s}$  in Eqs. (8.90) and (7.36), Eq. (8.90) becomes

$$U_B = \frac{1}{2} \int \mathbf{J}(\mathbf{r}) \cdot \mathbf{A}(\mathbf{r}) d^3 \mathbf{r} = \frac{I}{2} \oint d\mathbf{s} \cdot \left[ \frac{\mu_0}{4\pi} \int \frac{\mathbf{J}(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d^3 \mathbf{r}' \right]$$
$$= \frac{I^2}{2} \frac{\mu_0}{4\pi} \oint \oint \frac{d\mathbf{s} \cdot d\mathbf{s}'}{|\mathbf{r} - \mathbf{r}'|} = \frac{LI^2}{2}.$$
(8.110)

Inductors are commonly made of solenoids. Let us calculate the inductance of an infinitely long linear solenoid. Because inductance is related to the magnetic flux enclosed by the wire loop, we only need to calculate the **B**-field inside the solenoid. Let the axis of the solenoid be the z-axis. By Eq. (7.1) we know that **B** can only have the z-component and the r-component, because **J** is in the  $\theta$ -direction. The symmetry between the +z and -z directions makes all the contributions to the r-component cancel. Therefore we only need to calculate  $B_z$ . By cylindrical symmetry and translational symmetry in z,  $B_z$  can be a function of r only. Let us choose a rectangular loop of integration that goes up along the z-axis and comes back parallel to the z-axis at a distance r from the z-axis. Ampere's law yields  $B_z(0) = B_z(r)$ , since the loop does not enclose any current. Therefore inside the solenoid  $B_z$  is a constant. Using Eq. (7.1) in cylindrical coordinates, we can calculate  $B_z(0)$ . Let R be the radius of the solenoid, we have

$$B_{z} = \frac{\mu_{0}}{4\pi} \int_{-\infty}^{\infty} \frac{J_{s} 2\pi R}{R^{2} + z^{2}} \frac{R}{\sqrt{R^{2} + z^{2}}} dz$$
$$= \frac{\mu_{0} J_{s}}{2} \int_{-\infty}^{\infty} \frac{1}{[1 + (z^{2}/R^{2})]^{3/2}} d\left(\frac{z}{R}\right).$$
(8.111)

By a change of variable  $\tan \theta = z/R$ , the integral can be evaluated.

$$B_{z} = \frac{\mu_{0}J_{s}}{2} \int_{-\infty}^{\infty} \frac{1}{(1 + \tan^{2}\theta)^{3/2}} d(\tan\theta)$$
  
=  $\frac{\mu_{0}J_{s}}{2} \int_{-\pi/2}^{+\pi/2} \cos\theta d\theta$   
=  $\mu_{0}J_{s} = \mu_{0}nI$ , (8.112)

where n is the number of turns per unit length. The electromotive force per unit length is

$$\mathcal{E} = -\frac{d}{dt}(nB_z A) = -\mu_0 n^2 A \frac{dI}{dt},$$
(8.113)

hence the inductance per unit length is

$$L = \mu_0 n^2 A, \tag{8.114}$$

Another example of inductor is a toroid of rectangular cross section. Assume the inner radius of the toroid is a and the outer radius is b, and the height is h. Using Ampere's law, the magnetic flux density at r is

$$B_{\theta}(r)2\pi r = \mu_0 NI, \qquad (8.115)$$

where N is the total number of turns. The magnetic flux is

$$\phi_m = \int_a^b \frac{\mu_0 NI}{2\pi r} h \, dr = \frac{\mu_0 NIh}{2\pi} \ln\left(\frac{b}{a}\right). \tag{8.116}$$

Since each turn picks up an  $\mathcal{E} = -d\phi_m/dt$ , the inductance is

$$L = \frac{\mu_0 N^2 h}{2\pi} \ln\left(\frac{b}{a}\right). \tag{8.117}$$

Similar to capacitors, the inductance of a solenoid or toroid can be greatly increased by using a paramagnetic material of large  $\mu$  as the core of the solenoid or toroid. For the same current hence the same **H**, the magnetic flux is proportional to  $\mu$ **H** instead of  $\mu_0$ **H**. Therefore the factor of increase is  $\mu/\mu_0 = \kappa_m$ .

A transformer is made of two inductors sharing the same magnetic flux. Because the magnetic flux is the same, the ratio of the electromotive force in the two inductors is equal to the ratio of the number of turns  $N_2/N_1$ . By driving one inductor with an alternating voltage  $V_1 \cos \omega t$ , one can induce an electromotive force equal to  $(N_2/N_1)V_1 \cos \omega t$  in the other inductor. Note that this does not violate energy conservation, because to produce the same magnetic flux the ratio of current is inversely proportional to the numbers of turns. Therefore  $V_1I_I = V_2I_2$ , which means the input power is equal to the output power. In long-distance transmission of electricity it is important to reduce the current, because the power loss due to resistance in the electric cable is equal to  $I^2R$ . By using a step-up transformer in the transmitting end and a step-down transformer in the receiving end, the current can be reduced. Without transformers the modern power distribution system we are enjoying is impossible.

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# 8.8 Dipole Radiation

Let us consider the radiation field of an oscillating dipole  $\mathbf{p}(t) = \mathbf{p}_0 e^{-i\omega t}$ . The current density corresponding to this oscillating dipole satisfies the following equation:

$$\int \mathbf{J}(\mathbf{r}',t') \, d^3 \mathbf{r}' = \sum_i q_i \mathbf{v}_i = -i\omega \sum_i q_i \mathbf{r}_i = -i\omega \mathbf{p} = -i\omega \mathbf{p}_0 e^{-i\omega t'}, \quad (8.118)$$

where  $\mathbf{v}_i$  and  $\mathbf{r}_i$  are the velocity and the displacement of the *i*th particle respectively. If the location of the observation point is far away from the dipole, we may replace  $|\mathbf{r} - \mathbf{r}'|$  by r in Eq. (8.71). Then we have

$$\mathbf{A}(\mathbf{r},t) = \frac{\mu_0}{4\pi r} \int \mathbf{J}(\mathbf{r}',t') d^3 \mathbf{r}' = \frac{-i\mu_0\omega}{4\pi r} \mathbf{p}_0 e^{-i\omega t'}$$
$$= \frac{-i\mu_0\omega}{4\pi r} \mathbf{p}_0 e^{i(kr-\omega t)}, \qquad (8.119)$$

where  $k = \omega/c$  and the factor  $e^{ikr}$  comes from the relation t' = t - r/c. **E** and **B** can be obtained by

$$\mathbf{B} = \nabla \times \mathbf{A}$$
$$-i\omega\mu_0\epsilon_0 \mathbf{E} = \nabla \times \mathbf{B}.$$
(8.120)

Namely,

$$\mathbf{B} = \frac{-i\mu_0\omega}{4\pi} \left(\frac{ik}{r} - \frac{1}{r^2}\right) e^{i(kr - \omega t)} \hat{\mathbf{r}} \times \mathbf{p}_0$$
(8.121)

$$\approx \quad \frac{\mu_0 ck^2}{4\pi} \hat{\mathbf{r}} \times \mathbf{p}_0 \frac{e^{i(kr - \omega t)}}{r}, \tag{8.122}$$

where we have assumed  $kr \gg 1$ . Under the same approximation

$$\mathbf{E} \approx -\frac{k^2}{4\pi\epsilon_0} \hat{\mathbf{r}} \times (\hat{\mathbf{r}} \times \mathbf{p}_0) \frac{e^{i(kr-\omega t)}}{r} = -c\hat{\mathbf{r}} \times \mathbf{B}.$$
(8.123)

If  $\mathbf{p}$  is in the  $\hat{\mathbf{z}}$ -direction, we have

$$\mathbf{B} \approx -\frac{\mu_0 ck^2}{4\pi} \frac{|\mathbf{p}_0| e^{i(kr-\omega t)}}{r} \sin\theta \hat{\boldsymbol{\phi}},\tag{8.124}$$

and

$$\mathbf{E} \approx -\frac{k^2}{4\pi\epsilon_0} \frac{|\mathbf{p}_0| e^{i(kr-\omega t)}}{r} \sin\theta \hat{\boldsymbol{\theta}}.$$
(8.125)

By Eq. (8.98), the intensity of the radiation field at a faraway location is

$$\overline{|\mathbf{E} \times \mathbf{H}|} = \frac{ck^4}{32\pi^2\epsilon_0} \frac{|\mathbf{p}_0|^2 \sin^2 \theta}{r^2}.$$
(8.126)

The radiation intensity is maximum in the directions perpendicular to the dipole, and zero in the direction parallel to the dipole. The total radiation power is

$$\int \overline{\mathbf{E} \times \mathbf{H}} \cdot d\mathbf{a} = \int \overline{|\mathbf{E} \times \mathbf{H}|} \sin \theta \, d\theta d\phi = \frac{ck^4 |\mathbf{p}_0|^2}{12\pi\epsilon_0}.$$
(8.127)

# 8.9 Radiation from Relativistic Particles

According to Eq. (8.71), acceleration of charged particles will yield a timevarying **J**, and consequently a time-varying **A** which represents the radiation field. If the velocity of the particle v is not much smaller than c, it is not possible to make the approximation  $|\mathbf{r} - \mathbf{r}'| \approx r$  as we have done in deriving the formulas for dipole radiation. This is because during the retardation time  $t - t' = |\mathbf{r} - \mathbf{r}'|/c$  the particle has moved a distance v(t - t'), which is not much smaller than  $|\mathbf{r} - \mathbf{r}'|$  itself no matter how far the observation point is. For a single particle the charge density and current density can be written as

$$\rho(\mathbf{r}, t) = q\delta(\mathbf{r} - \mathbf{r}_0(t)), \qquad (8.128)$$

$$\mathbf{J}(\mathbf{r},t) = q\mathbf{v}(t)\delta(\mathbf{r} - \mathbf{r}_0(t)), \qquad (8.129)$$

where  $\mathbf{r}_0(t)$  and  $\mathbf{v}(t)$  are the position and velocity of the particle at time t respectively. The vector potential can be written as

$$\mathbf{A}(\mathbf{r},t) = \int \frac{\mu_0}{4\pi} \frac{q\mathbf{v}(t')}{|\mathbf{r} - \mathbf{r}'|} \delta(\mathbf{r}' - \mathbf{r}_0(t')) \, d^3\mathbf{r}'. \tag{8.130}$$

where

$$t' = t - \frac{|\mathbf{r} - \mathbf{r}'|}{c}.\tag{8.131}$$

To evaluate  $\mathbf{A}(\mathbf{r}, t)$ , we need to invert Eq. (8.131) and write t' as a function of t. This is a difficult task. Alternatively, we may impose the constraint of

### 8.9. RADIATION FROM RELATIVISTIC PARTICLES

Eq. (8.131) by writing Eq. (8.130) as

$$\mathbf{A}(\mathbf{r},t) = \int \frac{\mu_0}{4\pi} \frac{q\mathbf{v}(s)}{|\mathbf{r}-\mathbf{r}'|} \delta(\mathbf{r}'-\mathbf{r}_0(s)) \delta\left(s-t+\frac{|\mathbf{r}-\mathbf{r}'|}{c}\right) d^3\mathbf{r}' ds$$
$$= \int \frac{\mu_0}{4\pi} \frac{q\mathbf{v}(s)}{|\mathbf{r}-\mathbf{r}_0(s)|} \delta\left(s-t+\frac{|\mathbf{r}-\mathbf{r}_0(s)|}{c}\right) ds.$$
(8.132)

The  $\delta$ -function in Eq. (8.132) is not of the usual form  $\delta(x - x_0)$ . Instead it is of the form  $\delta(f(x) - f(x_0))$ . To evaluate  $\delta(f(x) - f(x_0))$ , we note that the  $\delta$ -function is only sensitive to its argument around zero. Therefore we have

$$\delta(f(x) - f(x_0)) = \delta(f'(x_0)(x - x_0)) = \frac{\delta(x - x_0)}{f'(x_0)}.$$
(8.133)

Let us calculate the derivative of  $s - t + |\mathbf{r} - \mathbf{r}_0(s)|/c$  with respect to s.

$$\frac{d}{ds}\left(s-t+\frac{|\mathbf{r}-\mathbf{r}_0(s)|}{c}\right) = 1 - \frac{[\mathbf{r}-\mathbf{r}_0(s)]\cdot\mathbf{v}_0(s)}{|\mathbf{r}-\mathbf{r}_0(s)|c},\tag{8.134}$$

where  $\mathbf{v}_0(s) = d\mathbf{r}_0(s)/ds$ . Eq. (8.132) can then be written as

$$\mathbf{A}(\mathbf{r},t) = \frac{\mu_0}{4\pi} \int \frac{q\mathbf{v}(s)}{|\mathbf{r} - \mathbf{r}_0(s)|} \frac{\delta(s-t')}{[1-\mathbf{n}(s)\cdot\boldsymbol{\beta}(s)]} ds$$
$$= \frac{\mu_0}{4\pi} \frac{q\mathbf{v}(t')}{|\mathbf{r} - \mathbf{r}_0(t')|} \frac{1}{[1-\mathbf{n}(t')\cdot\boldsymbol{\beta}(t')]}$$
(8.135)

where

$$\mathbf{n}(t') = \frac{\mathbf{r} - \mathbf{r}_0(t')}{|\mathbf{r} - \mathbf{r}_0(t')|},\tag{8.136}$$

and  $\boldsymbol{\beta}(t') = \mathbf{v}_0(t')/c$ . Similarly we have

$$\phi(\mathbf{r},t) = \frac{1}{4\pi\epsilon_0} \frac{q}{|\mathbf{r} - \mathbf{r}_0(t')|} \frac{1}{[1 - \mathbf{n}(t') \cdot \boldsymbol{\beta}(t')]}.$$
(8.137)

The potentials in Eqs. (8.135) and (8.137) are known as the **Liénard-Wiechert** potentials.



Fig. 8.1: LC-transmission line.



Fig. 8.2: Fly-wheel circuit.

# 8.10 Exercises

**Exercise 8.1.** An infinite chain made of small inductors and capacitors is shown in Fig. 8.1. The inductance of each inductor is  $\epsilon L$  and the capacitance of each capacitor is  $\epsilon C$ . What is the impedance of this chain when  $\epsilon \rightarrow 0$ ? Hint: Assume its impedance is Z. Because it is an infinite chain, its impedance does not change when we remove a basic section enclosed in the dashed box.

**Exercise 8.2.** Consider the circuit shown in Fig. 8.2. Capacitor  $C_1$  is charged to a voltage V initially. Show that by manipulating switches  $S_1$  and  $S_2$  with proper timing, the output can reach a peak voltage  $\sqrt{nV}$ , if  $C_1/C_2 = n$ . Draw a diagram to show the timing sequence of  $S_1$  and  $S_2$ . Hint: Consider the energy stored in the inductor and the capacitor, and the analogy between an LC circuit and a harmonic oscillator.

**Exercise 8.3.** We have shown that acceleration of charges generates electromagnetic wave. We have also shown that a static current generates only a static **B**-field. Consider a static current in a ring. The current does not change with time, therefore **B** is time-independent. However, electrons in the circular trajectory experience centrifugal acceleration, therefore they should generate electromagnetic wave. How would you explain this "paradox"? Hint: Compare the retarded vector potential for a ring current and a single circulating charge.
**Exercise 8.4.** An ideal battery of voltage V is employed to charge a capacitor of capacitance C. The wire that connects the battery and the capacitor is made of a superconducting material, namely a material of zero resistance. The charge q stored in the capacitor is equal to CV and the energy stored in the capacitor is  $CV^2/2$ . However, since the charge q comes from the battery, the energy delivered by the battery is  $qV = CV^2$ . It looks like that half of the energy delivered by the battery is missing. Where does it go?

**Exercise 8.5.** Most of the electronic appliances do not use the 110-VAC source of electricity directly. Instead, transformers are used to lower the voltage to a level more compatible to semiconductor devices. Since a transformer is made of two overlapping coils, it looks like that each coil of a transformer can be treated as an inductor. Assume the input voltage is  $V(t) = V_0 \cos \omega t$ , by the relation V = LdI/dt, we have  $I(t) = V_0 \sin \omega t/(\omega L)$ . The average power delivered to the transformer is therefore

$$\overline{P} = \frac{1}{T} \int_0^T \frac{V_0^2 \cos \omega t \sin \omega t}{\omega L} dt = 0,$$

where  $T = 2\pi/\omega$ . If this is true, how can a transformer deliver power to an electronic appliance? If we assume the coils has no resistance, can you show that the input power is equal to the output power?

**Exercise 8.6.** You are given two metal bars of identical appearance and weight. One of them is made of permanent magnet, and the other is made of unmagnetized iron. How do you tell which one is the bar-magnet without using an external magnetic field? If the unmagnetized iron bar is replaced by an alloy bar of identical appearance and weight that cannot be magnetized, how do you distinguish them? You are only allowed to arrange the two bars in various configurations and move them relative to each other and measure the force between them.

**Exercise 8.7.** The electric current flowing in the high-tension wires that deliver electricity from power plants is on the order of 1000 amperes. Consider an infinitely long copper wire carrying 1000 amperes of 60-Hz AC current in the z-axis. The diameter of the wire is 2 cm, and the conductivity of copper is  $5.81 \times 10^7/(\Omega \cdot m)$ . Assume the current density is uniformly distributed in the wire, what are the electric field and the magnetic field at a distance of 30 m from the wire? How does this electric field compare with the field required to ionize the hydrogen atom and the field required to polarize water at room temperature? How does this magnetic field compare with the magnetic field of the earth at the earth surface  $(3 \times 10^{-5} \text{ T})$ ?

Hint: Solve this exercise in cylindrical coordinates.

Step 1: Use

$$\mathbf{A}(\mathbf{r},t) = \frac{\mu_0}{4\pi} \int \frac{\mathbf{J}(\mathbf{r}',t')}{|\mathbf{r}-\mathbf{r}'|} d^3\mathbf{r}'$$

and

$$\mathbf{E} = -\nabla\phi - \frac{\partial \mathbf{A}}{\partial t}$$

to show that  $\mathbf{E}$  is in the z-direction and is only a function of r.

Step 2: Use  $\mathbf{B} = \nabla \times \mathbf{A}$  to show that  $\mathbf{B}$  is in the  $\theta$ -direction and is only a function of r.

Step 3: Assume the second term on the right-hand side of the the Ampere-Maxwell law shown below is negligible compared with the first term on the right-hand side.

$$\nabla \times \mathbf{B} = \mu_0 \mathbf{J} + \mu_0 \epsilon_0 \frac{\partial \mathbf{E}}{\partial t}$$

Step 4: Since the displacement current in the Ampere-Maxwell law is assumed to be negligible, you may now calculate **B** by using Ampere's law.

Step 5: Calculate E by using Faraday's law.

Step 6: Show that **E** satisfies the assumption in step 3 by integrating the Ampere-Maxwell law over a surface of 30-m radius on the x-y plane.

**Exercise 8.8.** A coaxial cable of infinite length is made of a thin wire of diameter d in the center and an outer cylindrical metal mesh of diameter D, where  $d \ll D$ . The space in between is filled with a polyethylene jacket of dielectric constant  $\kappa_e$ . Derive the speed of the charge density wave propagating in this cable. In this problem we assume both the center wire and the outer mesh have no resistance. Note that the voltage across an inductor is

$$V = L\frac{dI}{dt} = L\frac{d^2q}{dt},$$

and the voltage across a capacitor is

$$V = \frac{q}{C}.$$

If we treat V as the driving force and q as the response, then V acts like a mechanical force, q acts like the displacement, L acts like the mass, and 1/C acts like the spring constant. Under this analogy, it is well known that an *RLC* circuit is equivalent to a damped harmonic oscillator. Similarly, a coaxial cable is equivalent to a elastic string, where the voltage difference between the inner wire and the outer mesh at position x is equivalent to the tension of the string at x and the difference in charge density at x is equivalent to the string displacement at x. Further hints on this problem can be obtained with a price.

**Exercise 8.9.** A coaxial cable of infinite length is made of a thin wire of diameter d in the center and an outer cylindrical metal mesh of diameter D, where  $d \ll D$ . The space in between is filled with a polyethylene jacket of dielectric constant  $\kappa_e$ . Derive the impedance of this cable. In this problem we assume both the center wire and the outer mesh have no resistance.

**Exercise 8.10.** A cable of infinite length is made of two parallel thin wires of diameter d. The separation between the wires is D, where  $d \ll D$ . What is the inductance per unit length? What is the capacitance per unit length? In this problem we assume the wires have no resistance.

**Exercise 8.11.** Consider an inductor made of a long solenoid of N turns of thin stiff wire. The radius of the solenoid is R. The separation between adjacent coils is larger than the diameter of the wire, so that the solenoid can be compressed or expanded like a spring. The question is whether this spring will be compressed or expanded with a steady-state current I flowing through it. Peter thinks the spring will be compressed. His argument is that the currents that flow through the coils are parallel to each other, therefore the force between the coils is attractive. Paul thinks the spring will be expanded. His argument is that since the energy stored in the solenoid is  $U = LI^2/2$ , expanding the spring will reduce the inductance, thereby reduce the stored energy. The reduced energy can be used to do work to the outside world, therefore the spring will be expanded. Which argument is correct and why? Do a thorough analysis to support your answer.

**Exercise 8.12.** An instrument shown in Fig. 8.3 is built to analyze the charge-to-mass ratio of a group of particles. In the instrument, a uniform electric field and a uniform magnetic field between x = 0 and x = L are set up, both pointing to the z-direction. The charged particles fly across the fields in the x-direction. Behind the region of the fields, a phosphor screen at x = L facing the incoming particle is used to detect the deflection of the



Fig. 8.3: The mass spectrometer used by J. J. Thomson to discover isotopes of neon.

particles. Show that if the deflection is small, particles of the same chargeto-mass ratio falls on the same parabola on the screen, regardless of their velocity. Using this method, in 1913 J. J. Thomson observed two distinct parabolas for ionized neon atoms and thus discovered that the neon gas was composed of atoms of two different atomic masses (neon-20 and neon-22).

**Exercise 8.13.** In a rail gun the projectile is accelerated by passing a large current through it in the direction transverse to an external static magnetic field B that fills a gap of width w (see Fig. 8.4). Assume that both the barrel frame and the projectile are made of conductors of negligible resistance, then one might think the voltage needed to produce a large current can be arbitrarily small. Hence no energy is needed to drive such a rail gun. What is wrong with this argument? What is the voltage as a function of time to make a constant acceleration a for a projectile of mass m? In this problem we assume the magnetic field produced by the current is negligible comparing to the external field.

**Exercise 8.14.** In Bohr's model of hydrogen, the electron circulates the proton and the centrifugal force is balanced by the Coulomb force. However, the oscillatory motion of the electron will generate electromagnetic wave and thus cause energy loss. Calculate the energy loss rate r for the n = 1 electron orbit. Let  $\Delta t = E/r$ , where E is the kinetic energy of the electron in the n = 1 orbit. What is the numerical value of  $\Delta t$ ? For simplicity, in this problem we assume the proton has an infinitely large mass and v/c is negligibly small, where v is the speed of the electron and c is the speed of light.



Fig. 8.4: The barrel frame and the projectile of a rail gun.

# Chapter 9

# **Special Relativity**

# 9.1 The Mysterious Ether

In sections 3.5, 5.4, and 5.5 we have discussed the phenomena of string waves, sound waves, and water waves. In these systems the evolution of small disturbance is governed by the same wave equation that governs the electromagnetic waves. Therefore, it may seem that there is nothing special about the electromagnetic waves. However, in all the wave phenomena people have known previously, the wave equation is valid only in a reference frame in which the average motion of the medium is zero. This can be seen by applying the Galilean transformation

$$\mathbf{r}' = \mathbf{r} - \mathbf{v}t t' = t$$
 (9.1)

to the wave equation

$$\nabla^2 \psi - \frac{1}{c^2} \frac{\partial^2 \psi}{\partial t^2} = 0. \tag{9.2}$$

Using Eq. (1.270), we have

$$\frac{\partial}{\partial r_i} = \frac{\partial}{\partial r'_i} 
\frac{\partial}{\partial t} = \frac{\partial}{\partial t'} - v_i \frac{\partial}{\partial r'_i}.$$
(9.3)

The wave equation becomes

$$\nabla^{\prime 2}\psi - \frac{1}{c^2} \left(\frac{\partial}{\partial t'} - \mathbf{v} \cdot \nabla^{\prime}\right)^2 \psi = 0, \qquad (9.4)$$

which is by no means

$$\nabla^{\prime 2}\psi - \frac{1}{(c-v)^2}\frac{\partial^2\psi}{\partial t^{\prime 2}} = 0.$$
(9.5)

In the case of electromagnetic wave, what is the medium in which the electromagnetic disturbance propagates? Because the Maxwell equations agree well with all kinds of experiments, if there is such a medium, we must happen to be in a reference frame in which the medium is stationary. This hypothetical medium was called "ether".

Consider a long rod hanging in the center by a thread. One end of the rod has charge +q and the other end has charge -q. In a reference frame in which the rod is not moving, the rod experiences no torque, because the attraction force between the charges is in the same direction as their relative position vector. However, in a moving frame both charges are moving, so they correspond to two parallel current elements of opposite directions. The two current elements would repel each other by the magnetic force. By Eq. (7.22) the force between the two current elements is

$$\mathbf{F} = \frac{\mu_0}{4\pi} q^2 \frac{\mathbf{v} \times (\mathbf{v} \times \mathbf{L})}{L^3},\tag{9.6}$$

where **L** is the relative position vector. Therefore by measuring the torque experienced by the rod, we will know the speed of our reference frame relative to "ether". This kind of measurement has been carried out by Trouton and Noble, and the result is that v is much smaller than the orbital velocity of earth ( $\approx 30 \text{ km/s}$ ).

Another famous experiment for determining v is the Michelson-Morley experiment. In this experiment the two optical path lengths, one parallel to  $\mathbf{v}$ , the other perpendicular to  $\mathbf{v}$ , are compared by an interferometer. The arm parallel to  $\mathbf{v}$  has a length  $l_1$ , and the arm perpendicular to  $\mathbf{v}$  has a length  $l_2$ . In the parallel arm, the time it takes for light to travel a round trip from the beam splitter to the reflecting mirror and back is

$$t_1 = \frac{l_1}{c - v} + \frac{l_1}{c + v} = \frac{2l_1}{c(1 - \beta^2)},$$
(9.7)

#### 9.1. The Mysterious Ether

where  $\beta = v/c$ . In the perpendicular arm, the round trip time follows the equation

$$t_2 = \frac{2}{c}\sqrt{l_2^2 + \left(\frac{vt_2}{2}\right)^2},\tag{9.8}$$

or

$$t_2 = \frac{2l_2}{c\sqrt{1-\beta^2}}.$$
(9.9)

The optical path difference is

$$\Delta = c(t_1 - t_2) = \frac{2}{\sqrt{1 - \beta^2}} \left( \frac{l_1}{\sqrt{1 - \beta^2}} - l_2 \right).$$
(9.10)

If the interferometer is rotated by 90°, the optical path difference changes to

$$\Delta' = c(t_1' - t_2') = \frac{2}{\sqrt{1 - \beta^2}} \left( l_1 - \frac{l_2}{\sqrt{1 - \beta^2}} \right).$$
(9.11)

The difference is

$$\Delta' - \Delta = \frac{2(l_1 + l_2)}{\sqrt{1 - \beta^2}} \left( 1 - \frac{1}{\sqrt{1 - \beta^2}} \right).$$
(9.12)

As the interferometer rotates, the detector should see n cycles of constructive and destructive interference fringe shift, where

$$n = \frac{\Delta' - \Delta}{\lambda} = \frac{2(l_1 + l_2)}{\lambda\sqrt{1 - \beta^2}} \left(1 - \frac{1}{\sqrt{1 - \beta^2}}\right)$$
$$\approx -\frac{l_1 + l_2}{\lambda}\beta^2 \tag{9.13}$$

for small  $\beta$ . The experimental result again showed that v is much smaller than the orbital velocity of earth.

It is possible to imagine that the ether is dragged by the earth, much like that the air is dragged by a flying baseball. If that is the case, the ether surrounding the earth is moving together with the earth. Then both the Trouton-Noble experiment and the Michelson-Morley experiment will not detect the relative velocity with respect to the ether. However, such an idea is in direct conflict with the observation of star light aberration.

Let us imagine watching the rain fall in a rapidly moving train. The rain drops fall vertically down, but because the train is moving, the tracks they leave on the window is not vertical. The angle follows  $\tan \theta = v_t/v_r$ , where  $v_t$  is the velocity of the train and  $v_r$  is the velocity of the rain drops. If the air surrounding the train is moving with the train, we will not see this angle. We can imagine that after the rain drops fall into the train from an opening on the roof, they will be dragged to move with the train in the same horizontal velocity. Then as a passenger in the train, all one sees is the vertical movement of the rain drops.

Similarly, when one watches a star in the zenith direction, the the star light does not fall on us in the vertical direction, instead it comes in an angle that follows  $\tan \theta = v/c \approx 10^{-4}$ , where v is the orbital velocity of the earth. Every half year the angle is reversed because the velocity of the earth is reversed. This phenomenon is called the star light aberration. If the ether does not move with the earth, or there is no ether at all, one will see the star light aberration. In contrast, if the ether is dragged by the earth, one will not see star light aberration. Fizeau measured this aberration, and the result showed that ether was not moving with the earth.

In summary, if we assume there is ether and it is the medium for the propagation of electromagnetic wave, then the Trouton-Noble experiment and the Michelson-Morley experiment showed that ether is dragged by the earth, whereas Fizeau's experiment showed that it is not. This is the difficult situation nature forced on us, which fostered the invention of relativity.

## 9.2 Lorentz Transformation

Another approach to the problem of ether is to abandon altogether the idea of ether as well as the Galilean transformation, and postulate that the speed of light is the same in every reference frame. There is simply no "preferred" frame for the electromagnetic wave. If we accept this postulate, then the next question will be what to replace the Galilean transformation that will make the Maxwell equations invariant.

Consider the case in which the relative velocity between two frames is in the x-direction. For simplicity, let us assume the coordinate transformation between different frames of different velocity is a linear transformation. Since the relative velocity is in the x-direction, it is reasonable to assume that the coordinates in the y- and z-directions are not affected.

$$x' = \alpha_{11}x + \alpha_{12}t,$$

$$y' = y,$$
  
 $z' = z,$   
 $t' = \alpha_{21}x + \alpha_{22}t.$  (9.14)

The inverse transformation is

$$x = \frac{\alpha_{22}x' - \alpha_{12}t'}{\alpha_{11}\alpha_{22} - \alpha_{12}\alpha_{21}},$$
  

$$y = y',$$
  

$$z = z',$$
  

$$t = -\frac{\alpha_{21}x' - \alpha_{11}t'}{\alpha_{11}\alpha_{22} - \alpha_{12}\alpha_{21}}.$$
(9.15)

The two frames have a relative velocity v in the x-direction means when x' = 0 we have x = vt, and when x = 0 we have x' = -vt'. These conditions yield

$$-\frac{\alpha_{12}}{\alpha_{11}} = v,$$
  
$$\frac{\alpha_{12}}{\alpha_{22}} = -v.$$
(9.16)

Therefore

$$\begin{array}{rcl}
\alpha_{11} &=& \alpha_{22}, \\
\alpha_{12} &=& -v\alpha_{11}.
\end{array} \tag{9.17}$$

The condition that the speed of light is c in both frames implies if  $x^2 + y^2 + z^2 - c^2 t^2 = 0$ , then

$$x^{\prime 2} + y^{\prime 2} + z^{\prime 2} - c^2 t^{\prime 2} = 0. (9.18)$$

Substituting Eq. (9.14) into Eq. (9.18) and using the condition  $x^2 + y^2 + z^2 - c^2 t^2 = 0$ , we have

$$\alpha_{12} = c^2 \alpha_{21}. \tag{9.19}$$

We also note that swapping (x, y, z, t) and (x', y', z', t') is equivalent to replacing v by -v in the transformation between (x, y, z, t) and (x', y', z', t'). This gives

$$\alpha_{11}\alpha_{22} - \alpha_{12}\alpha_{21} = 1. \tag{9.20}$$

Eqs. (9.17), (9.19), and (9.20) yield

$$\alpha_{11} = \alpha_{22} = \frac{1}{\sqrt{1 - v^2/c^2}},$$
  

$$\alpha_{12} = -\alpha_{11}v = \frac{-v}{\sqrt{1 - v^2/c^2}},$$
  

$$\alpha_{21} = -\frac{\alpha_{11}v}{c^2} = \frac{-v/c^2}{\sqrt{1 - v^2/c^2}}.$$
(9.21)

Hence we have

$$x' = \frac{x - vt}{\sqrt{1 - v^2/c^2}},\tag{9.22}$$

$$y' = y, \tag{9.23}$$

$$z' = z, \tag{9.24}$$

$$t' = \frac{t - (v/c^2)x}{\sqrt{1 - v^2/c^2}}.$$
(9.25)

and

$$x = \frac{x' + vt'}{\sqrt{1 - v^2/c^2}},\tag{9.26}$$

$$y = y',$$
 (9.27)  
 $z = z',$  (9.28)

$$z = z, (9.28) t' + (v/c^2)x' (9.29)$$

$$t = \frac{v + (v/c)x}{\sqrt{1 - v^2/c^2}}.$$
(9.29)

Eqs. (9.22)–(9.25) are known as the **Lorentz transformation** and Eqs. (9.26)–(9.29) are its inverse transformation. Note that by swapping (x, y, z, t) and (x', y', z', t') and changing v to -v we obtain Eqs. (9.26)–(9.29) directly from Eqs. (9.22)–(9.25) as expected. Because space-time coordinates must be real numbers, we have v < c. In other words, an observer cannot move faster than the speed of light.

It is customary to use the coordinate (x, y, z, ct) and write the Lorentz transformation as

$$x' = \gamma x - \beta \gamma ct, \qquad (9.30)$$

$$y' = y, \tag{9.31}$$

$$z' = z, \tag{9.32}$$

$$ct' = -\beta\gamma x + \gamma ct, \qquad (9.33)$$

where

$$\beta = \frac{v}{c}, \tag{9.34}$$

$$\gamma = \frac{1}{\sqrt{1 - v^2/c^2}}.$$
 (9.35)

From Eq. (1.270), we have

$$\frac{\partial}{\partial x} = \gamma \frac{\partial}{\partial x'} - \beta \gamma \left(\frac{1}{c} \frac{\partial}{\partial t'}\right), \qquad (9.36)$$

$$\frac{\partial}{\partial y} = \frac{\partial}{\partial y'},\tag{9.37}$$

$$\frac{\partial}{\partial z} = \frac{\partial}{\partial z'},\tag{9.38}$$

$$\frac{1}{c}\frac{\partial}{\partial t} = -\beta\gamma\frac{\partial}{\partial x'} + \gamma\left(\frac{1}{c}\frac{\partial}{\partial t'}\right), \qquad (9.39)$$

Inverting the transformation matrix, we have

$$\frac{\partial}{\partial x'} = \gamma \frac{\partial}{\partial x} + \beta \gamma \left(\frac{1}{c} \frac{\partial}{\partial t}\right), \qquad (9.40)$$

$$\frac{\partial}{\partial y'} = \frac{\partial}{\partial y},\tag{9.41}$$

$$\frac{\partial}{\partial z'} = \frac{\partial}{\partial z}, \tag{9.42}$$

$$\frac{1}{c}\frac{\partial}{\partial t'} = \beta\gamma\frac{\partial}{\partial x} + \gamma\left(\frac{1}{c}\frac{\partial}{\partial t}\right), \qquad (9.43)$$

The transformation for the derivatives is the inverse Lorentz transformation. Hence we can see immediately

$$\nabla^2 - \frac{1}{c^2} \frac{\partial^2}{\partial t^2} = \nabla^{\prime 2} - \frac{1}{c^2} \frac{\partial^2}{\partial t^{\prime 2}}.$$
(9.44)

In summary, the Lorentz transformation makes the speed of light and the Maxwell equations invariant. If we wish to make sense out of the experimental results, we are forced to adopt this transformation for the space-time coordinates between reference frames. This does not mean we were wrong to use the Galilean transformation before. In the limit  $\beta \to 0$ , the Lorentz transformation is the same as the the Galilean transformation. Hence the Galilean transformation is a good approximation when  $v \ll c$ .

### 9.3 Simultaneity and Causality

In non-relativistic physics, time is a common parameter shared by all reference frames. In contrast, Lorentz transformation tells that each reference frame has its own time. Two events that are simultaneous in frame 1 may not be simultaneous in frame 2. For instance, consider two events in frame 1. One occurred at  $(x_1, 0, 0, ct)$  and the other at  $(x_2, 0, 0, ct)$ . They were simultaneously because both of them occurred at time t. By Eqs. (9.30)– (9.33), in frame 2 they occurred at  $(\gamma x_1 - \beta \gamma ct, 0, 0, -\beta \gamma x_1 + \gamma ct)$  and  $(\gamma x_2 - \beta \gamma ct, 0, 0, -\beta \gamma x_2 + \gamma ct)$  respectively. The time difference in frame 2 is

$$c\Delta t' = t'_2 - t'_1 = \beta \gamma (x_1 - x_2). \tag{9.45}$$

To understand this nonintuitive result, we must inspect what we mean by simultaneity more carefully. Consider a simple experiment in which a person  $O_1$  at the origin sends out light signals in both the x-direction and the -x-direction simultaneously to two detectors at equal distance. For  $O_1$  the coordinates of the detectors are  $(d_1, 0, 0)$  and  $(-d_1, 0, 0)$ . Obviously, from  $O_1$ 's point of view the two light signals will arrive at the two detectors simultaneously. However, to another person  $O_2$  who is passing by  $O_1$  in the x-direction with a speed v when  $O_1$  is sending out the signals, the two light signals cannot arrive the two detectors simultaneously. From  $O_2$ 's point of view both detectors are moving in the -x-direction with a speed v, therefore one detector is moving toward the light and the other is moving away from the light. Assume for  $O_2$  the coordinates of the detectors are  $(d_2, 0, 0)$  and  $(-d_2, 0, 0)$ . Since the speed of light is constant, the difference in the arrival time will be

$$\Delta t = \frac{d_2}{(c+v)} - \frac{d_2}{(c-v)} = -2d_2\frac{\beta\gamma^2}{c}.$$
(9.46)

We see simultaneity cannot be a common fact to be agreed by observers with relative motion. Because there is no "preferred" reference frame, we cannot say  $O_1$  is more correct than  $O_2$  or vice versa. The lack of universal simultaneity is a direct consequence of the fact that light speed is a constant in all frames.

Let us consider the communication between two events separated in spacetime. Event 1 occurred at  $(x_1, 0, 0, t_1)$  and event 2 occurred at  $(x_2, 0, 0, t_2)$ . Let us also assume that the fastest signal one can use for communication has the speed of light. If  $t_2 > t_1$  and  $|x_2 - x_1| < c|t_2 - t_1|$ , we could send a signal

#### 9.4. Proper Length and Proper Time

from  $(x_1, 0, 0)$  at  $t_1$  to  $(x_2, 0, 0)$  such that the signal arrived  $(x_2, 0, 0)$  before  $t_2$ , when event 2 occurred. Since the signal can carry information, it may have caused event 2 to occur, therefore we say event 1 may have a causal influence on event 2. From Eq. (9.33), the time interval between these two events seen in a different frame is

$$\Delta t' = \gamma \Delta t \left( 1 - \beta \frac{\Delta x}{c \Delta t} \right), \qquad (9.47)$$

where  $\Delta t' = t'_2 - t'_1$ ,  $\Delta t = t_2 - t_1$  and  $\Delta x = x_2 - x_1$ . Since  $\Delta t > 0$ , if  $\Delta t' < 0$  we have a contradiction, because for observers in this frame event 1 occurred later than event 2, hence it cannot have a causal influence on event 2. Instead, for observers in this frame event 2 may have caused event 1 to occur. To avoid this contradiction we must have  $\Delta t' > 0$ . For  $|\beta| < 1$  this is indeed the case. As long as  $|\Delta x| < c|\Delta t|$ ,  $\Delta t'$  and  $\Delta t$  in Eq. (9.47) have the same sign. Therefore Lorentz transformation preserves the causal relation if there is no means of communicate faster than light with a speed u, than the causal condition in one frame will be  $|x_2 - x_1| < u|t_2 - t_1|$ , where u > c. In this case reversal of causal relation may occur in a different frame when  $u > c/\beta$ . To avoid this contradiction, we must rule out the possibility of communication faster than the speed of light.

## 9.4 Proper Length and Proper Time

In the relativistic regime, even things as simple as measuring the length of a rod or the time interval between two events can be tricky. Because the Lorentz transformation mixes up space and time coordinates, one must define clearly the conditions under which a measurement is carried out. The simplest measurements are the length of a rod and the time interval between two events where the observer has no relative velocity with respect to the rod or the events. In the case we say the observer is in the rest frame of the events. Under this condition, the measured length is called the proper length  $l_p$  of the rod, and the time interval is called the proper time  $t_p$  between two events. If the observer has a relative velocity, the most reasonable measurement for the length of a rod is to measure the space coordinates of the two ends of the rod simultaneously. In this case, by Eq. (9.26) we have

$$l_p = \gamma l, \tag{9.48}$$

where l is the difference in the space coordinates of the two ends of the rod. Because  $\gamma > 1$ , we see that  $l < l_p$ . Namely a rod appears shorter than its proper length to a moving observer. Because motion is relative, it is equally well to say that a moving rod appears shorter than its proper length. This effect is called length contraction.

For the measurement of the time interval  $\tau$  between two events, if the observer has a relative velocity, we know the result will depend on the distance between the two events in the rest frame. If the two events occur at the same location in the rest frame, by Eq. (9.25) we have

$$\tau = \gamma t_p. \tag{9.49}$$

Because  $\gamma > 1$ , we see that  $\tau > t_p$ . Namely the period of a clock appears longer to a moving observer. This effect is called time dilation.

A confusion that often occurs to beginners in this field is that if we imagine two observers each carrying a standard meter passing by each other with high speed, Eq. (9.48) says that each of them will see the meter carried by the other is shorter. Is this a contradiction? If there existed an instant common to both observers at which the two ends of one meter matched the two ends of the other meter, it would be a contradiction. But as we have explained in Section 9.3, such a common instant does not exist. For the two observers, a common simultaneity is possible only if the two events occur at the same place. When observer 1 measures the length of the meter carried by observer 2, the only meaningful measurement for him is to measure the space coordinates of the two ends of the meter simultaneously, then subtract the coordinates to obtain the length. However, when observer 1 does so, observer 2 does not agree that observer 1 measured the meter simultaneously. He thinks that observer 1 measured the space coordinates of the two ends of his meter at two instants with a time interval  $\Delta t'$  between the instants. Replacing  $2d_2$  in Eq. (9.46) by the proper length of the meter  $l_p$ , we know that observer 2 thinks  $\Delta t'$  is

$$\Delta t' = -l_p \frac{\beta \gamma^2}{c}.$$
(9.50)

Within this time interval observer 1 should have moved  $-v\Delta t$  in his own coordinate, where  $\Delta t = \Delta t'/\gamma$ . Without taking into account of the effect of this movement, observer 2 anticipates that observer 1 would have measured the length to be  $\gamma l_p$ , because after length contraction this quantity should be  $l_p$ . However, because the measurements are carried out at different times, the measured length should be

$$\gamma l_p - (-v\Delta t) = \gamma l_p - \beta^2 \gamma l_p = \frac{l_p}{\gamma}.$$
(9.51)

#### 9.5. Addition of Velocity

From observer 1's point of view, by Eq. (9.22) he would measured the length of observer 2's meter to be  $l_p/\gamma$ . From observer 2's point of view, by Eq. (9.51) he would also think that observer 1 would get the same value  $l_p/\gamma$ . Therefore there is no contradiction. The important point to realize is that simultaneity for observer 1 does not imply simultaneity for observer 2. This resolves the apparent contradiction.

Similarly, if observer 1 and observer 2 both carry a standard clock, each of them would see the other's clock runs slower. There is no contradiction either, because to each observer the other's clock is moving, and it is not possible to measure the time intervals of both clocks at the same place. Let the clock interval be  $t_p$ . As observer 1 measures observer 2's clock interval, observer 2 knows that observer 1 has moved a distance  $\Delta x' = -vt_p$  between the two measurements. Without taking into account the effect of this distance, observer 2 anticipates that observer 1 would have measured the time interval to be  $t_p/\gamma$ , because after time dilation this quantity should be  $t_p$ . However, because from observer 2's point of view the measurements are carried out at two different locations separated by  $\Delta x'$ , we must add the extra time interval that arises from the difference in simultaneity between the two observers as a result of  $\Delta x' \neq 0$ . This extra time interval can be obtained by replacing  $2d_2$  in Eq. (9.46) with  $\Delta x'$ . Therefore the measured time interval should be

$$\frac{1}{\gamma} \left[ t_p - (-vt_p) \frac{\beta \gamma^2}{c} \right] = \frac{t_p}{\gamma} (1 + \beta^2 \gamma^2) = \gamma t_p.$$
(9.52)

Again there is no contradiction.

## 9.5 Addition of Velocity

For a reference frame moving in the x-direction with velocity v, the transformation of velocities can be obtained directly from Eqs. (9.22)–(9.25).

$$u'_{x} = \frac{dx'}{dt'} = \frac{dx - vdt}{dt - (v/c^{2})dx} = \frac{u_{x} - v}{1 - (v/c^{2})u_{x}},$$
(9.53)

or equivalently

$$u_x = \frac{u'_x + v}{1 + (v/c^2)u'_x}.$$
(9.54)

$$u'_{y} = \frac{dy'}{dt'} = \frac{1}{\gamma} \left[ \frac{dy}{dt - (v/c^{2})dx} \right] = \frac{1}{\gamma} \left[ \frac{u_{y}}{1 - (v/c^{2})u_{x}} \right].$$
 (9.55)

$$u'_{z} = \frac{dz'}{dt'} = \frac{1}{\gamma} \left[ \frac{dz}{dt - (v/c^{2})dx} \right] = \frac{1}{\gamma} \left[ \frac{u_{z}}{1 - (v/c^{2})u_{x}} \right].$$
 (9.56)

By straightforward algebra, it can be shown that

$$1 - \frac{u^{\prime 2}}{c^2} = \frac{\left(1 - \frac{v^2}{c^2}\right)\left(1 - \frac{u^2}{c^2}\right)}{\left(1 - \frac{vu_x}{c^2}\right)^2}.$$
(9.57)

Because the right-hand side is always positive, we see  $u'^2 < c^2$ , which means the sum of two velocities will not exceed the speed of light, no matter how close to the speed of light they are.

### 9.6 Energy and Momentum

In the non-relativistic regime,  $v \ll c$ , the momentum conservation law can be expressed as

$$\sum_{i} m_i \mathbf{u}_i = \text{constant.} \tag{9.58}$$

before and after collisions. In other words,  $\sum_i m_i \mathbf{u}_i$  is invariant under collisions. The Galilean transformation does not change the momentum conservation law, because in a moving frame Eq. (9.58) becomes

$$\sum_{i} m_{i} \mathbf{u}_{i}^{\prime} = \sum_{i} m_{i} (\mathbf{u}_{i} - \mathbf{v}) = \sum_{i} m_{i} \mathbf{u}_{i} - \left(\sum_{i} m_{i}\right) \mathbf{v}, \qquad (9.59)$$

and the second term on the right-hand side is also a constant invariant under collisions. In the relativistic regime, Eq. (9.58) is not compatible with the formula for the addition of velocity. Assuming all the velocities are in the *x*-direction, in a frame moving also in the *x*-direction, Eq. (9.58) changes to

$$\sum_{i} m_{i} u_{i}' = \sum_{i} \frac{m_{i} (u_{i} - v)}{1 - (v/c^{2})u_{i}}.$$
(9.60)

This equation shows that  $\sum_{i} m_{i}u_{i}$  and  $\sum_{i} m_{i}u'_{i}$  cannot be both invariant under collisions.

Similarly, under the Galilean transformation the kinetic energy becomes

$$\sum_{i} \frac{m_i}{2} u_i^{\prime 2} = \sum_{i} \frac{m_i}{2} (u_i^2 - 2u_i v + v^2) = \sum_{i} \frac{m_i}{2} u_i^2 + \text{constant}, \quad (9.61)$$

which means if  $\sum_i m_i u_i^2/2$  is invariant under collisions, so is  $\sum_i m_i u_i'^2/2$ . Again, the formula for the addition of velocity ruins this invariance.

A way to maintain the energy and momentum conservation laws is to redefine the kinetic energy and momentum so that they are compatible with the Lorentz transformation. Let us consider a two-particle collision. Before the collision, the momenta of the two particles are  $\mathbf{p}_1$  and  $\mathbf{p}_2$ , and after the collision  $\mathbf{p}_3$  and  $\mathbf{p}_4$ . Similarly, before the collision the kinetic energy of the two particles are  $T_1$  and  $T_2$ , and after the collision  $T_3$  and  $T_4$ . To maintain the energy and momentum conservation laws, we demand

$$\mathbf{p}_1 + \mathbf{p}_2 = \mathbf{p}_3 + \mathbf{p}_4, T_1 + T_2 = T_3 + T_4.$$
 (9.62)

In order to satisfy the above relations, we must make the generalization that the mass a particle depends on its velocity. In other words, a particle has different masses in different reference frames. In addition, the form of the kinetic energy must also be modified accordingly. Let us postulate that

$$\mathbf{p} = m(u)\mathbf{u},$$
  

$$T = T(u),$$
(9.63)

where the exact form of m(u) and T(u) will be determined by considering energy and momentum conservation in an event of two-particle collision.

Imagine the collision of two identical particles in their center-of-mass frame. In this frame, the two particles move in opposite directions with velocity  $\mathbf{v}$ , and the energy and momentum conservation laws are

$$m(v)\mathbf{v} - m(v)\mathbf{v} = m(v')\mathbf{v}' + m(v'')\mathbf{v}'', T(v) + T(v) = T(v') + T(v''),$$
(9.64)

where  $\mathbf{v}'$  and  $\mathbf{v}''$  are the velocities after the collision. Because the two particles are identical, we must have  $\mathbf{v}'' = -\mathbf{v}'$ . Let us assume  $\mathbf{v}$  is in the *x*-direction and the angle between  $\mathbf{v}'$  and  $\mathbf{v}$  is  $\theta$ . After collision, the velocities are

$$\begin{aligned}
v'_x &= v \cos \theta, \\
v'_y &= v \sin \theta, \\
v''_x &= -v \cos \theta, \\
v''_y &= -v \sin \theta.
\end{aligned}$$
(9.65)

Let us now look at the event in a reference frame moving with velocity  $-\mathbf{v}$ . Before collision, one particle is at rest and the other particle moves with velocity

$$\mathbf{u} = \frac{2\mathbf{v}}{1 + \frac{v^2}{c^2}}.\tag{9.66}$$

After collision, the velocities  $\mathbf{u}'$  and  $\mathbf{w}'$  can be obtained from Eq. (9.65) and the formula for the addition of velocity.

$$u'_{x} = \frac{c\beta(1+\cos\theta)}{1+\beta^{2}\cos\theta},$$
  

$$u'_{y} = \frac{c\beta\sin\theta}{\gamma(1+\beta^{2}\cos\theta)},$$
  

$$w'_{x} = \frac{c\beta(1-\cos\theta)}{1-\beta^{2}\cos\theta},$$
  

$$w'_{y} = -\frac{c\beta\sin\theta}{\gamma(1-\beta^{2}\cos\theta)}.$$
(9.67)

Momentum conservation in the y-direction demands

$$m(u')\frac{c\beta\sin\theta}{\gamma(1+\beta^2\cos\theta)} - m(w')\frac{c\beta\sin\theta}{\gamma(1-\beta^2\cos\theta)} = 0.$$
 (9.68)

which reduces to

$$m(u') = m(w')\frac{1+\beta^2\cos\theta}{1-\beta^2\cos\theta}.$$
(9.69)

On the other hand, by straightforward calculation, it can be shown

$$\sqrt{1 - \frac{u'^2}{c^2}} = \frac{1 - \beta^2}{1 + \beta^2 \cos \theta}, 
\sqrt{1 - \frac{w'^2}{c^2}} = \frac{1 - \beta^2}{1 - \beta^2 \cos \theta}.$$
(9.70)

Hence

$$m(u')\sqrt{1-\frac{u'^2}{c^2}} = m(w')\sqrt{1-\frac{w'^2}{c^2}}.$$
 (9.71)

Since this equation holds for all possible pairs of v' and w', and the range of them can vary from 0 to c, we must have

$$m(v) = \frac{m_0}{\sqrt{1 - \frac{v^2}{c^2}}},\tag{9.72}$$

#### 9.6. Energy and Momentum

where v is the velocity of the particle and  $m_0$  is the mass of the particle at rest. Conventionally  $m_0$  is called the rest mass of the particle. Eq. (9.72) shows that as the velocity of the particle approaches the speed of light, its mass approaches infinity. This is why we cannot accelerate a particle of finite mass to the speed of light.

Let us go back to check if Eq. (9.72) also preserve the momentum in the *x*-direction. Using Eq. (9.66), before the collision we have

$$p_x = \frac{m_0 u}{\sqrt{1 - \frac{u^2}{c^2}}} = \frac{2m_0 v}{1 - \beta^2}.$$
(9.73)

Using Eqs. (9.70) and (9.67), after the collision we have

$$p_x = \frac{m_0}{\sqrt{1 - \frac{w'^2}{c^2}}} u'_x + \frac{m_0}{\sqrt{1 - \frac{w'^2}{c^2}}} w'_x$$
$$= \frac{2m_0 v}{1 - \beta^2}.$$
(9.74)

With the formula Eq. (9.72), the momentum in the *x*-direction is also conserved.

To derive the expression for the kinetic energy, we note that in addition to Eq. (9.70), from Eq. (9.66) we have

$$\sqrt{1 - \frac{u^2}{c^2}} = \frac{1 - \beta^2}{1 + \beta^2}.$$
(9.75)

Let w = 0, we have

$$\frac{1}{\sqrt{1 - \frac{w^2}{c^2}}} + \frac{1}{\sqrt{1 - \frac{u^2}{c^2}}} = \frac{1}{\sqrt{1 - \frac{w'^2}{c^2}}} + \frac{1}{\sqrt{1 - \frac{w'^2}{c^2}}}.$$
(9.76)

This gives a hint that

$$T(v) \propto \frac{1}{\sqrt{1 - \frac{v^2}{c^2}}} + \text{constant.}$$
 (9.77)

Dimensional consideration yields

$$T(v) = \frac{m_0 c^2}{\sqrt{1 - \frac{v^2}{c^2}}} + \text{constant.}$$
(9.78)

Because T(0) = 0, we have

$$T(v) = \frac{m_0 c^2}{\sqrt{1 - \frac{v^2}{c^2}}} - m_0 c^2.$$
(9.79)

We may define

$$E(v) = \frac{m_0 c^2}{\sqrt{1 - \frac{v^2}{c^2}}} = m(v)c^2,$$
(9.80)

so that T(v) = E(v) - E(0). The interpretation of this relation is that a particle carries an intrinsic amount of energy  $m_0c^2$  even when it is not moving. This is conventionally called the rest energy, and in general the energy of a particle is  $E = mc^2$ . From the relation

$$\mathbf{p} = \frac{m_0 \mathbf{v}}{\sqrt{1 - \frac{v^2}{c^2}}}\tag{9.81}$$

we have

$$\frac{v^2}{c^2} = \frac{p^2}{m_0^2 c^2 + p^2}.$$
(9.82)

Substituting Eq. (9.82) back into

$$E = \frac{m_0 c^2}{\sqrt{1 - \frac{v^2}{c^2}}},\tag{9.83}$$

we have

$$E^2 = m_0^2 c^4 + p^2 c^2. (9.84)$$

This is the relativistic energy-momentum relation.

From the definitions of the relativistic energy and momentum, we may define the relativistic force as

$$\mathbf{F} = \frac{d\mathbf{p}}{dt}.\tag{9.85}$$

The conversion of work to kinetic energy can be seen by considering the following integral:

$$\int \mathbf{F} \cdot d\mathbf{s} = \int \frac{d\mathbf{p}}{dt} \cdot d\mathbf{s}$$
$$= \int \mathbf{v} \cdot d\mathbf{p}.$$
(9.86)

### 9.7. Four-Vectors

Substituting Eq. (9.82) back into Eq. (9.81), we have

$$\mathbf{v} = \frac{\mathbf{p}c}{\sqrt{m_0^2 c^2 + p^2}}.\tag{9.87}$$

$$\int \mathbf{v} \cdot d\mathbf{p} = \int \frac{cp}{\sqrt{m_0^2 c^2 + p^2}} dp$$
$$= \Delta \sqrt{m_0^2 c^4 + p^2 c^2} = \Delta E.$$
(9.88)

# 9.7 Four-Vectors

The Lorentz transformation tells us how to transform the 3-dimensional position vector  $\mathbf{r}$  that marks the relative space coordinates of two events together with the time coordinates. Because the transformation is linear, we may imagine that  $(\mathbf{r}, t)$  is a vector in the 4-dimensional space-time, in which time is the fourth component. By convention, we denote a vector in the 4-dimensional space-time  $x_i$  (i = 0, 1, 2, 3), where  $(x_1, x_2, x_3)$  are the usual space components, and the time component ct is denoted by  $x_0$ . To derive the general Lorentz transformation where  $\mathbf{v}$  is in any direction, let us decompose  $\mathbf{r}$  into the parallel component and the perpendicular component.

$$\mathbf{r} = \mathbf{r}_l + \mathbf{r}_t, \tag{9.89}$$

where

$$\mathbf{r}_{l} = \frac{(\mathbf{r} \cdot \boldsymbol{\beta})}{\beta^{2}} \boldsymbol{\beta}, \qquad (9.90)$$

$$\mathbf{r}_t = \mathbf{r} - \frac{(\mathbf{r} \cdot \boldsymbol{\beta})}{\beta^2} \boldsymbol{\beta}, \qquad (9.91)$$

(9.92)

and  $\boldsymbol{\beta} = \mathbf{v}/c$ . Using Eqs. (9.30)–(9.33), we have

$$\begin{aligned} x'_{0} &= \gamma(x_{0} - \boldsymbol{\beta} \cdot \mathbf{r}), \\ \mathbf{r}'_{l} &= \gamma\left(\frac{\mathbf{r} \cdot \boldsymbol{\beta}}{\beta^{2}}\boldsymbol{\beta} - \boldsymbol{\beta}x_{0}\right), \\ \mathbf{r}'_{t} &= \mathbf{r} - \frac{\mathbf{r} \cdot \boldsymbol{\beta}}{\beta^{2}}\boldsymbol{\beta}. \end{aligned}$$
(9.93)

In terms of  $(x_0, x_1, x_2, x_3)$ , we have

$$\begin{aligned} x'_{0} &= \gamma(x_{0} - \boldsymbol{\beta} \cdot \mathbf{x}), \\ \mathbf{x}' &= \mathbf{r}'_{l} + \mathbf{r}'_{t} = \mathbf{x} + \frac{\gamma - 1}{\beta^{2}} (\boldsymbol{\beta} \cdot \mathbf{x}) \boldsymbol{\beta} - \gamma \boldsymbol{\beta} x_{0}. \end{aligned}$$
(9.94)

In the matrix notation, Eq. (9.94) is

$$\begin{pmatrix} x'_{0} \\ x'_{1} \\ x'_{2} \\ x'_{3} \end{pmatrix} = \begin{bmatrix} \gamma & -\gamma\beta_{1} & -\gamma\beta_{2} & -\gamma\beta_{3} \\ -\gamma\beta_{1} & 1 + \frac{(\gamma-1)\beta_{1}^{2}}{\beta^{2}} & \frac{(\gamma-1)\beta_{1}\beta_{2}}{\beta^{2}} & \frac{(\gamma-1)\beta_{1}\beta_{3}}{\beta^{2}} \\ -\gamma\beta_{2} & \frac{(\gamma-1)\beta_{1}\beta_{2}}{\beta^{2}} & 1 + \frac{(\gamma-1)\beta_{2}^{2}}{\beta^{2}} & \frac{(\gamma-1)\beta_{2}\beta_{3}}{\beta^{2}} \\ -\gamma\beta_{3} & \frac{(\gamma-1)\beta_{1}\beta_{3}}{\beta^{2}} & \frac{(\gamma-1)\beta_{2}\beta_{3}}{\beta^{2}} & 1 + \frac{(\gamma-1)\beta_{2}^{2}}{\beta^{2}} \end{bmatrix} \begin{pmatrix} x_{0} \\ x_{1} \\ x_{2} \\ x_{3} \end{pmatrix}.$$
(9.95)

A scalar in the 4-dimensional space-time is a physical quantity that is invariant under a change of reference frame. Similarly, a vector quantity in the 4-dimensional space-time that transforms according to the Lorentz transformation is called a 4-vector. We have shown  $(ct, \mathbf{r})$  is a 4-vector, what about other physical quantities such as momentum, energy, charge density, current density, scalar potential, vector potential, etc?

To begin with, let us consider  $J_i$  (i = 0, 1, 2, 3), where  $(J_1, J_2, J_3)$  is the 3-dimensional current density and  $J_0$  is the charge density times the speed of light  $c\rho$ . Because

$$\frac{\partial}{\partial x_i} = \left(\frac{1}{c}\frac{\partial}{\partial t}, \nabla\right),\tag{9.96}$$

the continuity equation for the charge reads

$$\frac{\partial J_i}{\partial x_i} = 0. \tag{9.97}$$

Because charge cannot be created or annihilated by a change of reference frame, we have

$$\frac{\partial J_i'}{\partial x_i'} = 0 \tag{9.98}$$

in another reference frame. According to Eqs. (1.263) and (1.270),

$$\frac{\partial}{\partial x_i'} = M_{ik}^{\mathrm{T}} \frac{\partial}{\partial x_k},\tag{9.99}$$

### 9.7. Four-Vectors

where  $M_{ik}^{-1}$  is the matrix in Eq. (9.95). If we choose

$$J'_i = M_{im}^{-1} J_m, (9.100)$$

we have

$$\frac{\partial J'_{i}}{\partial x'_{i}} = M_{ik}^{\mathrm{T}} M_{im}^{-1} \frac{\partial J_{m}}{\partial x_{k}}$$

$$= M_{ki} M_{im}^{-1} \frac{\partial J_{m}}{\partial x_{k}} = \delta_{km} \frac{\partial J_{m}}{\partial x_{k}}$$

$$= \frac{\partial J_{k}}{\partial x_{k}}.$$
(9.101)

Hence the invariance of the continuity equation demands that  $J_i$  transforms in the same way as  $x_i$ . Namely we should use the same Lorentz transform on  $(c\rho, \mathbf{J})$  to obtain  $(c\rho', \mathbf{J}')$  in another reference frame. Hence  $(c\rho, \mathbf{J})$  is a 4-vector.

Similarly, the phase of a wave  $\mathbf{k} \cdot \mathbf{x} - \omega t$  measures the cycles of oscillation the wave has gone through. Hence it is a quantity that is invariant under a change of reference frame. Let us define  $k_0 \equiv -\omega/c$ . Because

$$x_i' = M_{im}^{-1} x_m, (9.102)$$

if we choose

$$k_i' = M_{il}^{\mathrm{T}} k_l, \tag{9.103}$$

we have

$$x'_{i}k'_{i} = M_{il}^{\mathrm{T}}M_{im}^{-1}x_{m}k_{l} = M_{li}M_{im}^{-1}x_{m}k_{l} = x_{m}k_{m}.$$
(9.104)

Hence the invariance of the phase demands that  $k_i$  transforms the same way as  $\partial/\partial x_i$ . Note that  $M(-\beta) = M^{-1}(\beta)$ , and from Eq. (9.95) we see  $M^{\mathrm{T}}(-\beta) = M(-\beta)$ . Hence  $M^{\mathrm{T}}$  is also a Lorentz transformation. This means both  $(-\omega/c, \mathbf{k})$  and  $[\partial/(c\partial t), \nabla]$  are 4-vectors.

Let consider the vector potential **A** and the scalar potential  $\phi$  together. If we define  $A_0 \equiv \phi/c$ , Eqs. (8.27) and (8.28) can be written as

$$\left(\nabla^2 - \frac{1}{c^2} \frac{\partial^2}{\partial t^2}\right) A_i = -\mu_0 J_i.$$
(9.105)

Since

$$\nabla^2 - \frac{1}{c^2} \frac{\partial^2}{\partial t^2}$$

is invariant under Lorentz transformation,  $A_i$  must transform in the same way as  $J_i$ . Hence  $(\phi/c, \mathbf{A})$  is also a 4-vector. The condition we imposed on  $\mathbf{A}$ , Eq. (8.26), becomes

$$\frac{\partial A_i}{\partial x_i} = 0. \tag{9.106}$$

This is automatically satisfied for all reference frames, in view of Eq. (9.101) and the same transformation for  $J_i$  and  $A_i$ .

The velocity transformation in Eqs. (9.53), (9.55), and (9.56) is different from the Lorentz transform. Therefore velocity itself is not part of a 4-vector. To construct a relativistic form of the velocity that is a 4-vector, we note that

$$1 - \frac{u^{\prime 2}}{c^2} = \frac{\left(1 - \frac{v^2}{c^2}\right)\left(1 - \frac{u^2}{c^2}\right)}{\left(1 - \frac{vu_x}{c^2}\right)^2}.$$
(9.107)

Therefore by defining

$$\gamma_u \equiv \sqrt{\frac{1}{1 - \frac{u^2}{c^2}}}$$

Eqs. (9.53), (9.55), and (9.56) can be written as

$$\begin{aligned}
\gamma_{u'}u'_x &= \gamma_v(\gamma_u u_x - \beta c \gamma_u), \\
\gamma_{u'}u'_y &= \gamma_u u_y, \\
\gamma_{u'}u'_z &= \gamma_u u_z,
\end{aligned} \tag{9.108}$$

and

$$c\gamma_{u'} = \gamma_v (-\beta \gamma_u u_x + c\gamma_u) \tag{9.109}$$

follows directly from Eq. (9.57). These equation shows that  $(c\gamma_u, \gamma_u \mathbf{u})$  is a 4-vector. By Eqs. (9.81) and (9.83), we see that  $(E/c, \mathbf{p})$  is also a 4-vector.

At this point you must have noticed that there are two kinds of 4-vectors. The first kind is called contravariant vectors. They are written as  $A^i$  (i = 0, 1, 2, 3) from now on, and transform according to

$$A'^{i} = M_{im}^{-1}(\mathbf{v})A^{m}.$$
(9.110)

The second kind is called covariant vectors. They are written as  $A_i$  (i = 0, 1, 2, 3) from now on, and transform according to

$$A'_i = M_{il}^{\mathrm{T}}(\mathbf{v})A_l. \tag{9.111}$$

### 9.7. Four-Vectors

Because  $M_{il}^{\mathrm{T}}(\mathbf{v}) = M_{il}^{-1}(-\mathbf{v})$ , we have

$$A'_{i} = M_{il}^{-1}(-\mathbf{v})A_{l}.$$
(9.112)

Here is a list of contravariant vectors and covariant vectors we have learned. Contravariant vectors:  $(ct, \mathbf{r}), (c\rho, \mathbf{J}), (\phi/c, \mathbf{A}), (c\gamma_u, \gamma_u \mathbf{u}), (E/c, \mathbf{p})$ . Covariant vectors:  $(-\omega/c, \mathbf{k}), [\partial/(c\partial t), \nabla]$ .

Because

$$A'_{i}B'^{i} = M^{\mathrm{T}}_{il}(\mathbf{v})M^{-1}_{im}(\mathbf{v})A_{l}B^{m} = \delta_{lm}A_{l}B^{m} = A_{m}B^{m}, \qquad (9.113)$$

we see that the inner product between a contravariant vector  $B^m$  and a covariant  $A_m$  is a scaler, which is invariant under Lorentz transformation. Examples are:

$$\mathbf{k} \cdot \mathbf{r} - \omega t = \phi,$$
  

$$\nabla \cdot \mathbf{J} + \frac{\partial \rho}{\partial t} = 0,$$
  

$$\nabla \cdot \mathbf{A} + \frac{\partial \phi}{c^2 \partial t} = 0.$$
(9.114)

Note that Eq. (9.95) can be written as

$$\begin{pmatrix} -x'_{0} \\ x'_{1} \\ x'_{2} \\ x'_{3} \end{pmatrix}$$

$$= \begin{bmatrix} \gamma & \gamma \beta_{1} & \gamma \beta_{2} & \gamma \beta_{3} \\ \gamma \beta_{1} & 1 + \frac{(\gamma - 1)\beta_{1}^{2}}{\beta^{2}} & \frac{(\gamma - 1)\beta_{1}\beta_{2}}{\beta^{2}} & \frac{(\gamma - 1)\beta_{1}\beta_{3}}{\beta^{2}} \\ \gamma \beta_{2} & \frac{(\gamma - 1)\beta_{1}\beta_{2}}{\beta^{2}} & 1 + \frac{(\gamma - 1)\beta_{2}^{2}}{\beta^{2}} & \frac{(\gamma - 1)\beta_{2}\beta_{3}}{\beta^{2}} \\ \gamma \beta_{3} & \frac{(\gamma - 1)\beta_{1}\beta_{3}}{\beta^{2}} & \frac{(\gamma - 1)\beta_{2}\beta_{3}}{\beta^{2}} & 1 + \frac{(\gamma - 1)\beta_{2}^{2}}{\beta^{2}} \end{bmatrix} \begin{pmatrix} -x_{0} \\ x_{1} \\ x_{2} \\ x_{3} \end{pmatrix} . (9.115)$$

Hence we see that a contravariant vector can be converted to a covariant vector and vice versa by reversing the sign of the 0th component. For example, since  $(-\omega/c, \mathbf{k})$  is a covariant vector,  $(\omega/c, \mathbf{k})$  is a contravariant vector. For the same reason the inner product between  $(A_0, A_1, A_2, A_3)$  and  $(-A_0, A_1, A_2, A_3)$  is a scaler. Similarly, the inner product between  $(B^0, B^1, B^2, B^3)$  and  $(-B^0, B^1, B^2, B^3)$  is a also scaler. Examples are:

$$|\mathbf{r}|^2 - c^2 t^2 = -c^2 \tau^2,$$

$$\begin{split} |\mathbf{p}|^2 &- \frac{E^2}{c^2} = -m_0^2 c^2, \\ |\mathbf{k}|^2 &- \frac{\omega^2}{c^2} = -\frac{m_0^2 c^2}{\hbar^2}, \\ &\mathbf{J}\cdot\mathbf{A} - \rho\phi, \\ \nabla^2 &- \frac{\partial^2}{c^2\partial t^2}. \end{split}$$

# 9.8 Transformation of Electromagnetic Fields

We may work out the transformation of electromagnetic fields by transforming  $(\phi/c, \mathbf{A})$  first and then use the relations

$$\mathbf{E} = -\nabla \phi - \frac{\partial \mathbf{A}}{\partial t},$$
  
 
$$\mathbf{B} = \nabla \times \mathbf{A}.$$
 (9.116)

Assuming the relative velocity is in the x-direction, we have

$$E'_{x} = -\frac{\partial \phi'}{\partial x'} - \frac{\partial A'_{x}}{\partial t'}$$

$$= -\left(\gamma \frac{\partial}{\partial x} + \frac{\beta \gamma}{c} \frac{\partial}{\partial t}\right) (-c\beta\gamma A_{x} + \gamma\phi) - \left(c\beta\gamma \frac{\partial}{\partial x} + \gamma \frac{\partial}{\partial t}\right) \left(\gamma A_{x} - \beta\gamma \frac{\phi}{c}\right)$$

$$= -\frac{\partial \phi}{\partial x} - \frac{\partial A_{x}}{\partial t} = E_{x}.$$
(9.117)

$$E'_{y} = -\frac{\partial \phi'}{\partial y'} - \frac{\partial A'_{y}}{\partial t'}$$
  
$$= -\frac{\partial}{\partial y} \left( -c\beta\gamma A_{x} + \gamma\phi \right) - \left( c\beta\gamma \frac{\partial}{\partial x} + \gamma \frac{\partial}{\partial t} \right) A_{y}$$
  
$$= \gamma (E_{y} - c\beta B_{z}). \qquad (9.118)$$

$$E'_{z} = -\frac{\partial \phi'}{\partial z'} - \frac{\partial A'_{z}}{\partial t'}$$
  
=  $-\frac{\partial}{\partial z} \left( -c\beta\gamma A_{x} + \gamma\phi \right) - \left( c\beta\gamma \frac{\partial}{\partial x} + \gamma \frac{\partial}{\partial t} \right) A_{z}$   
=  $\gamma (E_{z} + c\beta B_{y}).$  (9.119)

$$B'_{x} = \frac{\partial A'_{z}}{\partial y'} - \frac{\partial A'_{y}}{\partial z'}$$
$$= \frac{\partial A_{z}}{\partial y} - \frac{\partial A_{y}}{\partial z}$$
$$= B_{x}.$$
(9.120)

$$B'_{y} = \frac{\partial A'_{x}}{\partial z'} - \frac{\partial A'_{z}}{\partial x'}$$
  
$$= \frac{\partial}{\partial z} \left( \gamma A_{x} - \beta \gamma \frac{\phi}{c} \right) - \left( \gamma \frac{\partial}{\partial x} + \frac{\beta \gamma}{c} \frac{\partial}{\partial t} \right) A_{z}$$
  
$$= \gamma \left( B_{y} + \frac{\beta}{c} E_{z} \right). \qquad (9.121)$$

$$B'_{z} = \frac{\partial A'_{y}}{\partial x'} - \frac{\partial A'_{x}}{\partial y'}$$
$$= \left(\gamma \frac{\partial}{\partial x} + \frac{\beta \gamma}{c} \frac{\partial}{\partial t}\right) A_{y} - \frac{\partial}{\partial y} \left(\gamma A_{x} - \beta \gamma \frac{\phi}{c}\right)$$
$$= \gamma \left(B_{z} - \frac{\beta}{c} E_{y}\right).$$
(9.122)

These equations can be combined into two vector equations:

$$\mathbf{E}' = \gamma (\mathbf{E} + c\boldsymbol{\beta} \times \mathbf{B}) - \frac{\gamma^2}{\gamma + 1} (\boldsymbol{\beta} \cdot \mathbf{E}) \boldsymbol{\beta}, \qquad (9.123)$$

$$\mathbf{B}' = \gamma \left( \mathbf{B} - \frac{\boldsymbol{\beta}}{c} \times \mathbf{E} \right) - \frac{\gamma^2}{\gamma + 1} (\boldsymbol{\beta} \cdot \mathbf{B}) \boldsymbol{\beta}.$$
(9.124)

## 9.9 Exercises

**Exercise 9.1.** Consider two identical space ships of length L, one moving in the x-direction and the other in the -x-direction. They pass by each other at a negligible distance. At the tail of each space ship there is a gunner controlling a gun that can be pointed to any direction perpendicular to the x-axis. To maintain the peace of the galaxy, the rule of engagement set by the congress is that the gunner can only fire the gun before the time when the tail of the opponent ship is aligned with the head of his own ship. By length contraction, at this time the head of the opponent ship has not reached the tail position of his own ship yet. Therefore from his point of view, the gun will not hit the opponent ship. However, thinking in the opponent's position, he becomes worried. When the head of the opponent ship is aligned with the tail of the opponent ship, by length contraction the tail of the opponent ship. How can this be right? After all, the two ships are in symmetric positions. Can you explain what went wrong?

**Exercise 9.2.** The wavelength  $\lambda_0$  of light emitted by hydrogen atoms as a result of transition from state 3p to state 2s is 656 nm. By measuring the optical spectrum of a distant star, one finds that this line emission is redshifted by 50%. Namely,  $(\lambda - \lambda_0)/\lambda_0 = 0.5$ . How fast is that star moving away from us?

**Exercise 9.3.** A photon with 1.5-eV energy propagating in the z-direction collides with an electron moving in the x-direction. The electron energy is 1.5 GeV. After the collision, what is the photon energy and at what angle does it propagate with respect to the x-axis?

**Exercise 9.4.** Two gamma-ray photons of the same energy E collide to create an electron-position pair. The rest mass of the electron or the position is  $m_e$ . The angle between the k-vectors of the gamma-ray photons is  $\theta$ . What is the minimum of E for this process to occur?

**Exercise 9.5.** A smart student proposes to build a spaceship that can move by itself without propellant. In the proposal two identical atoms are fixed at the two ends of a spaceship. One atom makes a transition from the state  $E_2$  to the state  $E_1$  and emits a photon in the x-direction at t = 0, and the photon is absorbed by the other atom at t = L/c by making a transition from the state  $E_1$  to the state  $E_2$ , where L is the length of the spaceship. Between t = 0 and t = L/c, the spaceship moves toward the -x-direction due to

#### 9.9. EXERCISES

recoil. The velocity is  $v = h/(\lambda M)$ , where  $\lambda$  is the wavelength of the photon and M is the mass of the spaceship. At t = L/c the spaceship has moved a distance  $D = hL/(\lambda Mc)$ . After that the astronaut on board swaps the two atoms quickly enough, so that the atom that has absorbed the photon before can now emit also in the x-direction, and the atom that has emitted before can now absorb the photon. By repeating this process many times, the spaceship will move in the -x-direction as far as the astronaut wants. You may wonder how one can control the direction of photon emission. This is a technical problem that in principle can be solved, for example by putting the two atoms at the two foci of an ellipsoid. Light emitting from one focus will always propagate to the other one. Explain what is wrong in this proposal, and show by correct calculation that the spaceship cannot move by itself this way.

**Exercise 9.6.** A stationary charged test particle is at a distance d from a straight long conducting neutral wire. In the wire the positive charges are stationary and the negative charges moving at velocity  $v\hat{\mathbf{x}}$  produce a current I. Since the test particle is not moving, and the wire is charge-neutral, there is no force between the wire and the particle, hence d does not change with time. For an observer moving at the same velocity as the negative charges in the wire, the current is still I, except that from his/her point of view it is the positive charges that are moving. However, from his/her point of view the test particle is moving at  $-v\hat{\mathbf{x}}$ , therefore it feels the magnetic force produced by the wire. In that case d changes with time. How do you resolve this apparent paradox?

**Exercise 9.7.** Consider a long rod hanging in the center by a thread. The thread is parallel to the *y*-axis and the rod is in the *x-y* plane making an angle  $\theta \neq 0$  with respect to the *x*-axis. One end of the rod has charge +q and the other end has charge -q. In a reference frame in which the rod is not moving, the rod experiences no torque, because the attraction force between the charges is in the same direction as their relative position vector. However, in a moving frame both charges are moving, so they correspond to two parallel current elements of opposite directions. In addition to the attractive Coulomb force between them, there should be a repulsive magnetic force **F** between the two current elements given by

$$\mathbf{F} = \frac{\mu_0}{4\pi} q^2 \frac{\mathbf{v} \times (\mathbf{v} \times \mathbf{L})}{L^3}$$

where **L** is the relative position vector. Because the direction of **F** is in the +y-direction for one charge and in the -y-direction for the other charge, one



Fig. 9.1: A detector for moving charge.

might think that this force will produce a torque to rotate the rod. Use your knowledge of relativity to show that actually there is no torque in the moving frame.

**Exercise 9.8.** A light source of 632.8-nm wavelength is mounted on the edge of a rotating disk. The radius of the disk is 1 m, and z-axis is the axis of rotation. An observer at a far-away place on the z-axis with no motion relative to the center of the disk finds the wavelength to be 650.2 nm. What is the angular velocity of the disk?

**Exercise 9.9.** A detector for moving charges is shown in Fig. 9.1. As a charged particle flies through the center of the ring of radius r and cross section A, which is made of a material with a large permeability  $\mu$ , a changing magnetic field is induced in the ring. The changing magnetic field then induces a voltage V(t) in the N-turn pick-up coil. For a particle of charge q moving at a velocity v, passing the center of the ring in the normal direction of the plane of the ring, what is V(t)? For simplicity we assume the thickness of the ring is negligibly small compared with the radius of the ring, and v is also negligibly small compared with the speed of light. Since one can use the induced V(t) to do work, where does this energy come from?

# Chapter 10

# Optics

# 10.1 Refraction and Reflection of Plane Waves

In section 3.6 we have shown the general solutions of the 1-dimensional wave equation can be written as

$$a(x,t) = \sum_{k} \alpha(k) \exp i(kx - \omega t + \phi_k), \qquad (10.1)$$

where  $v = \omega/k$  is the phase velocity. By the same procedure, the general solutions for the 3-dimensional wave equation can be written as

$$a(\mathbf{r},t) = \sum_{\mathbf{k}} \alpha(\mathbf{k}) \exp i(\mathbf{k} \cdot \mathbf{r} - \omega t + \phi_{\mathbf{k}}), \qquad (10.2)$$

and the phase velocity is still  $\omega/k$ . Therefore the general electromagnetic waves have the following form:

$$\mathbf{E}(\mathbf{r},t) = \sum_{\mathbf{k}} \mathbf{a}(\mathbf{k}) \exp i(\mathbf{k} \cdot \mathbf{r} - \omega t + \phi_{\mathbf{k}}),$$
  
$$\mathbf{B}(\mathbf{r},t) = \sum_{\mathbf{k}} \mathbf{b}(\mathbf{k}) \exp i(\mathbf{k} \cdot \mathbf{r} - \omega t + \phi'_{\mathbf{k}}).$$
 (10.3)

For a particular  $\mathbf{k}$ , because

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}.$$
 (10.4)

we have

$$\mathbf{k} \times \mathbf{E} = \omega \mathbf{B},\tag{10.5}$$

$$\phi'_{\mathbf{k}} = \phi_{\mathbf{k}}.\tag{10.6}$$

Therefore **B** is perpendicular to both **E** and **k**. The equation  $\nabla \cdot \mathbf{E} = 0$  leads to

$$\mathbf{k} \cdot \mathbf{E} = 0. \tag{10.7}$$

Therefore **k** is also perpendicular to **E**. Eqs. (10.6) and (10.7) lead to  $k|\mathbf{a}| = \omega |\mathbf{b}|$ . These solutions are called plane waves because in the 3-dimensional space the surface of constant phase is a plane. Namely the equation

$$\mathbf{k} \cdot \mathbf{r} - \omega t + \phi_{\mathbf{k}} = \text{constant} \tag{10.8}$$

represents a plane perpendicular to  $\mathbf{k}$ .

Since for each **k** there are two possible directions of **E**, there are two plane waves associated with each **k**. We use the variable  $\alpha = 1, 2$  to distinguish these two waves.

$$\mathbf{E}(\mathbf{r},t) = \sum_{\mathbf{k},\alpha} \mathbf{a}_{\alpha}(\mathbf{k}) \exp i(\mathbf{k} \cdot \mathbf{r} - \omega t + \phi_{\mathbf{k},\alpha}),$$
  
$$\mathbf{B}(\mathbf{r},t) = \sum_{\mathbf{k},\alpha} \frac{\mathbf{k}}{\omega} \times \mathbf{a}_{\alpha}(\mathbf{k}) \exp i(\mathbf{k} \cdot \mathbf{r} - \omega t + \phi_{\mathbf{k},\alpha}).$$
(10.9)

For a particular  $\mathbf{k}$ , if  $\phi_{\mathbf{k},1} = \phi_{\mathbf{k},2}$  or  $\phi_{\mathbf{k},1} = \phi_{\mathbf{k},2} + \pi$  we call the plane wave linearly polarized, because the electric field and the magnetic field oscillate along a fixed direction in the plane perpendicular to  $\mathbf{k}$ . In contrast, if  $\phi_{\mathbf{k},1} = \phi_{\mathbf{k},2} \pm \pi/2$ , we call the plane wave circularly polarized, because the directions of the electric field and the magnetic field change with time in the same way as the position vector of a particle moving in a circle. In general  $\phi_{\mathbf{k},1} = \phi_{\mathbf{k},2} + \theta$ , if  $\theta$  is not 0,  $\pi$ , or  $\pm \pi/2$ , we call the plane wave elliptically polarized, because the electric field and the magnetic field follow an elliptical trajectory.

Let us consider a plane wave propagating through the interface between two media. Because the phase velocities are different in these two media, part of the wave will be reflected and part will be transmitted. If the wave vector  $\mathbf{k}$  of the incident wave is not normal to the interface, the transmitted wave does not follow the same direction as the incident wave. The change of propagation direction for the transmitted wave is called refraction. Similar

to the case of string waves, refraction and reflection are required by the boundary conditions at the interface.

For an incident wave of a particular  $\mathbf{k}$ , we may write the incident wave, the refracted wave, and the reflected wave as

$$\mathbf{E}_{i}(\mathbf{r},t) = \mathbf{a}_{i} \exp\left[i(\mathbf{k}_{i} \cdot \mathbf{r} - \omega t + \phi_{i})\right], \\
\mathbf{B}_{i}(\mathbf{r},t) = \frac{\mathbf{k}_{i}}{\omega} \times \mathbf{a}_{i} \exp\left[i(\mathbf{k}_{i} \cdot \mathbf{r} - \omega t + \phi_{i})\right]. \quad (10.10)$$

$$\mathbf{E}_{t}(\mathbf{r},t) = \mathbf{a}_{t} \exp\left[i(\mathbf{k}_{t} \cdot \mathbf{r} - \omega t + \phi_{t})\right], \\ \mathbf{B}_{t}(\mathbf{r},t) = \frac{\mathbf{k}_{t}}{\omega} \times \mathbf{a}_{t} \exp\left[i(\mathbf{k}_{t} \cdot \mathbf{r} - \omega t + \phi_{t})\right].$$
(10.11)

$$\mathbf{E}_{r}(\mathbf{r},t) = \mathbf{a}_{r} \exp\left[i(\mathbf{k}_{r} \cdot \mathbf{r} - \omega t + \phi_{r})\right], \\
\mathbf{B}_{r}(\mathbf{r},t) = \frac{\mathbf{k}_{r}}{\omega} \times \mathbf{a}_{r} \exp\left[i(\mathbf{k}_{r} \cdot \mathbf{r} - \omega t + \phi_{r})\right]. \quad (10.12)$$

Assume the interface is the x-y plane. The plane defined by the incident wave and the reflected wave is call the incidence plane. Let us decompose  $\mathbf{E}_i$  into two components. The  $\alpha = 1$  mode, which is conventionally called the s-wave, is the one in which  $\mathbf{E}_i$  is perpendicular to the incidence plane. On the other hand, the  $\alpha = 2$  mode, which is conventionally called the p-wave, is the one in which  $\mathbf{E}_i$  is in the incidence plane.

When there is no free charge or current, the boundary conditions at the interface are that the tangential components of  $\mathbf{E}$  and  $\mathbf{H}$  are continuous, and the normal components of  $\mathbf{D}$  and  $\mathbf{B}$  are continuous. The first condition can be seen by imagining a rectangular loop for line integration. The length of the rectangle is l and the width is w. Let us put the loop in such a way that one of the long sides is in medium 1 and the other in medium 2, and both sides are parallel to the interface. Because

$$\oint \mathbf{E} \cdot d\mathbf{s} = -\frac{\partial}{\partial t} \int \mathbf{B} \cdot d\mathbf{a}, \qquad (10.13)$$

if we let  $w \to 0$  the right-hand side becomes zero, and the left-hand side becomes  $E_{\parallel 1}l - E_{\parallel 2}l$ , where  $E_{\parallel 1}$  and  $E_{\parallel 2}$  are the components of **E** that are parallel to the interface in medium 1 and medium 2 respectively. Hence we have  $E_{\parallel 1} = E_{\parallel 2}$ . For the same reason, because

$$\oint \mathbf{H} \cdot d\mathbf{s} = \frac{\partial}{\partial t} \int \mathbf{D} \cdot d\mathbf{a}, \qquad (10.14)$$

we have  $H_{\parallel 1} = H_{\parallel 2}$ . The second condition can be seen by imagining a rectangular box for surface integration. The length and width of the box are l and the height is h. Because

$$\int \nabla \cdot \mathbf{D} \, d^3 \mathbf{r} = \int \mathbf{D} \cdot d\mathbf{a} = 0, \qquad (10.15)$$

when  $h \to 0$  we have  $D_{\perp 1}l^2 - D_{\perp 2}l^2 = 0$ , that is  $D_{\perp 1} = D_{\perp 2}$  where  $D_{\perp 1}$  and  $D_{\perp 2}$  are the components of **D** that are normal to the interface in medium 1 and medium 2 respectively. Similarly, from  $\nabla \cdot \mathbf{B} = 0$  we have  $B_{\perp 1} = B_{\perp 2}$ .

Let us consider the reflection and refraction of the *s*-wave first. Applying these boundary conditions to the *s*-wave, we have

$$a_{i}^{s} \exp\left[i(\mathbf{k}_{i} \cdot \mathbf{r} - \omega t + \phi_{i})\right] + a_{r}^{s} \exp\left[i(\mathbf{k}_{r} \cdot \mathbf{r} - \omega t + \phi_{r})\right]$$
  
=  $a_{t}^{s} \exp\left[i(\mathbf{k}_{t} \cdot \mathbf{r} - \omega t + \phi_{t})\right],$  (10.16)

where the superscript s in the amplitudes denotes s-waves. This condition must be satisfied at the whole plane of z = 0, therefore we have

$$a_i^s + a_r^s = a_t^s, (10.17)$$

$$\phi_i = \phi_r = \phi_t,$$
  
 $k_{\parallel i} = k_{\parallel r} = k_{\parallel t}.$  (10.18)

In terms of the angle between  $\mathbf{k}$  and the surface normal, Eq. (10.18) reads

$$k_i \sin \theta_i = k_r \sin \theta_r = k_t \sin \theta_t. \tag{10.19}$$

Since  $k_i = k_r$ ,  $k_i/n_i = k_t/n_t$ , where  $n_i/c = \sqrt{\epsilon_1 \mu_1}$  is the index of refraction of medium 1, and  $n_t/c = \sqrt{\epsilon_2 \mu_2}$  is that of medium 2, we have

$$\theta_i = \theta_r, \tag{10.20}$$

$$n_i \sin \theta_i = n_t \sin \theta_t. \tag{10.21}$$

Eq. (10.21) is known as the **Snell's law**.

For the *s*-wave, the boundary condition for the normal components of **D** is satisfied automatically, because  $\mathbf{a}_i$ ,  $\mathbf{a}_r$ , and  $\mathbf{a}_t$  have no normal components. The boundary condition for the normal components of **B** reads

$$k_i \sin \theta_i a_i^s + k_r \sin \theta_r a_r^s = k_t \sin \theta_t a_t^s.$$
(10.22)
From Eqs. (10.17) and (10.19), we see it is also automatically satisfied. The last condition left is for the tangential components of **H**, which reads

$$\frac{1}{\mu_1}(k_i a_i^s \cos \theta_i - k_r a_r^s \cos \theta_r) = \frac{1}{\mu_2}(k_t a_t^s \cos \theta_t), \qquad (10.23)$$

For dielectric media that are not magnetizable, we have  $\mu_1 = \mu_2 = \mu_0$ . In this case Eq. (10.23) is reduced to

$$k_{\perp i}a_i^s - k_r a_r^s = k_{\perp t}a_t^s, \tag{10.24}$$

where the subscript  $\perp$  denotes the component normal to the interface. That is

$$k_{\perp i}(a_i^s - a_r^s) = k_{\perp t} a_t^s. \tag{10.25}$$

Eqs. (10.17) and (10.25) lead to

$$\frac{a_{t}^{s}}{a_{i}^{s}} = \frac{2k_{\perp i}}{k_{\perp i} + k_{\perp t}}, 
\frac{a_{r}^{s}}{a_{i}^{s}} = \frac{k_{\perp i} - k_{\perp t}}{k_{\perp i} + k_{\perp t}},$$
(10.26)

or

$$\frac{a_t^s}{a_i^s} = \frac{2n_i \cos \theta_i}{n_i \cos \theta_i + n_t \cos \theta_t}, 
\frac{a_r^s}{a_i^s} = \frac{n_i \cos \theta_i - n_t \cos \theta_t}{n_i \cos \theta_i + n_t \cos \theta_t}.$$
(10.27)

Note that Eq. (10.26) is the same as Eq. (3.112) for the string waves.

Now we shall consider the reflection and refraction of the p-wave. As before, we consider the case in which  $\mu_1 = \mu_2 = \mu_0$ . Continuity of the tangential components of  $\mathbf{H}$  leads to

$$\mathbf{k}_{i} \times a_{i}^{p} \exp\left[i(\mathbf{k}_{i} \cdot \mathbf{r} - \omega t + \phi_{i})\right] + \mathbf{k}_{r} \times a_{r}^{p} \exp\left[i(\mathbf{k}_{r} \cdot \mathbf{r} - \omega t + \phi_{r})\right]$$
  
= 
$$\mathbf{k}_{t} \times a_{t}^{p} \exp\left[i(\mathbf{k}_{t} \cdot \mathbf{r} - \omega t + \phi_{t})\right], \qquad (10.28)$$

which yields

$$n_i(a_i^p + a_r^p) = n_t a_t^p,$$

$$\phi_i = \phi_r = \phi_t,$$
(10.29)

$$k_{\parallel i} = k_{\parallel r} = k_{\parallel t}. \tag{10.30}$$

$$c_{\parallel i} = k_{\parallel r} = k_{\parallel t}.$$
 (10.3)

Eq. (10.30) again leads to the Snell's law. Continuity of the tangential components of  $\mathbf{E}$  leads to

$$\cos\theta_i(a_i^p - a_r^p) = \cos\theta_t a_t^p. \tag{10.31}$$

The condition for the normal components of **B** is automatically satisfied because **B** is parallel to the interface, and the condition for the normal components of **D** leads to the Eq. (10.29) again. Eqs. (10.29) and (10.31) leads to

$$\frac{a_t^p}{a_i^p} = \frac{2n_i \cos \theta_i}{n_t \cos \theta_i + n_i \cos \theta_t},\tag{10.32}$$

$$\frac{a_r^p}{a_i^p} = \frac{n_t \cos \theta_i - n_i \cos \theta_t}{n_t \cos \theta_i + n_i \cos \theta_t}.$$
(10.33)

If  $n_t > n_i$ , by Snell's law we have  $\cos \theta_t > \cos \theta_i$ , and vice versa. Therefore it is seen from Eq. (10.27) that the reflection of the *s*-wave cannot be zero. In contrast, for a special incidence angle  $\theta_B$  the reflection of the *p*-wave can be zero. This angle is called Brewster's angle. The equation for Brewster's angle is

$$n_t \cos \theta_B = n_i \sqrt{1 - \frac{n_i^2 \sin^2 \theta_B}{n_t^2}}.$$
 (10.34)

Let  $r = n_t/n_i$  and solve for  $\cos^2 \theta_B$ , we have

$$\cos^2 \theta_B = \frac{1}{r^2 + 1}.$$
 (10.35)

That is

$$\tan \theta_B = \frac{n_t}{n_i}.\tag{10.36}$$

For example, the index of refraction for ordinary glass is  $\approx 1.5$ . When a plane wave propagates from air into glass, the condition for no *p*-wave reflection at the interface is  $\theta_B \approx 56^{\circ}$ .

If  $n_i > n_t$  and  $\sin \theta_i > n_t/n_i$ , from Snell's law we see it is not possible to have refraction. The interface functions as a perfect mirror. This phenomenon is called total reflection. But how can the boundary conditions be satisfied if there is no refraction? The answer lies in the transition from Eq. (10.18) to Eq. (10.19). If we use Eq. (10.18) in conjunction with the following equations

$$\begin{aligned} k_{\perp i}^2 + k_{\parallel i}^2 &= n_i^2 k_0^2, \\ k_{\perp t}^2 + k_{\parallel t}^2 &= n_t^2 k_0^2, \end{aligned} \tag{10.37}$$

where  $k_{\perp}$  is the z-component of **k** and  $k_0 = \omega/c$ , we have

$$k_{\perp t}^2 = (n_t^2 - n_i^2)k_0^2 + k_{\perp i}^2.$$
(10.38)

Because  $k_{\perp i} = n_i k_0 \cos \theta_i$ ,

$$k_{\perp t}^2 = k_0^2 (n_t^2 - n_i^2 \sin^2 \theta_i).$$
(10.39)

when  $\sin \theta_i > n_t/n_i$ , that is when total reflection occurs,  $k_{\perp t}^2 < 0$ . This means when the refracted wave is written as

$$\mathbf{E}_{t}(\mathbf{r},t) = \mathbf{a}_{t} \exp\left[i(\mathbf{k}_{t} \cdot \mathbf{r} - \omega t)\right], \\
\mathbf{B}_{t}(\mathbf{r},t) = \frac{\mathbf{k}_{t}}{\omega} \times \mathbf{a}_{t} \exp\left[i(\mathbf{k}_{t} \cdot \mathbf{r} - \omega t)\right], \quad (10.40)$$

the z-component of  $\mathbf{k}_t$  is imaginary. Namely

$$\mathbf{k}_{t} = (k_{xi}, k_{yi}, ik_{0}\sqrt{n_{i}^{2}\sin^{2}\theta_{i} - n_{t}^{2}}).$$
(10.41)

Hence both  $\mathbf{E}_t$  and  $\mathbf{B}_t$  decay exponentially in the z-direction. That is

$$\mathbf{E}_{t}(\mathbf{r},t) = \mathbf{a}_{t} \exp\left[-\eta z + i(\mathbf{k}_{\parallel t} \cdot \mathbf{r} - \omega t)\right],$$
  
$$\mathbf{B}_{t}(\mathbf{r},t) = \frac{\mathbf{k}_{t}}{\omega} \times \mathbf{a}_{t} \exp\left[-\eta z + i(\mathbf{k}_{\parallel t} \cdot \mathbf{r} - \omega t)\right], \qquad (10.42)$$

where  $\eta = k_0 \sqrt{n_i^2 \sin^2 \theta_i - n_t^2}$ . This exponential decaying waves leaking out of the interface are called evanescent waves.

In the above discussions we have assumed the media are polarizable but not magnetizable. This assumption is generally valid in the optical frequency range for the following reason. A medium is polarized by the displacement of electrons in response to the external field. In the optical frequency range, the displacement occurs in a time scale shorter than the period of light. Therefore a dense transparent medium is generally polarizable in the optical frequency range. In contrast, magnetization involves the rotation of atoms or molecules so that their magnetic dipole moment can be aligned with the external field. In the optical frequency range, the rotation occurs in a much longer time scale than the period of light, therefore the medium can be considered effectively non-magnetizable.

# 10.2 Huygen's principle

Consider a scalar wave of a fixed frequency  $\omega$ ,  $\psi(\mathbf{r}, t) = \phi(\mathbf{r})e^{-i\omega t}$ . We may write  $\phi(\mathbf{r})$  as a superposition of plane waves.

$$\phi(\mathbf{r}) = \sum_{k=\omega/c} u(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{r}},\tag{10.43}$$

where the summation is over all the **k** that satisfies the condition  $k = \omega/c$ . Multiplying both sides by  $e^{-i\mathbf{k}'\cdot\mathbf{r}}$  and integrating over a large box with length, width and height all equal to L, we see the integration on the right-hand side is zero for all the **k** except when  $\mathbf{k} = \mathbf{k}'$ . Therefore we have

$$u(\mathbf{k}) = \frac{1}{L^3} \int \phi(\mathbf{r}') e^{-i\mathbf{k}\cdot\mathbf{r}'} d^3\mathbf{r}'.$$
 (10.44)

Combining Eqs. (10.43) and (10.44), we have

$$\phi(\mathbf{r}) = \frac{1}{L^3} \sum_{k=\omega/c} \int \phi(\mathbf{r}') e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')} d^3\mathbf{r}'.$$
 (10.45)

Because  $\mathbf{k}$  satisfies the periodic boundary conditions, we have

$$k_x L = 2n_x \pi,$$
  

$$k_y L = 2n_y \pi,$$
  

$$k_z L = 2n_z \pi,$$
(10.46)

where  $n_x$ ,  $n_y$ , and  $n_z$  are integers. The interval between consecutive **k** is

$$\Delta k_i = \frac{2\pi}{L}.\tag{10.47}$$

Since  $|\mathbf{k}|$  is fixed to  $\omega/c$ , in the continuous limit the summation over  $\mathbf{k}$  can be changed to integration over the surface of a sphere in the  $\mathbf{k}$ -space with a radius of  $\omega/c$  by the following replacement.

$$\sum_{k=\omega/c} = \frac{L^2}{4\pi^2} \int_0^\pi \int_0^{2\pi} k^2 d\phi \,\sin\theta \,d\theta, \qquad (10.48)$$

where  $\theta$  is the angle between **k** and **r** - **r**'. Hence we have

$$\begin{split} \phi(\mathbf{r}) &= \frac{1}{L^3} \sum_{k=\omega/c} \int \phi(\mathbf{r}') e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')} d^3\mathbf{r}' \\ &= \frac{1}{2\pi L} \int \int_0^{\pi} \phi(\mathbf{r}') e^{ik|\mathbf{r}-\mathbf{r}'|\cos\theta} k^2 \sin\theta \, d\theta \, d^3\mathbf{r}' \\ &= \frac{1}{2\pi L} \int \phi(\mathbf{r}') \frac{\sin k|\mathbf{r}-\mathbf{r}'|}{k|\mathbf{r}-\mathbf{r}'|} 2k^2 \, d^3\mathbf{r}'. \end{split}$$
(10.49)

#### 10.2. HUYGEN'S PRINCIPLE

In terms of  $\psi(\mathbf{r}, t)$ , we have

$$\psi(\mathbf{r},t) = \frac{1}{2\pi L} \int \psi(\mathbf{r}',t') \frac{\sin k|\mathbf{r}-\mathbf{r}'|}{k|\mathbf{r}-\mathbf{r}'|} e^{-i\omega(t-t')} 2k^2 d^3 \mathbf{r}'$$

$$= \frac{-ik}{2\pi L} \int \psi(\mathbf{r}',t') \frac{e^{i[k|\mathbf{r}-\mathbf{r}'|-\omega(t-t')]}}{|\mathbf{r}-\mathbf{r}'|} d^3 \mathbf{r}'$$

$$+ \frac{ik}{2\pi L} \int \psi(\mathbf{r}',t') \frac{e^{-i[k|\mathbf{r}-\mathbf{r}'|+\omega(t-t')]}}{|\mathbf{r}-\mathbf{r}'|} d^3 \mathbf{r}'. \quad (10.50)$$

This equation shows that the wave at  $\mathbf{r}$  can be constructed from the wave at  $\mathbf{r}'$ . The fields at these two positions are linked by an outgoing spherical wave as well as an incoming spherical wave.

If the source of the wave is at distance much larger than L, within the box of integration the phase front will be close to a plane. Let us choose the normal vector of the phase front to be the z-direction and decompose  $\mathbf{r}'$  into  $\mathbf{r}' = \mathbf{r}'_t + z'\hat{\mathbf{z}}$ , where  $\mathbf{r}'_t$  is perpendicular to  $\hat{\mathbf{z}}$ . In this case we have

$$\psi(\mathbf{r}', t') \approx \Phi(\mathbf{r}'_t) e^{i(kz' - \omega t')}.$$
(10.51)

If the angle  $\theta$  between  $\mathbf{r} - \mathbf{r}'_t$  and the z-axis is small, we have

$$|\mathbf{r} - \mathbf{r}'| = \sqrt{|\mathbf{r} - \mathbf{r}'_t|^2 - 2|\mathbf{r} - \mathbf{r}'_t|z'\cos\theta + z'^2} \approx |\mathbf{r} - \mathbf{r}'_t| - z'. \quad (10.52)$$

Substituting Eqs. (10.51) and (10.52) into Eq. (10.50), we obtain

$$\psi(\mathbf{r},t) = \frac{-ik}{2\pi L} \int \Phi(\mathbf{r}'_t) \frac{e^{i(k|\mathbf{r}-\mathbf{r}'_t|-\omega t)}}{|\mathbf{r}-\mathbf{r}'_t|} d^2 \mathbf{r}'_t dz' + \frac{ik}{2\pi L} \int \Phi(\mathbf{r}'_t) \frac{e^{2ikz'}e^{-i(k|\mathbf{r}-\mathbf{r}'_t|+\omega t)}}{|\mathbf{r}-\mathbf{r}'_t|} d^2 \mathbf{r}'_t dz', \qquad (10.53)$$

where we have replaced  $d^3\mathbf{r}'$  by  $d^2\mathbf{r}'_t dz'$ . In the first term on the right-hand side the integrand is independent of z' and the second term averages to zero because of the fast oscillating factor  $e^{2ikz'}$ . Hence we have

$$\psi(\mathbf{r},t) = \frac{-ik}{2\pi} \int \Phi(\mathbf{r}'_t) \frac{e^{i(k|\mathbf{r}-\mathbf{r}'_t|-\omega t)}}{|\mathbf{r}-\mathbf{r}'_t|} d^2 \mathbf{r}'_t.$$
 (10.54)

The wave amplitude at  $(\mathbf{r}, t)$  is the superposition of all the spherical waves whose sources are  $\Phi(\mathbf{r}'_t)$ . This is a form of the **Huygen's principle** that most commonly appears in its application.

### **10.3** Paraxial Approximation and Fresnel's Diffraction

Consider a scalar wave  $\phi(\mathbf{r})e^{-i\omega t}$  of a fixed frequency  $\omega = ck$  propagating essentially in the z-direction. The wave can be written as a superposition of plane waves, and each of its plane-wave components  $e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}$  has a wave vector pointing close to the z-direction. If  $\mathbf{k}$  points close to the z-direction, we must have  $|k_x| \ll k_z$  and  $|k_y| \ll k_z$ . Under these conditions, we have

$$k_z = \sqrt{k^2 - k_x^2 - k_y^2} \approx k - \frac{k_x^2 + k_y^2}{2k}.$$
 (10.55)

This is called the paraxial approximation. Under the paraxial approximation  $k_z$  is a function of  $k_x$  and  $k_y$  as shown above, hence in the expansion of  $\phi(\mathbf{r})$  we only use the two independent variables  $k_x$  and  $k_y$ .

$$\phi(\mathbf{r}) = \left(\frac{1}{\sqrt{2\pi}}\right)^2 \int u(k_x, k_y) e^{i\mathbf{k}\cdot\mathbf{r}} dk_x dk_y$$
$$\approx e^{ikz} \left(\frac{1}{\sqrt{2\pi}}\right)^2 \int u(k_x, k_y) e^{i\left(k_x + k_y y - \frac{k_x^2 + k_y^2}{2k}z\right)} dk_x dk_y.$$
(10.56)

At z = 0, this equation becomes

$$\phi(x, y, 0) = \left(\frac{1}{\sqrt{2\pi}}\right)^2 \int u(k_x, k_y) e^{i(k_x x + k_y y)} dk_x dk_y$$
(10.57)

Using the inverse Fourier transform, we may express  $u(k_x, k_y)$  in terms of the field in the z = 0 plane.

$$u(k_x, k_y) = \left(\frac{1}{\sqrt{2\pi}}\right)^2 \int \phi(x', y', 0) e^{-i(k_x x' + k_y y')} \, dx' dy'.$$
(10.58)

Put this back into Eq. (10.56), we have

$$\phi(\mathbf{r}) = \frac{e^{ikz}}{4\pi^2} \int \int \phi(x', y', 0) e^{i \left[k_x(x-x')+k_y(y-y')-\frac{k_x^2+k_y^2}{2k}z\right]} dk_x dk_y \, dx' dy'.$$
(10.59)

By using the formula

$$\int_{-\infty}^{\infty} e^{-x^2} e^{-ikx} \, dx = \int_{-\infty}^{\infty} e^{-x^2} \cos kx \, dx = \sqrt{\pi} e^{-k^2/4}, \tag{10.60}$$

#### 10.4. INDEX OF REFRACTION

we can reduce Eq. (10.59) to

$$\phi(\mathbf{r}) = \frac{-ike^{ikz}}{2\pi z} \int \phi(x', y', 0) e^{\frac{ik}{2z}[(x-x')^2 + (y-y')^2]} dx' dy'.$$
 (10.61)

This is known as **Fresnel's diffraction integral**. Since in the paraxial approximation we have  $x - x' \ll z$ ,  $y - y' \ll z$ , for z' = 0 we may expand  $|\mathbf{r} - \mathbf{r}'|$  as

$$\sqrt{(x-x')^2 + (y-y')^2 + z^2} \approx z + \frac{(x-x')^2 + (y-y')^2}{2z}.$$
 (10.62)

Therefore we have

$$\frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} \approx \frac{e^{ik\left[z + \frac{(x-x')^2 + (y-y')^2}{2z}\right]}}{z}.$$
(10.63)

Eq. (10.61) can be written as

$$\phi(\mathbf{r}) = \frac{-ik}{2\pi} \int \phi(x', y', 0) \frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} dx' dy'.$$
(10.64)

For z' = 0 we can write  $\mathbf{r}'$  as  $\mathbf{r}'_t$ , then Eq. (10.64) is the same as Eq. (10.54). We see under the paraxial approximation Fresnel's diffraction integral is an equivalent expression of Huygen's principle.

# 10.4 Index of Refraction

Consider the displacement of electrons in a medium caused by external fields. If the medium is not a conductor, we may assume the electrons are bounded by a potential well V(x). Let us expand V(x) in Taylor series and assume x = 0 is the equilibrium point.

$$V(x) = V(0) + V'(0)x + \frac{V''(0)}{2}x^2 \cdots$$
(10.65)

Because at the equilibrium point the force is zero, we have V'(0) = 0. Therefore in the first-order approximation, we may treat the motion of the electrons as a harmonic oscillator. The equation of motion is

$$\ddot{\mathbf{r}} + \gamma \dot{\mathbf{r}} + \omega_0^2 \mathbf{r} = \frac{e\mathbf{E} + e\mathbf{v} \times \mathbf{B}}{m_e},$$
(10.66)

where **E** and **B** are the external fields and  $m_e$  is the electron mass. For plane waves  $|\mathbf{B}| = |\mathbf{E}|/c$ , hence the contribution from the magnetic force  $e\mathbf{v} \times \mathbf{B}$  is much smaller than that of the electric force  $e\mathbf{E}$  when  $v \ll c$ . In this case the electron displacement is

$$\mathbf{r} = \frac{e\mathbf{E}_0 e^{-i\omega t}}{m_e(\omega_0^2 - \omega^2 - i\gamma\omega)}.$$
(10.67)

If the electron density is  $n_e$ , the polarization is

$$\mathbf{P} = \frac{n_e e^2 \mathbf{E}_0 e^{-i\omega t}}{m_e (\omega_0^2 - \omega^2 - i\gamma\omega)}.$$
(10.68)

Hence

$$\epsilon_0 \chi_e = \frac{n_e e^2}{m_e (\omega_0^2 - \omega^2 - i\gamma\omega)}.$$
(10.69)

In the optical frequency range we may assume  $\mu = \mu_0$ . From Eqs. (6.43) and (6.44), we have

$$n = \sqrt{\frac{\epsilon}{\epsilon_0}} = \sqrt{1 + \frac{n_e e^2}{\epsilon_0 m_e (\omega_0^2 - \omega^2 - i\gamma\omega)}}.$$
 (10.70)

This formula is valid only when the electron density is small. If the electron density is large, the displacement of the electrons will generate an additional **E**-field. In that case, the **E**-field on the right-hand side of Eq. (10.66) must include this additional field. In this Section we shall consider only the case of small  $n_e$ . The general case will be discussed in Section 10.5. Therefore we have

$$n \approx 1 + \frac{n_e e^2}{2\epsilon_0 m_e (\omega_0^2 - \omega^2 - i\gamma\omega)}.$$
(10.71)

We may separate n into the real part and the imaginary part:

$$\operatorname{Re}[n] = 1 + \frac{n_e e^2 (\omega_0^2 - \omega^2)}{2\epsilon_0 m_e [(\omega_0^2 - \omega^2)^2 + \gamma^2 \omega^2]},$$
(10.72)

$$Im[n] = \frac{n_e e^2 \gamma \omega}{2\epsilon_0 m_e [(\omega_0^2 - \omega^2)^2 + \gamma^2 \omega^2]},$$
 (10.73)

and correspondingly,

$$k = \frac{n\omega}{c} = \beta + i\frac{\alpha}{2}.$$
(10.74)

#### 10.4. INDEX OF REFRACTION

The plane wave propagating in the z-direction becomes

$$\mathbf{E}(z,t) = \mathbf{E}_0 e^{-\frac{\alpha}{2}z} e^{i(\beta z - \omega t)}.$$
(10.75)

We see that if  $\gamma \neq 0$ , the electromagnetic wave will be absorbed by the medium. Both the **E**-field and the **B**-field decay exponentially in the propagation direction, and  $\alpha$  is called the absorption coefficient. The absorption is maximum at resonance, *i.e.*, when  $\omega = \omega_0$ . Near the resonance, we may write

$$\omega_0^2 - \omega^2 \approx 2\omega(\omega_0 - \omega). \tag{10.76}$$

Then we have

$$k \operatorname{Im}[n] = \frac{\alpha}{2} \approx \frac{n_e e^2 \gamma}{8\epsilon_0 m_e c [(\omega_0 - \omega)^2 + \frac{\gamma^2}{4}]}.$$
(10.77)

The width of the resonance  $\Delta \omega$  is defined by the frequency range within which the absorption drops to half. Hence  $\Delta \omega = \gamma/2$ , which means the smaller the  $\gamma$ , the sharper the resonance. At resonance,

$$\frac{\alpha}{2} \approx \frac{n_e e^2}{2\epsilon_0 m_e c \gamma},\tag{10.78}$$

which means the smaller the  $\gamma$ , the stronger the absorption at resonance. The total absorption coefficient integrated over all the frequencies is

$$\alpha_t \approx \int \frac{n_e e^2 \gamma}{4\epsilon_0 m_e c [(\omega_0 - \omega)^2 + \frac{\gamma^2}{4}]} \, d\omega = \frac{n_e e^2 \pi}{2\epsilon_0 m_e c},\tag{10.79}$$

which is independent of  $\omega_0$  and  $\gamma$ .

If the medium has many resonance frequencies, Eq. (10.70) becomes

$$n = \sqrt{1 + \sum_{i} \frac{n_i e^2}{\epsilon_0 m_e(\omega_i^2 - \omega^2 - i\gamma_i \omega)}},$$
(10.80)

where  $\omega_i$  and  $\gamma_i$  are the resonance frequency and the damping factor respectively for the *i*th oscillator, and  $n_i$  is the density of the electron associated with the *i*th oscillator. For most small molecules, resonance frequencies are in the ultraviolet range. They are much larger than optical frequencies. This is why materials made of small molecules are mostly transparent in the optical region. Because each atom or molecule has its own characteristic resonance frequencies, by measuring the locations of the absorption peaks, it is possible to identify the composition of an unknown material, or to determine the structure of a molecule of known chemical composition. Such techniques are known as optical spectroscopy.

The real part of the index of refraction also shows a resonance structure. If there is only a single resonance,  $\operatorname{Re}[n] = 1$  at resonance,  $\operatorname{Re}[n] > 1$  when  $\omega < \omega_0$  and vice versa. In general, atoms and molecules have many resonance frequencies. Most of them are in the ultraviolet range, and all of them contribute to  $\operatorname{Re}[n]$ . As can be seen in Eq. (10.80), because optical frequencies are much smaller than most of the resonance frequencies, even if there are some resonance frequencies happen to be in the optical region, their contribution to  $\operatorname{Re}[n]$  are outweighed. Therefore the index of refraction for most materials in the optical region is larger than 1.

In conductors the electrons can move freely, hence  $\omega_0 = 0$ . In most conductors continuous acceleration of electrons does not occur. This is because the electrons suffers from many collisions. Therefore the motion is a random walk with drift. The average drift velocity is the acceleration times the mean free time. Let us define the conductivity  $\sigma$  by  $\mathbf{J} = \sigma \mathbf{E}$ . Because  $\mathbf{J} = n_e e \mathbf{v}$  we have

$$\mathbf{v} = \frac{\sigma}{n_e e} \mathbf{E},\tag{10.81}$$

$$\mathbf{r} = \frac{i\sigma}{\omega n_e e} \mathbf{E}.$$
 (10.82)

From Eq. (10.67) we may write  $\sigma$  as

$$\sigma = \frac{in_e e^2}{m_e(\omega + i\gamma)}.$$
(10.83)

Since in general the conducting electrons are not the only contribution to polarization; there are contributions from other bound electrons, we have

$$\mathbf{P} = \left(\epsilon_0 \chi_b + \frac{i\sigma}{\omega}\right) \mathbf{E},\tag{10.84}$$

where  $\chi_b$  is the susceptibility of the bound electrons. Consequently, the index of refraction for a conductor is

$$n = \sqrt{1 + \chi_b + \frac{i\sigma}{\epsilon_0 \omega}}.$$
(10.85)

#### 10.4. INDEX OF REFRACTION

We see that electromagnetic waves suffer from an exponential decay in the direction of propagation. The depth of 1/e amplitude attenuation is called the skin-depth  $\delta$ , which is equal to  $2/\alpha$ . Eqs. (10.83) and (10.85) show that the skin depth increases with frequency. For a good conductor

$$\frac{\sigma}{\epsilon_0\omega} \gg 1 + \chi_b,\tag{10.86}$$

we have

$$n \approx (1+i)\sqrt{\frac{\sigma}{2\epsilon_0\omega}},\tag{10.87}$$

and the skin-depth is

$$\delta = \frac{2}{\alpha} = \sqrt{\frac{2\epsilon_0}{\omega\sigma}} c \tag{10.88}$$

If we coat the surface of glass with silver or aluminum to make a mirror, the thickness of coating must be several times larger than the skin-depth, otherwise part of the light will be transmitted. Similarly if we wish to shield an electromagnetic wave with a metal box, the thickness of the wall must be several times larger the skin-depth, otherwise the shielding will not be effective. For example, the density of free electron in aluminum is  $1.8 \times 10^{29} \text{ m}^{-3}$ , and the DC-conductivity is  $3.64 \times 10^7 \Omega^{-1} \text{m}^{-1}$ . Substituting them into Eq. (10.83) yields  $\gamma = 1.39 \times 10^{14} \text{ s}^{-1}$ . Therefore, for frequency much smaller than  $10^{14} \text{ Hz}$ , we may ignore the frequency dependence of  $\sigma$ . For a 60-Hz wave the skin-depth is 1.1 cm, therefore it is not possible to shield the magnetic field leaked out from a power transformer with a thin aluminum box. In contrast, for a 1.8-GHz wave the skin-depth is 2.0  $\mu$ m, therefore the radio wave from a GSM mobile phone can be easily shielded with aluminum foil.

Finally let us consider the case in which both the damping and the resonance effects are negligible. This is the case of dilute plasma, in which the electrons move freely and the collision rate is low, or the case of very high frequency light in which the contribution from  $\omega_0^2$  and  $\gamma \omega$  are negligible compared with that from  $\omega^2$ . The polarization is

$$\mathbf{P} = -\frac{n_e e^2 \mathbf{E}_0 e^{-i\omega t}}{m_e \omega^2},\tag{10.89}$$

and the index of refraction is

$$n = \sqrt{1 - \frac{\omega_p^2}{\omega^2}},\tag{10.90}$$

where

$$\omega_p^2 = \frac{n_e e^2}{\epsilon_0 m_e} \tag{10.91}$$

is called the plasma frequency. For  $\omega > \omega_p$ , electromagnetic waves can propagate with an index of refraction less than 1, namely with a phase velocity larger than c. For  $\omega < \omega_p$ , n has an imaginary part, and the wave will be attenuated. At the surface of such a medium, electromagnetic waves will be reflected completely because transmission into such a medium is not possible. An important application of this effect was radio communication beyond horizon. Before the advent of satellite communication, reflection of radio waves below 7 MHz by the ionosphere was a key technique for long distance radio communication.

### 10.5 Clausius-Mossotti Equation

Eq. (10.68) is derived under the assumption that the medium is dilute, so that we can use the external **E** in the right-hand side of Eq. (10.66). In a dense medium atoms and molecules do not experience directly the external field. Instead, they are driven by the local field that is a combination of the external field  $\mathbf{E}_e$  and the field  $\mathbf{E}_p$  produced by the polarization. Therefore Eq. (10.67) should be changed to

$$\mathbf{r} = \frac{e}{m_e(\omega_0^2 - \omega^2 - i\gamma\omega)} (\mathbf{E}_e + \mathbf{E}_p).$$
(10.92)

Consider a test charge in a medium of polarization **P**. The charge will experience an electric field in the opposite of the direction of **P**. For simplicity, let us consider the charge distribution of a polarized sphere of radius R. The polarized sphere can be treated as two uniformly charged spheres of opposite sign separated by a small distance  $2d \ll R$ . Let the center of the positively charged sphere be at (d, 0, 0) and that of the negatively charged sphere be at (-d, 0, 0). By the Shell theorem, a test charge placed at the origin will experience an electric field as if all the positive charge within a radius d from (d, 0, 0) is concentrated at (d, 0, 0) and all the negative charge within a radius d from (-d, 0, 0) is concentrated at (-d, 0, 0). Therefore the test charge experiences a field equal to

$$E_p = \frac{2}{4\pi\epsilon_0} \frac{\rho\left(\frac{4\pi}{3}d^3\right)}{d^2} = \frac{2\rho d}{3\epsilon_0} = \frac{P}{3\epsilon_0}.$$
(10.93)

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#### 10.6. LIGHT PROPAGATING IN DISPERSIVE MEDIA

Let us define the atomic or molecular polarizability  $\gamma_p$  by

$$\mathbf{p} = \gamma_p (\mathbf{E}_e + \mathbf{E}_p), \tag{10.94}$$

where  $\mathbf{p}$  is the dipole induced by the local field. We have

$$\mathbf{P} = \mathcal{N}\gamma_p(\mathbf{E}_e + \mathbf{E}_p) = \mathcal{N}\gamma_p\left(\mathbf{E}_e + \frac{\mathbf{P}}{3\epsilon_0}\right), \qquad (10.95)$$

where  $\mathcal{N}$  is the atomic or molecular density. Because  $\mathbf{P} = (\epsilon - \epsilon_0) \mathbf{E}_e$ , we have

$$\epsilon = \epsilon_0 \left( 1 + \frac{\frac{N\gamma_p}{\epsilon_0}}{1 - \frac{N\gamma_p}{3\epsilon_0}} \right), \tag{10.96}$$

or conversely

$$\frac{\mathcal{N}\gamma_p}{3\epsilon_0} = \frac{\kappa_e - 1}{\kappa_e + 2},\tag{10.97}$$

where  $\kappa_e = \epsilon/\epsilon_0 = n^2$ . This is known as the **Clausius-Mossotti equation**. With  $\gamma_p$  given by

$$\sum_{i} \frac{e^2 f_i}{m_e(\omega_i^2 - \omega^2 - i\gamma_i\omega)},\tag{10.98}$$

where  $f_i$  is the number of electrons in the *i*th potential well per atom or molecule, we obtain

$$\frac{n^2 - 1}{n^2 + 2} = \frac{\mathcal{N}e^2}{3\epsilon_0} \sum_i \frac{f_i}{m_e(\omega_i^2 - \omega^2 - i\gamma_i\omega)}.$$
(10.99)

## 10.6 Light Propagating in Dispersive Media

If the index of refraction of a medium is frequency dependent, we say the medium is dispersive. In fact, all the media are dispersive, it is only a matter of degree. Because the index of refraction is frequency dependent, so is the refraction angle. This is how a prism splits white light into a band of rainbow colors.

Consider the propagation of a time-dependent waveform in a dispersive medium and assume the propagation is along the z-direction. Define the

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propagation constant  $\beta \equiv n(\omega)k$ , where  $n(\omega)$  is the frequency-dependent index of refraction and  $k = \omega/c$ . A general waveform can be written as a superposition of plane waves in the z-direction, where each plane-wave component has a different frequency.

$$A(z,t) = \frac{1}{\sqrt{2\pi}} \int \tilde{A}(\omega) e^{i\beta(\omega)z - i\omega t} d\omega.$$
 (10.100)

Within the bandwidth of the pulse, if  $\beta$  depends weakly on  $\omega$ , one may expand  $\beta$  around the central frequency  $\omega_0$  in Taylor series up to the quadratic term,

$$A(z,t) = \frac{1}{\sqrt{2\pi}} \int \tilde{A}(\omega) e^{i \left[\beta_0 + \beta'(\omega - \omega_0) + \frac{\beta''}{2}(\omega - \omega_0)^2\right]^2} e^{-i\omega t} d\omega.$$
(10.101)

To simplify the mathematics, let us consider the amplitude of A(z,t) defined by  $A(z,t) = a(z,t)e^{i(\beta_0 z - \omega_0 t)}$ , where  $\beta_0 = \beta(\omega_0)$ . a(z,t) varies with z and t much slower than A(z,t), because  $e^{i(\beta_0 z - \omega_0 t)}$  is the rapidly varying component.

$$a(z,t) = \frac{1}{\sqrt{2\pi}} \int \tilde{A}(\omega) e^{i \left[\beta'(\omega-\omega_0) + \frac{\beta''}{2}(\omega-\omega_0)^2\right]^2} e^{-i(\omega-\omega_0)t} d\omega$$
$$= \frac{1}{\sqrt{2\pi}} \int \tilde{A}(\omega) e^{i \left[(\beta'z-t)(\omega-\omega_0) + \frac{\beta''}{2}(\omega-\omega_0)^2z\right]} d\omega.$$
(10.102)

By a change of variables

$$t' = t - \frac{z}{v_q},$$
 (10.103)

where  $v_g = 1/\beta'$ , we have

$$i\frac{\beta''}{2}\frac{\partial^2 a(z,t')}{\partial t'^2} + \frac{\partial a(z,t')}{\partial z} = 0.$$
(10.104)

Eqs. (10.103)–(10.104) reveals that the pulse travels as a group with a velocity  $v_g$ . Even though each component travels with a different phase velocity, the envelope of the waveform moves with velocity  $v_g$ . Hence  $v_g$  is called the group velocity. If  $\beta'' = 0$ , a(z, t') is independent of z, which means the pulse will not change its shape during propagation.

If  $\beta'' \neq 0$ , the pulse will change shape as it propagates. A particular solution of Eq. (10.104) is the Gaussian pulse

$$a(z,t') = \frac{e^{-i\theta(z)}}{\sqrt{\tau}} \exp\left(-\frac{t'^2}{2\tau^2} - \frac{i\eta t'^2}{2}\right),$$
(10.105)

where

$$b = -\frac{\tau_0^2}{\beta''}, \tag{10.106}$$

$$\tau^2(z) = \tau_0^2 \left( 1 + \frac{z^2}{b^2} \right), \qquad (10.107)$$

$$\eta(z) = \frac{1}{\beta''} \frac{z}{z^2 + b^2}, \qquad (10.108)$$

$$\theta(z) = \frac{1}{2}\arctan\frac{z}{b}.$$
 (10.109)

We see the pulse duration  $\tau$  has a minimum at z = 0 and increases according to Eq. (10.107). For any initially given  $\tau$  and  $\eta$ , we can use Eqs. (10.107) and (10.108) to determine  $\tau_0$  and z, then the waveform at any other z and t'is determined by Eqs. (10.106)–(10.109).

## 10.7 Scattering

In Section 10.4 we have seen that charge oscillation driven by the external field is the origin of the index of refraction. In this Section we shall see that charge oscillation is also the origin of scattering. Consider an oscillating charge driven by the external field. According to Eq. (8.71), the oscillating charge will also radiate electromagnetic wave at the same frequency. The dipole moment associated with the oscillating charge can be written as  $\mathbf{p}(t) = \mathbf{p}_0 e^{-i\omega t}$ , where  $\omega$  is the angular frequency of the external field. The radiation fields from this oscillating dipole are given by Eqs. (8.122) and (8.123). According to Eq. (10.67), if the frequency of the driving wave is much smaller than the resonance frequencies, the electron oscillation amplitude is insensitive to  $\omega$ . In other words,  $\mathbf{p}_0$  is nearly independent of  $\omega$ . This is the case when the scatters are small molecules that comprise the air and  $\omega$  is in the optical frequency range. In this case Eq. (8.126) shows that the intensity of the scattered wave is proportional to  $\omega^4$ . In the daylight if we look into the sky not in the direction of the Sun, we see scattered light. This explains why the color of the sky is blue. It is not purple because our eyes are much more sensitive to green than purple. For the same reason, as we look at the Sun at sunset, the dominant color is orange. This is because at sunset sunlight travels through much thicker atmosphere than at noon. Consequently light of higher frequencies suffer from more scattering, and what is left is the orange light. Again, it is not red because our eyes are much more sensitive to yellow than red.

Scattering is not only related to the charge oscillation in individual atoms and molecules, but also to the density fluctuation. In a completely uniform medium, the scattered waves from different spatial locations have different phases. If all the wave have equal amplitude, they tend to cancel each other. Density fluctuation breaks the uniformity, hence makes the cancelation incomplete. This is why density fluctuation enhances scattering. Let us consider an oscillating charge distribution driven by a plane wave  $\mathbf{E}_0 e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}$ . According to the generalized version of Eq. (10.67), the electron displacement at  $\mathbf{r}'$  is

$$\mathbf{d}(\mathbf{r}', t') = \left[\sum_{i} \frac{e\mathbf{E}_{0}}{m_{e}(\omega_{i}^{2} - \omega^{2} - i\gamma_{i}\omega)}\right] e^{i(\mathbf{k}\cdot\mathbf{r}'-\omega t')}$$
(10.110)  
$$\equiv \mathbf{d}_{0}e^{i(\mathbf{k}\cdot\mathbf{r}'-\omega t')}.$$
(10.111)

Hence at a location  $\mathbf{r} \gg \mathbf{r}'$ , the vector potential is

$$\mathbf{A}(\mathbf{r},t) = \frac{\mu_0}{4\pi} \int \frac{\mathbf{J}(\mathbf{r}',t')}{|\mathbf{r}-\mathbf{r}'|} d^3 \mathbf{r}' = \frac{\mu_0}{4\pi} \int \frac{\rho(\mathbf{r}')\mathbf{v}(\mathbf{r}',t')}{|\mathbf{r}-\mathbf{r}'|} d^3 \mathbf{r}'$$
$$= \left(\frac{\mu_0}{4\pi}\right) (-i\omega \mathbf{d}_0) \int \frac{e^{i(\mathbf{k}\cdot\mathbf{r}'-\omega t')}\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} d^3 \mathbf{r}'$$
$$= \left(\frac{\mu_0}{4\pi}\right) (-i\omega \mathbf{d}_0) e^{-i\omega t} \int \frac{e^{i(\mathbf{k}\cdot\mathbf{r}'+k|\mathbf{r}-\mathbf{r}'|)}\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} d^3 \mathbf{r}', \quad (10.112)$$

where in the last step we have used the relation  $t' = t - |\mathbf{r} - \mathbf{r}'|/c$ . Using the approximations  $|\mathbf{r} - \mathbf{r}'| \approx r$  and  $e^{ik|\mathbf{r} - \mathbf{r}'|} \approx e^{ik(r - \hat{\mathbf{r}} \cdot \mathbf{r}')}$ , we have

$$\mathbf{A}(\mathbf{r},t) \approx \frac{\mu_0}{4\pi} \left[ \frac{-i\omega \mathbf{d}_0 e^{i(k\mathbf{r}-\omega t)}}{r} \right] \int e^{i(\mathbf{k}\cdot\mathbf{r}'-k\hat{\mathbf{r}}\cdot\mathbf{r}')} \rho(\mathbf{r}') \, d^3\mathbf{r}'.$$
(10.113)

The integral in the right-hand side of Eq. (10.113) will be very small if the integration volume is larger than  $\lambda^3$  and  $\rho(\mathbf{r}')$  is uniform. In the case of scattering by air, we may write the integral as a sum of the contribution from each molecule at random position.

$$\int e^{-i\Delta\mathbf{k}\cdot\mathbf{r}'}\rho(\mathbf{r}') d^3\mathbf{r}' = \sum_i e^{-i\Delta\mathbf{k}\cdot\mathbf{r}_i},$$
(10.114)

where  $\Delta \mathbf{k} = k\hat{\mathbf{r}} - \mathbf{k}$ . Note that  $k\hat{\mathbf{r}}$  is the wave vector of the outgoing wave, whereas  $\mathbf{k}$  is that of the incoming wave. Comparing Eq. (10.113) with Eq. (8.119), we can see that the intensity of the scattered wave is proportional to  $|\sum_{i} e^{-i\Delta \mathbf{k} \cdot \mathbf{r}_{i}}|^{2}$ .

$$|\sum_{i} e^{-i\Delta \mathbf{k} \cdot \mathbf{r}_{i}}|^{2} = \sum_{i} \sum_{j} e^{-i\Delta \mathbf{k} \cdot (\mathbf{r}_{i} - \mathbf{r}_{j})}$$
$$= \sum_{i} \sum_{j} \delta_{ij} + \sum_{i} \sum_{j \neq i} e^{-i\Delta \mathbf{k} \cdot (\mathbf{r}_{i} - \mathbf{r}_{j})}.$$
(10.115)

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#### 10.8. DIFFRACTION OF X-RAY

If the integration volume is larger than  $\lambda^3$  and there are many molecules in the integration volume, the summation over  $j \neq i$  yields a number near zero because  $-\Delta \mathbf{k} \cdot (\mathbf{r}_i - \mathbf{r}_j)$  is a random distribution. In this case

$$|\sum_{i} e^{-i\Delta \mathbf{k} \cdot \mathbf{r}_{i}}|^{2} \approx N, \qquad (10.116)$$

where N is the total number of molecule in the integration volume. Therefore the intensity of the wave scattered from a localized region is proportional to the total number of molecules in that region. In other words, the scattering intensity is proportional to the molecular density.

If the electron density is not uniform, Eq. (10.113) shows that the vector potential of the scattered wave is proportional to the Fourier coefficient of the electron density for the component  $e^{i\Delta \mathbf{k}\cdot\mathbf{r}'}$ . Therefore, in principle by measuring  $\mathbf{A}(\mathbf{r})$  for all  $\Delta \mathbf{k}$ , one can determine  $\rho(\mathbf{r}')$ , which gives essential information about the structure of the scattering material. The wavelength employed for the scattering experiments must be comparable to the length scale of the density variation. If the wavelength is much longer, we get only the averaged structure information. If the wavelength is much shorter, the integral in Eq. (10.113) will be averaged out, and the scattering amplitude will be small. For optical frequencies and higher, it is very difficult to measure the phase of  $\mathbf{A}(\mathbf{r},t)$ , therefore the information obtained from the scattering intensity alone, which is proportional to  $|\mathbf{A}(\mathbf{r},t)|^2$ , does not provide complete information of  $\rho(\mathbf{r}')$ . How to determine the phase of the scattering wave for x-ray scattering is currently an active research topic. The phase information in x-ray scattering is essential for determining the structures of large complex molecules such as proteins.

### 10.8 Diffraction of X-Ray

Consider 3-dimensional crystal whose charge density distribution is periodic in three directions. Namely

$$\rho(\mathbf{r}) = \rho(\mathbf{r} + \mathbf{a}) = \rho(\mathbf{r} + \mathbf{b}) = \rho(\mathbf{r} + \mathbf{c}), \qquad (10.117)$$

where  $\mathbf{a}$ ,  $\mathbf{b}$ , and  $\mathbf{c}$  are three basis vectors that represent the translation invariance of the lattice cells. Because of the translation invariance, we have

$$\rho(\mathbf{r} + m\mathbf{a} + n\mathbf{b} + l\mathbf{c}) = \rho(\mathbf{r}), \qquad (10.118)$$

for any integers m, n, and l. Note that these lattice basis vectors are not necessarily orthogonal to each other. We may define the basis vectors of the reciprocal lattice by

$$\mathbf{a}_{r} = \frac{2\pi}{v_{c}} \mathbf{b} \times \mathbf{c},$$
  

$$\mathbf{b}_{r} = \frac{2\pi}{v_{c}} \mathbf{c} \times \mathbf{a},$$
  

$$\mathbf{c}_{r} = \frac{2\pi}{v_{c}} \mathbf{a} \times \mathbf{b},$$
(10.119)

where  $v_c = \mathbf{a} \cdot (\mathbf{b} \times \mathbf{c})$  is the volume of the basic lattice cell. A general vector  $\mathbf{g}$  in the reciprocal lattice is

$$\mathbf{g} = m\mathbf{a}_r + n\mathbf{b}_r + l\mathbf{c}_r. \tag{10.120}$$

In terms of  $\mathbf{g}$ , we have

$$\rho(\mathbf{r}') = \sum_{\mathbf{g}} n_{\mathbf{g}} e^{i\mathbf{g}\cdot\mathbf{r}'}.$$
(10.121)

Substituting into Eq. (10.113), we have

$$\mathbf{A}(\mathbf{r},t) = \frac{\mu_0}{4\pi} \frac{-i\omega \mathbf{d}_0 e^{i(kr-\omega t)}}{r} \sum_{\mathbf{g}} n_{\mathbf{g}} \int e^{-i(\Delta \mathbf{k}-\mathbf{g})\cdot\mathbf{r}'} d^3 \mathbf{r}'.$$
 (10.122)

We see that **A** is not close to zero only when  $\Delta \mathbf{k} = \mathbf{g}$ . Therefore the scattered waves point to discrete directions in space. The condition  $|k\hat{\mathbf{r}}|^2 = |\mathbf{k} + \mathbf{g}|^2$  leads to

$$-2\mathbf{k} \cdot \mathbf{g} = g^2. \tag{10.123}$$

For a particular  $\mathbf{g} = n\mathbf{a}_r$ , we have  $g = 2\pi n/d$ , where *d* is the spacing between two parallel layers of lattice cells normal to  $\mathbf{a}_r$ . The condition in Eq. (10.123) becomes

$$n\lambda = 2d\sin\theta,\tag{10.124}$$

where  $\theta$  is the angle between **k** and the layers. This is Bragg's condition. Hence Bragg's condition is a special case of the general scattering condition in Eq. (10.123).

### 10.9 Exercises

**Exercise 10.1.** The refractive index of glass can be changed by doping of heavy metals. The more the doping concentration is, the larger the refractive index. If the doping is not uniform in space, the refractive index can be a function of position. A graded-index lens is made of a thin slab of glass of radius R and thickness d in which the index of refraction varies with position according to  $n(r) = n_0 - hr^2/2$ , where h is a small positive constant and r is the distance from the center. The constant h is small enough such that  $hR^2/2 \ll n_0$ . The thickness of the slab is also small enough such that  $hRd/2 \ll 1$ . What is the focal length of this device?

**Exercise 10.2.** Calculate the reflectivity of a glass slab for incident light of 600-nm wavelength. The index of refraction is 1.5, and the thickness of the slab is 300  $\mu$ m. Show that the reflectivity depends on the polarization of the incident light. Calculate the reflectivity for both *s*-wave and *p*-wave for an incidence angle of 60°. Note that both surfaces of the slab reflect. Do not forget to consider multiple reflection.

**Exercise 10.3.** An interferometer is shown in Fig. 10.1. The intensity of each input beam is I, which means the amplitude of each input beam is  $E = \sqrt{I/(c\epsilon_0)}$ . The power reflectivity and transmittance of the beam splitter are R and T respectively. Because the beam splitter is made of a glass that does not absorb light, we have R + T = 1. However, if the power reflectivity is R, the amplitude reflectivity  $\mathcal{R}$  should be  $\sqrt{R}$ . Similarly, the amplitude transmittance  $\mathcal{T}$  should be  $\sqrt{T}$ . Therefore, one might derive that the amplitude of each output beam is  $(\sqrt{R} + \sqrt{T})E$ , and the total intensity of both output beams is  $2I + 4\sqrt{RT}I$ . But energy conservation requires the total intensity of both output beams to be equal to that of the input beams, namely 2I. Therefore such a derivation violates the energy conservation law. Explain what is wrong in the above argument and derive the correct amplitudes of both output beams.

**Exercise 10.4.** Show that the group velocity of light in plasma is smaller than c even though the phase velocity is larger than c. Here we consider only the case when the frequency of the light wave is larger than the plasma frequency, otherwise the light wave cannot propagate.

**Exercise 10.5.** In radio communication the ionosphere of the earth is used as the reflector to bounce the radio wave over the horizon. This technique



Fig. 10.1: An interferometer with two input beams.

can only be used for frequencies below 7 MHz. From this number can you estimate the electron density in the ionosphere? In this exercise we assume the electron density in the ionosphere is uniform and ignore the effect of the magnetic field of the earth.

**Exercise 10.6.** The electric field of an x-polarized plane wave propagating in the z-direction can be written as

$$\mathbf{E}(\mathbf{r},t) = E_0 e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)} \,\hat{\mathbf{x}},$$

where  $\mathbf{k} = k\hat{\mathbf{z}}$ . A transmission grating is made of parallel gold lines coated on glass. The spacing between the lines is d and the width of the lines is also d, where  $kd \gg 1$ . After this plane wave propagates through the grating, the amplitude  $E_0$  becomes spatially modulated such that the electric field becomes

$$\mathbf{E}(\mathbf{r},t) = h(x)E_0e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}\,\hat{\mathbf{x}}$$

where

$$h(x) = \begin{cases} 1 & \text{if } (2n-1)d < x - \frac{d}{2} \le 2nd, & n \text{ is an integer} \\ 0 & \text{otherwise} \end{cases}$$

Show that the plane wave is split into many plan waves and each of them propagates in an angle  $\theta_m$  with respect to the z-axis that satisfies the following condition.

$$2d\sin\theta_m = m\lambda,$$

where m is an integer.



Fig. 10.2: Transmission of evanescent wave across a gap.

**Exercise 10.7.** A pair of polarizers can block the transmission of a plane wave propagating in the z-direction when one is aligned in the x-direction  $(\theta = 0)$  while the other in the y-direction  $(\theta = \frac{\pi}{2})$ . However, if a third polarizer aligned in the  $\theta = \frac{\pi}{4}$  is inserted between the two polarizers, 1/4 of the intensity that has passed the first polarizer can go through the rest two. Hence we see inserting one more polarization filter may actually increase transmission. Consider inserting N polarizers between the two cross-aligned filters. The angle of the kth filter is set at  $\frac{k\pi}{2(N+1)}$ . If the intensity after the first polarizer is  $I_0$  and the intensity after the last polarizer is  $I_{N+1}$ , show that as  $N \to \infty$ ,  $I_{N+1}/I_0 \to 1$ .

**Exercise 10.8.** A light beam of wavelength  $\lambda$  propagates through two prisms separated by a gap of thickness d as shown in Fig. 10.2. The polarization of the incident beam is normal to both k-vectors of the incident and the reflected beams. In other words, the incident beam is an *s*-wave with respect to the gap surfaces. The refractive index of the prisms is 2.0 with permeability  $\mu = \mu_0$ , and the beam incidents on the gap at an angle of 45°. By considering the boundary conditions at the two surfaces of the gap, calculate the reflectivity and transmission coefficients of intensity as functions of d and  $\lambda$ . Note that you cannot assume that  $d \gg \lambda$ . In this exercise we assume all the surfaces except the two of the gap are anti-reflection coated.

**Exercise 10.9.** The surface temperature of the Sun is 5780 K. The radius of the Sun is  $6.96 \times 10^8$  m. Estimate the surface temperature of the Earth by using the Stefan-Boltzmann law. The Stefan-Boltzmann law is given by

 $I = \sigma T^4,$ 

where I is the total power emitted at all wavelengths per unit surface area, T is the absolute temperature, and

$$\sigma = \frac{2\pi^5 k^4}{15c^2h^3}.$$

In this problem we assume both the Sun and the Earth are blackbodies, and the Earth has no atmosphere and thus there is no need to consider the greenhouse effect. In reality 30% of the radiation energy from the Sun is reflected back to the space, and the greenhouse effect also reduces the Earth's loss of energy due to blackbody radiation.

**Exercise 10.10.** When the Earth was formed many many years ago, it was a ball of molten rock. Let  $t_1$  be the time when the surface temperature of the Earth was 1500 K, and  $t_2$  be the time when the surface temperature was 300 K. Assuming the Earth is a blackbody, use the Stefan-Boltzmann law to estimate how long it takes for the Earth to cool down from 1500 K to 300 K (*i.e.*,  $t_2 - t_1$ ) if the Earth does not receive the radiation energy from the Sun. For simplicity we assume the temperature of the Earth is uniform during the cool-down process, and the specific heat of the Earth is 0.8 J/(g· K).

**Exercise 10.11.** An optical fiber made by a thin thread of graded-index glass can be used to guide the propagation of light. The action of the graded-index glass as a continuous distribution of lens balances the diffraction, so that light can be confined in a thin thread without leaking out by diffraction. Because in the optical fiber the light can only propagate in the z-direction, we may assume the light has the following waveform

$$A(x, y, z, t) = a(x, y)e^{i(kz - \omega t)}.$$

Show that a(x, y) satisfies the following equation:

$$\left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} - k^2 + \frac{n(x,y)^2 \omega^2}{c^2}\right] a(x,y) = 0,$$

where

$$n(x,y) = n_0 - h\left(\frac{x^2 + y^2}{2}\right)$$

For small h one can make the following approximation:

$$n(x,y)^2 = \left[n_0 - h\left(\frac{x^2 + y^2}{2}\right)\right]^2 \approx n_0^2 - n_0 h(x^2 + y^2).$$

#### 10.9. Exercises

Now the equation looks like a two-dimensional time-independent Schrödinger equation for the harmonic oscillator. The equation can be solved by assuming that

$$a(x,y) = a_x(x)a_y(y).$$

Show that the equation for  $a_x(x)$  and  $a_y(y)$  is the one-dimensional timeindependent Schrödinger equation. Copy the solution from the lecture notes, and show that there are different modes for the light propagating in the fiber. The modes can be labeled by two integers m and n, just like the wavefunctions of the two-dimensional harmonic oscillator. For each mode labeled by (m, n), what is the dispersion relation  $k(\omega)$ ?

**Exercise 10.12.** The structure of gold is a cubic crystal in which the structure repeats itself every 0.40788 nm in all the three directions of  $\hat{\mathbf{x}}$ ,  $\hat{\mathbf{y}}$ , and  $\hat{\mathbf{z}}$ . Consider the scattering of a 10-keV x-ray beam by a powder sample of gold crystal. Because the sample is in the powder form, each grain of the gold crystal in the powder has a random orientation with respect to the direction of the x-ray beam. An x-ray film normal to the x-ray beam is placed at 1 m behind the sample. Show that the scattering pattern on the x-ray film forms concentric rings. Determine the radii of the first four rings, starting from the smallest ring.

# Chapter 11

# Quantum Phenomena

### 11.1 Rayleigh-Jeans Formula for Blackbody Radiation

How matter radiates light has been an intriguing problem in physics for a long time. In the beginning of the 20th century, Rayleigh and Jeans attempted to understand the spectrum of blackbody radiation from classical statistical mechanics. Treating light as classical electromagnetic waves, they first calculated the mode density of light waves, then assigned each mode an average energy kT as one would do for mechanical waves. This way they obtained a formula for the power spectrum of blackbody radiation.

Assume light waves exist only in an isolated space with length, width and height all equal to L. Then only light waves which satisfy the following boundary condition exist.

$$k_i L = 2n_i \pi \quad i = x, y, z.$$
 (11.1)

where  $k_i$  are the components of the wave vector and  $n_i$  are integers. The condition for light waves with frequency smaller than  $\nu_m$  is

$$\frac{c}{2\pi}\sqrt{k_x^2 + k_y^2 + k_z^2} \le \nu_m. \tag{11.2}$$

or

$$\sqrt{n_x^2 + n_y^2 + n_z^2} \le \frac{L\nu_m}{c}.$$
(11.3)

The total number of modes with frequency lying between 0 and  $\nu_m$  is

$$2 \times \frac{4\pi}{3} \left(\frac{L\nu_m}{c}\right)^3 = \frac{8\pi}{3} \frac{L^3 \nu_m^3}{c^3}.$$
 (11.4)

The factor 2 in the above expression accounts for the two polarization of light. The number of modes per unit volume in the frequency interval between  $\nu$ and  $\nu + d\nu$  is therefore

$$\frac{1}{L^3} \frac{d}{d\nu} \left( \frac{8\pi}{3} \frac{L^3 \nu^3}{c^3} \right) d\nu = \frac{8\pi \nu^2}{c^3} d\nu.$$
(11.5)

From Boltzmann distribution the average energy per mode is

$$\frac{1}{Z} \int \int \left(\frac{p^2}{2m} + \frac{kq^2}{2}\right) e^{-\frac{1}{kT}\left(\frac{p^2}{2m} + \frac{kq^2}{2}\right)} dp \, dq = kT, \tag{11.6}$$

where

$$Z = \int \int e^{-\frac{1}{kT} \left(\frac{p^2}{2m} + \frac{kq^2}{2}\right)} dp \, dq.$$
(11.7)

Multiplying Eqs. (11.5) and (11.10), the power spectrum of the light is

$$P(\nu)d\nu = \frac{8\pi\nu^2 kT}{c^3} \, d\nu.$$
 (11.8)

One can immediately recognize a serious problem in Eq. (11.8). If the equation were correct, then any matter at any finite temperature would emit much more X-ray than visible light, not to mention the  $\gamma$ -rays! The power spectrum diverges at high frequency. Needless to say, such a spectrum does not agree with experimental observations. But Eq. (11.8) is derived from very fundamental principles, it was hard to understand what went wrong. It turned out that the quantum nature of light has a subtle but important effect on the blackbody spectrum. The problem was solved by Max Planck with his revolutionary hypothesis of quantized light energy.

# 11.2 Planck's Theory of Blackbody Radiation

Planck showed that if light energy is not continuously variable, instead, if the energy level spacing for light with frequency  $\nu$  is

$$\Delta E = h\nu, \tag{11.9}$$

then a blackbody spectrum which is free of divergence and agrees with experimental observations can be derived using the same idea of statistical mechanics. Using Eq. (11.9), the average energy per mode becomes

$$\frac{\sum_{n=0}^{\infty} nh\nu \, e^{-\frac{m\nu}{kT}}}{\sum_{n=0}^{\infty} e^{-\frac{nh\nu}{kT}}} = \frac{h\nu}{e^{\frac{h\nu}{kT}} - 1}.$$
(11.10)

#### 11.3. Photoelectric Effect

The spectrum of light is then

$$P(\nu) d\nu = \frac{8\pi\nu^2}{c^3} \frac{h\nu}{e^{\frac{h\nu}{kT}} - 1} d\nu.$$
(11.11)

The rapid decrease of average mode energy with increasing frequency saves the spectrum from diverging at high frequency.

## 11.3 Photoelectric Effect

When light is shined on the surface of metal, it can kick out electrons. This is called the photoelectric effect. Experimentally it is found that the kinetic energy T of the electrons follows the following equation.

$$T = \hbar\omega - W,\tag{11.12}$$

where W is a material-dependent constant called the work function. Great difficulties are encountered when one tries to explain this experimental observation by classical electromagnetic theories. First of all, in classical theories the intensity of light is  $c\epsilon_0 |\mathbf{E}|^2$ , which does not depend on  $\omega$ . Since the kinetic energy of the electron must come from the energy of light, why does it depend on  $\omega$  instead of  $|\mathbf{E}|^2$ ? If one increase the intensity of light, more electrons are kicked out, but their kinetic energy still follows Eq. (11.12). Second, according to classical theories, there should be a delay before the electron can be kicked out, because it takes time to accumulate the energy. Therefore the weaker the light is, the longer delay it should take. However, experimentally one finds that weaker light only reduce the probability of kicking out an electron. There is no delay between the arrival of the light and the departure of the electrons.

Einstein showed that by thinking light as particles, the photoelectric effect can be easily explained. Following Planck's suggestion, the energy of a photon is  $\hbar\omega$ , therefore Eq. (11.12) is simply an instance of the energy conservation law. Clearly we need a theory to describe light as particles.

## **11.4** Taylor's Interference Experiment

If light is made of particles after all, can a single particle of light interfere with itself? Using the same experimental set-up as the Young's interference experiment except an extremely weak light source, in 1909 G. I. Taylor proved

that a single photon does interfere with itself. The light source was attenuated to the extent that on the average less than one photon existed in the experimental set-up. In other words, on the average a photon did not leave the light source until the previous photon had arrived at the photographic plate which served as the detector. In a short time, only individual random dots appeared on the photographic plate. However, in a long time as one accumulated many dots, it became clear that the dots prefer to appear at certain positions and never appear at some other positions. The density distribution of dots follows exactly as the classical interference pattern. Taylor's interference experiment forces us to treat light as both wave and particle.

### 11.5 Emission Spectrum of the Hydrogen Atom

Using grating spectrometry, one can analyze the frequency spectrum of a light source with great resolution. Experimentally is was found that the wavenumber of the emission is given by the following formula:

$$k = R\left(\frac{1}{m^2} - \frac{1}{n^2}\right),$$
(11.13)

where R is a constant and m, n are positive integers. The series of lines corresponding to m = 1 is called the Lyman series. The m = 2 series is called the Balmer series, and the m = 3 series is called the Paschen series. J. J. Thomson explained the discrete atomic lines by the harmonic oscillation of electrons at the bottom of each potential well. However, the  $\alpha$ -particle scattering experiment by Rutherford disagree with this picture seriously.

Under the inspection of spectroscopy with even higher resolution, the emission lines of hydrogen atoms are found to have a fine structure described by

$$k = R \left[ f(m, m_{\theta}) - f(n, n_{\theta}) \right], \qquad (11.14)$$

where

$$f(m, m_{\theta}) = \frac{1}{m^2} \left[ 1 + \frac{\alpha^2}{m} \left( \frac{1}{m_{\theta}} - \frac{3}{4m} \right) \right],$$
 (11.15)

and

$$m_{\theta} - n_{\theta} = \pm 1. \tag{11.16}$$

The dimensionless constant  $\alpha$  is called the fine structure constant. No classical theory was able to explain these mysterious rules for the hydrogen spectrum.

### **11.6** Franck-Hertz Experiment

When measuring the voltage-current relation for a vacuum tube filled with mercury vapor, J. Franck and G. Hertz discovered in 1913 that the differential conductivity dI/dV showed resonant structures. It appeared that when electrons collided with the mercury atoms, the loss of electron kinetic energy is discrete. This is in agreement with the hypothesis that atomic energy levels are discrete.

## 11.7 Problem of Specific Heat

Boltzmann's invention of statistical mechanics turns out to be a tremendous achievement in physics. However, at the time Boltzmann proposed the idea of energy equipartition, he faced strong objection. One of the objections is that statistical mechanics was not able to explain the specific heat of even the simplest systems. Consider a polyatomic molecule made of n atoms. The degree of freedom is 3n, and among them 3 are the translational motion, three are the rotational motion, and the rest are the vibrations. From Eq. (11.6), the specific heat for each vibrational degree of freedom is k, therefore for a diatomic molecule such as H<sub>2</sub>, the specific heat should be

$$c_V = \frac{3k}{2} + \frac{3k}{2} + k = 4k.$$
(11.17)

If the two atoms are treated as points of zero radius, one may argue that there is no rotation along the axis connecting the two atoms. In this case we have

$$c_V = \frac{3k}{2} + \frac{2k}{2} + k = \frac{7}{2}k.$$
(11.18)

However, at room temperature the experimental result is close to 5k/2. As the number of atoms in the molecule increases, the discrepancy becomes more significant. Experimentally the specific heat is a function of temperature, but Boltzmann's prediction is independent of temperature. Worst of all, because atoms have internal degrees of freedom, for instance the neon atom contains 10 electrons, if all these internal degrees of freedom contribute to the specific heat, even the ideal gas made of neon atoms will have a specific heat much larger than the experimental value 3k/2.

The solution of this contradiction comes from quantum mechanics. By the analogy between waves and harmonic oscillators shown in Section 3.5, the energy levels of simple harmonic oscillators must also be  $\Delta E = h\nu$ , the same as the energy of light. From Eq. (11.10), we see that a vibrational degree of freedom contributes to the specific heat only if  $h\nu \ll kT$ . For  $h\nu \ll kT$ , we have

$$c_V = \frac{d}{dT} \left[ \frac{h\nu}{e^{\frac{h\nu}{kT}} - 1} \right] \approx k.$$
(11.19)

In contrast, for  $h\nu \gg kT$ ,

$$c_V \approx k \left(\frac{h\nu}{kT}\right)^2 e^{-\frac{h\nu}{kT}},$$
 (11.20)

which is negligibly small. For diatomic molecules  $h\nu/k$  is in the range of thousands K, therefore at room temperature the vibrational motion of diatomic molecules contributes little to the specific heat. The internal degrees of freedom of atoms have even larger energy. For instance, the energy of the first excited state of hydrogen is 10.2 eV. At room temperature it contributes only about  $10.2 \times e^{-392}$  eV to the internal energy and  $(392)^2 \times e^{-392} k$  to the specific heat. It was a pity that Boltzmann did not know the problem of specific heat was not in statistical mechanics, but in using classical mechanics to describe atoms and molecules. He was unduely bothered by this problem only because he was truly a genius ahead of his time.

### 11.8 Wilson-Sommerfeld Quantization Rule

In 1911 Rutherford showed by  $\alpha$  particle scattering that most of the positive charge in an atom is concentrated in the center, called the nucleus. But such an atomic model cannot explain the stability of atoms. According to classical mechanics, the only way for the electrons not to fall into the nucleus is by circulating. However, according to the classical electromagnetic theory, circulating electrons lose energy by emitting a continuous spectrum of electromagnetic wave, therefore cannot maintain their orbits. Even more puzzling is the experimental fact that atomic spectra consist of sharp discrete ordered lines that no theory was able to explain. In 1913 Bohr discovered a rule for the quantization of electron orbits,

$$L = \frac{nh}{2\pi},\tag{11.21}$$

where L is the angular momentum n is a positive integer. This simple rule accurately describes the hydrogen spectrum. But why the electron orbits

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#### 11.9. EXERCISES

follow this rule was still not explained. In 1916 Wilson and Sommerfeld found a more general quantization condition,

$$\oint \mathbf{p}(\mathbf{r}) \cdot d\mathbf{r} = nh, \qquad (11.22)$$

where  $\mathbf{p}$  is the momentum and  $\mathbf{r}$  is the coordinate. For the hydrogen atom, the Wilson-Sommerfeld quantization rule yields

$$\oint \mathbf{p}(\mathbf{r}) \cdot d\mathbf{r} = \oint pr \, d\theta = 2\pi L = nh, \qquad (11.23)$$

which is the same as Bohr's rule. For the harmonic oscillator the same rule yields

$$nh = \oint \mathbf{p}(\mathbf{r}) \cdot d\mathbf{r} = \oint \sqrt{2mE - mkx^2} \, dx = 2\pi E \sqrt{\frac{m}{k}},\tag{11.24}$$

which gives Planck's rule  $E = nh\nu$ . The Wilson-Sommerfeld quantization rule not only unifies Planck's quantization rule for the harmonic oscillator and Bohr's for the hydrogen atom, it can also be applied to any integrable system in which **p** can be solved as a function of **r**. An important achievement of the Wilson-Sommerfeld quantization rule is that when combined with relativity, it explained accurately the fine structure of the hydrogen spectrum.

### 11.9 Exercises

**Exercise 11.1.** In textbooks the calculation of the heat capacity at room temperature (300 °K) of hydrogen gas is done by including only 3 translational degrees of freedom and two rotational degrees of freedom to obtain the value 5k/2. Let us call the axis connecting the two protons the z-axis. Assuming the mass distribution of proton is a uniform sphere with a diameter equal to  $10^{-15}$  m, and on the average the two electrons circulate around the z-axis at a radius of  $0.5 \times 10^{-10}$  m, what is the moment of inertia of the hydrogen molecule with respect to the z-axis? By the Wilson-Sommerfeld rule the angular momentum along a particular axis is quantized according to  $L = n\hbar$ . How much does the rotation along the z-axis contribute to the heat capacity at room temperature? Hint: It is sufficient to estimate the contribution from the first few energy levels.

**Exercise 11.2.** In the lecture note we have derived the total number of modes for an isolated space with length, width and height all equal to L.

Use this result to derive the formula for the Fermi energy of free electrons in a box,

$$E_F = \frac{\hbar^2}{2m_e} \left(3\pi^2 n_e\right)^{\frac{2}{3}},$$

where  $n_e$  is the electron density and  $m_e$  is the electron mass.

**Exercise 11.3.** Heisenberg's uncertainty principle can be used to estimate the radii of electron orbits in atoms. If the 3-dimensional root-mean-square position of an electron is r, show that by Heisenberg's uncertainty principle the minimum 3-dimensional root-mean-square momentum of the electron is  $3\hbar/(2r)$ . Consider the inner most electron of an atom of atomic number Z. Write down the total energy of the electron when it is at a distance rfrom the nucleus. For simplicity you may treat all the electrons around the nucleus as independent particles and ignore the contribution of other electrons in potential energy. Use Heisenberg's uncertainty principle to estimate the minimum kinetic energy of the electron. Find the radius  $r_0$  that gives the lowest total energy for the electron under consideration for Z = 1 and Z = 100. Show that when Z is larger than a certain number, no minimum energy can be found, and in that case the inner most electron will fall into the nucleus. This sets an upper bound for the number of elements in the universe. Note that when the kinetic energy T of the electron is small comparing with the rest energy  $m_0c^2$ , we have  $T \approx p^2/(2m_0)$ , otherwise we have  $T = \sqrt{m_0^2 c^4 + p^2 c^2} - m_0 c^2.$ 

**Exercise 11.4.** Bohr obtained the radii of electron orbits in the hydrogen atom from the following equation

$$\frac{e^2}{4\pi\epsilon_0 r^2} = \frac{m_e v^2}{r},$$

with the quantization condition  $L = mvr = n\hbar$ . The equation can be written as

$$\frac{e^2}{4\pi\epsilon_0 r} = \frac{L^2}{m_e r^2} = \frac{p^2}{m_e}$$

with the quantization condition  $p = L/r = n\hbar/r$ . We may understand these equations in the following way. Consider the total energy of the electron as a function of r. The potential energy is  $-e^2/(4\pi\epsilon_0 r)$  and the kinetic energy is  $p^2/(2m_e) = L^2/(2m_e r^2)$ . Since L is a conserved quantity, we may find the radius  $r_0$  for the electron orbit by minimizing the total energy while keeping L constant. This yields the above equations. Now consider the inner most electron of an atom of atomic number Z in the ground (n = 1) state. Write down the total energy of the electron when it is at a distance r from the nucleus. For simplicity you may treat all the electrons around the nucleus as independent particles and ignore the contribution of other electrons in potential energy. Find the radius  $r_0$  that gives the lowest total energy for the electron under consideration for Z = 1 and Z = 100. Show that when Z is larger than a certain number, no minimum energy can be found, and in that case the inner most electron will fall into the nucleus. This sets an upper bound for the number of elements in the universe.

**Exercise 11.5.** In exercises 11.3 and 11.4, we estimated the radii of electron orbits in two different ways. The results do not completely agree with each other. Show that the results can be made to agree with each other by changing the dimension from 3 to 2 in exercise 11.3. Explain why such a change is reasonable when we compare with exercise 11.4?

**Exercise 11.6.** The Fermi energy of copper is 7.0 eV that corresponds to a temperature of  $8.12 \times 10^4 \text{ K}$ . At 0 K the maximum energy of the electrons is the Fermi energy. When we touch the surface of copper at 0 K, why don't we feel hot?

**Exercise 11.7.** In applying the Wilson-Sommerfeld quantization rule to the hydrogen model, one may restrict the motion of the electron to be circular to get a simple result:  $2\pi L = nh$ . However, since the electron trajectory can be an ellipse, one should consider the motion in the  $\hat{\mathbf{r}}$ -direction as well as in the  $\hat{\boldsymbol{\theta}}$ -direction. The quantization rules become

$$\oint \mu(r\dot{\theta})(rd\theta) = n_{\theta}h$$

and

$$\oint \mu \dot{r} \, dr = n_r h,$$

where  $\mu$  is the reduced mass of the electron-proton pair. Show that the energy levels are determined by the following equation

$$E = -\frac{\mu e^4}{2(4\pi\epsilon_0)^2\hbar^2 n^2},$$

where  $n = n_r + n_{\theta}$  is the principal quantum and  $n_{\theta}$  is the azimuthal quantum number. For each n,  $n_{\theta}$  can go from 1 to n.

**Exercise 11.8.** At low temperature the main contribution of the specific heat of a solid is lattice vibration. Show that the specific heat is proportional to  $T^3$  by using Planck's quantization rule  $E = nh\nu$ .

# Chapter 12

# Matter Waves

# 12.1 Schrödinger Equation

In 1924, De Broglie presented the idea of matter wave. De Broglie noted that if an electron moves like a wave, with wavelength  $\lambda = h/p$ , then the Wilson-Sommerfeld quantization rule is simply the common periodic condition for waves, and the photon quantization rule  $E = h\nu$  is just a special case. Finally, one saw a good reason behind the Wilson-Sommerfeld quantization rule. This astonishing idea was soon verified by electron diffraction experiments in 1927 (Davisson and Germer, G. P. Thomson), in which the effect of constructive and destructive interference can only be explained by wave and not by particle motion. In 1925 Schrödinger derived the matter wave equation by replacing  $\mathbf{p}$  with  $-i\hbar\nabla$  and E with  $i\hbar\partial/\partial t$  in the classical relation  $p^2/(2m) + V(\mathbf{r}) = E$ . The result is the Schrödinger equation

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V(\mathbf{r})\psi = i\hbar\frac{\partial\psi}{\partial t}.$$
(12.1)

The replacement was based on the obvious fact that when  $-i\hbar\nabla$  operates on a wave of wave number **k**, it multiplies the wave by  $\hbar \mathbf{k} = \mathbf{p}$ , and when  $i\hbar\partial/\partial t$  operates on a wave of angular frequency  $\omega$ , it multiplies the wave by  $\hbar\omega = E$ . This can be seen clearly by representing the wavefunction in terms of its Fourier components, namely

$$-i\hbar\nabla\sum_{k}a_{k}e^{i(\mathbf{k}\cdot\mathbf{r}-\omega_{k}t)} = \hbar\sum_{k}\mathbf{k}a_{k}e^{i(\mathbf{k}\cdot\mathbf{r}-\omega_{k}t)},$$
(12.2)

#### CHAPTER 12. MATTER WAVES

$$i\hbar\frac{\partial}{\partial t}\sum_{k}a_{k}e^{i(\mathbf{k}\cdot\mathbf{r}-\omega_{k}t)} = \hbar\sum_{k}\omega_{k}a_{k}e^{i(\mathbf{k}\cdot\mathbf{r}-\omega_{k}t)}.$$
(12.3)

In fact, the first quantum wave equation Schrödinger derived was the relativistic wave equation, now known as the Klein-Gordon equation,

$$-\hbar^2 \frac{\partial^2 \psi}{\partial t^2} = -\hbar^2 c^2 \nabla^2 \psi + m^2 c^4 \psi, \qquad (12.4)$$

which was based on the relativistic energy-momentum relation  $E^2 = p^2 c^2 + m^2 c^4$ . However, when he added the electromagnetic potential ( $\phi$ , **A**) to Eq. (12.4) to take into account the interaction between the charges, it did not give the correct fine structure of the hydrogen spectrum. This forced Schrödinger to fall back to the non-relativistic approximation Eq. (12.1). Now we know the reason Eq. (12.4) does not work is because the electron has spin, therefore its wavefunction cannot be a scalar. It was Dirac who derived the correct relativistic wave equation for electrons. In the Dirac equation the wavefunction of an electron has four components. Two of the components represent the spin components of the positive-energy states, and the other two represent that of the negative-energy states. Now we know the negative-energy states actually represent the states of the positron, which is the anti-particle of the electron.

## 12.2 Probabilistic Interpretation of Wavefunction

Although the Schrödinger equation looks not particularly different from other wave equations in classical physics, we must note that matter wave is very different from classical waves. For classical waves, it is possible to separate the wave into small pieces and measure the intensity of them independently. For example, the sound wave produced by a loudspeaker can be measured at different corners of a music hall. The measurement made at one corner will not affect the result made at another corner. However, if the matter wave represents the state of a single microscopic object, it is not possible to detect the matter wave at the same time at different locations. Otherwise one would say that the object has been split into pieces. It is an experimental fact that one cannot split an electron into several fractional electrons. Even though the wavefunction can spread all over the space, it still represents a single nonsplitable electron. Therefore, we must interpret the wavefunction differently from classical waves.

Whether there is a satisfactory interpretation of the wavefunction is still

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#### 12.2. PROBABILISTIC INTERPRETATION OF WAVEFUNCTION

an unsettled issue, but from the experimental point of view, the probability interpretation is consistent with all the experiments so far. Under the probability interpretation,  $\psi(x,t)$  is called the probability amplitude and  $|\psi(x,t)|^2$  is the probability density. If  $\psi(x,t)$  describes the state of a particle at time t, then the probability of finding the particle in the space interval (x, x + dx) at time t is

$$P(x,t) dx = |\psi(x,t)|^2 dx.$$
(12.5)

Such an interpretation allows us to explain why an electron can behave like wave in diffraction experiments, yet only one detector will receive the scattered electron at one of the diffraction peaks. The diffraction pattern will not show up until we repeat the scattering event many times and accumulate the result. For a single scattering event, we do not know how to predict which direction the electron will go. We only know the probability distributions of the electron's position and momentum.

One of the most strange result of the probability interpretation is that the detectors seem to be able to "collaborate" over a large distance in the measurement. Imagine we put several detectors each at one diffraction peak. By placing the detectors far away from the scattering site, it is possible to make the spatial separation of the detectors arbitrarily large. Yet, if one detector detects the electron, the other detectors must not, even though the matter wave has similar intensity at each detector. How does the detectors know how to act in perfect correlation? Or has the electron already decided which way to go, only we don't know?

Some early physicists (possibly including Einstein) believed that there are hidden variables in quantum mechanics. Similar to statistical mechanics, these hidden variables determine which way the electron will go, only we don't know. If this is true, the Schrödinger equation cannot be the full story because it leaves no room for the "hidden variables". However, modern experiments have provided strong evidences to rule out the possibility of hidden-variable theories. Therefore, how does a group of detectors turn the wavefunction into a measurement result is still a mystery.

A more fundamental picture of the quantum measurement process comes from treating the detector as another quantum system. This is possible theoretically, but extremely difficult practically because the detector must be made of a large number of particles with many degrees of freedom in order to amplify the small change produced by the incoming electron. For instance, the detector may be a inert-gas tube under high voltage. The incoming electron collides with the gas atoms and knocks off a few electrons from the atoms. These electrons are accelerated by the high voltage and then knock off more electrons from the atoms that collide with them subsequently. After such an avalanche process, finally there is enough electrons to turn the needle of an ampere meter for us to see. If we describe all the atoms and electrons in the detector also by matter waves, we make the problem much more complicated. Worst of all, doing so does not help to understand why the matter waves in different detectors separated far apart are correlated. However, without doing so, it is not even possible to define clearly what is a measurement, because eventually one must define what kind of change to occur in the detector means "detecting" an incoming electron. Ironically, if the wavefunction of the electron is in a superposition state of "arriving at this detector" and "not arriving at this detector", which is perfectly meaningful in quantum mechanics, will the needle of the ampere meter also in a superposition state of "turning" and "not turning"? Would our brain, which processes the visual signals of watching the needle, also be in a superposition state of "seeing the needle turn" and "not seeing the needle turn"?

Such questions cannot be answered experimentally yet, because in practice the detectors are not free from the interference of the thermal environment. There are always random fluctuations coming from the environment. Therefore experimentally we can only relate the reading of the ampere meter with the incoming electrons in a statistical way. Even if one could isolate the environment to a satisfactory degree, one would still need a quantum amplifier that is completely free of noise to amplify the state of the incoming electron truthfully. It seems that quantum mechanics itself would not allow such an amplifier, because in quantum mechanics even the vacuum is full of zero-point fluctuation. There is simply no quiet amplifier in quantum mechanics.

# **12.3** Stationary States and State Evolution

Each solution of the Schrödinger equation describes a state of the quantum system. If a quantum state has a probability density that is independent of t, it is called a stationary state. Obviously, a solution of the form  $\Psi(\mathbf{r}, t) = \psi(\mathbf{r})e^{i\phi(t)}$  describes a stationary state. To find out the form of  $\phi(t)$ , let us assume the solution can be written as

$$\Psi(\mathbf{r},t) = \psi(\mathbf{r})f(t). \tag{12.6}$$

#### 12.3. STATIONARY STATES AND STATE EVOLUTION

Substituting into the Schrödinger equation, we have

$$\left[-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r}) + V(\mathbf{r})\psi(\mathbf{r})\right]f(t) = i\hbar\frac{\partial f}{\partial t}\psi(\mathbf{r}).$$
(12.7)

Dividing both sides by  $\psi(\mathbf{r})f(t)$ , we have

$$-\frac{1}{\psi(\mathbf{r})}\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r}) + V(\mathbf{r}) = i\hbar\frac{1}{f}\frac{\partial f}{\partial t}.$$
(12.8)

Since the left-hand side is a function of  $\mathbf{r}$  and the right-hand side is a function of t, they must be equal to a constant E. Therefore we have

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})\right]\psi(\mathbf{r}) = E\psi(\mathbf{r})$$
(12.9)

and

$$f(t) = e^{-iEt/\hbar}.$$
 (12.10)

The Hamiltonian operator H is defined as

$$H = \frac{p^2}{2m} + V(\mathbf{r}) = -\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}).$$
 (12.11)

Since H is a linear operator operated on  $\psi$ , if  $\psi$  satisfies Eq. (12.9), it is an eigenfunction of H with eigenvalue E. In general H has a set of eigenfunctions  $\psi_i$  with corresponding eigenvalues  $E_i$ , where all the  $\psi_i$  form a complete orthonormal set. Therefore the general solution of the Schrödinger equation can be written as

$$\Psi(\mathbf{r},t) = \sum_{i} a_i \psi_i(\mathbf{r}) e^{-iE_i t/\hbar}.$$
(12.12)

Set t = 0, multiply both sides by  $\psi_k^*(\mathbf{r})$  and integrate, we have

$$\int \psi_k^*(\mathbf{r}) \Psi(\mathbf{r}, 0) \, d^3 \mathbf{r} = \sum_i a_i \int \psi_k^*(\mathbf{r}) \psi_i(\mathbf{r}) \, d^3 \mathbf{r}.$$
(12.13)

Because  $\psi_k(\mathbf{r})$  and  $\psi_i(\mathbf{r})$  are orthonormal eigenfunctions, we have

$$\int \psi_k^*(\mathbf{r})\psi_i(\mathbf{r})\,d^3\mathbf{r} = \delta_{ik}.$$
(12.14)

Therefore, the coefficients  $a_i$  can be determined by the initial wavefunction  $\Psi(\mathbf{r}, 0)$ .

$$a_i = \int \psi_i^*(\mathbf{r}) \Psi(\mathbf{r}, 0) \, d^3 \mathbf{r}.$$
(12.15)

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Since the Schrödinger equation is a first-order differential equation in t, the time evolution of its solution  $\Psi(\mathbf{r}, t)$  is completely determined by the initial value  $\Psi(\mathbf{r}, 0)$ . Now that  $a_i$  is completely determined by the initial value  $\Psi(\mathbf{r}, 0)$  through Eq. (12.15), we see that Eq. (12.12) is not only a general solution, but also the unique solution after  $a_i$  is set by the initial value  $\Psi(\mathbf{r}, 0)$ .

# 12.4 Uncertainty Relation of Position and Momentum

One of well-cited statements in quantum mechanics is that one cannot measure both the position and the momentum of a particle accurately. This is one instance of the uncertainty principle. To see why this is true, let us consider an important inequality in linear algebra, the Cauchy-Schwartz inequality.

$$|\mathbf{a}|^2 |\mathbf{b}|^2 \ge |\mathbf{a}^* \cdot \mathbf{b}|^2, \tag{12.16}$$

where  $\mathbf{a}$  and  $\mathbf{b}$  are complex vectors. To prove this inequality, we decompose  $\mathbf{a}$  into a vector parallel to  $\mathbf{b}$  and a vector perpendicular to  $\mathbf{b}$ . That is

$$\mathbf{a} = \alpha \mathbf{b} + \mathbf{h},\tag{12.17}$$

where **h** is perpendicular to **b**. Multiplying both sides from the left by  $\mathbf{b}^*$  and remembering that  $\mathbf{b}^* \cdot \mathbf{h} = 0$ , we have

$$\mathbf{b}^* \cdot \mathbf{a} = \alpha |\mathbf{b}|^2. \tag{12.18}$$

The Cauchy-Schwartz inequality comes directly from the following one.

$$|\mathbf{h}|^{2} = \left|\mathbf{a} - \frac{(\mathbf{b}^{*} \cdot \mathbf{a})}{|\mathbf{b}|^{2}}\mathbf{b}\right|^{2} \ge 0.$$
(12.19)

Let  $\psi(x)$  be the wavefunction of a particle. From the probabilistic interpretation of wavefunction we have

$$\overline{x} = \int \psi^*(x) x \psi(x) \, dx, \qquad (12.20)$$

where  $\overline{x}$  is the expectation value of x. The variance of x is

$$(\Delta x)^2 = \int \psi^*(x)(x-\overline{x})^2 \psi(x) \, dx. \tag{12.21}$$

If  $|\psi(x)|^2$  is the probability density of finding the particle at position x, what is the probability density of finding the particle having a momentum  $\hbar k$ ? To

answer this question, we need to expand the wavefunction  $\psi(x)$  into a linear combination of its Fourier components, each having a definite k.

$$\psi(x) = \frac{1}{\sqrt{2\pi}} \int \phi(k) e^{ikx} dk. \qquad (12.22)$$

Because of the one-to-one correspondence between  $\psi(x)$  and  $\phi(k)$ , the quantum state of the particle is equally well described by  $\phi(k)$ . The symmetric roles played by  $\psi(x)$  and  $\phi(k)$  yield the interpretation of  $|\phi(k)|^2$  as the probability density of finding the particle having a momentum  $\hbar k$ . Therefore we have

$$\overline{k} = \int \phi^*(k) k \phi(k) \, dk, \qquad (12.23)$$

where  $\overline{k}$  is the expectation value of k. The variance of k is

$$(\Delta k)^{2} = \int \phi^{*}(k)(k-\bar{k})^{2}\phi(k) \, dk.$$
 (12.24)

Using the inverse Fourier transform, in terms of  $\psi(x)$  Eq. (12.23) can be written as

$$\overline{k} = \frac{1}{2\pi} \int \left[ \int \psi^*(x') e^{ikx'} dx' \right] k \left[ \int \psi(x) e^{-ikx} dx \right] dk,$$
  
$$= \frac{1}{2\pi} \int \left[ \int \psi^*(x') e^{ikx'} dx' \right] \left[ \int \psi(x) \left( i \frac{\partial}{\partial x} e^{-ikx} \right) dx \right] dk,$$
  
$$= \frac{1}{2\pi} \int \left[ \int \psi^*(x') e^{ikx'} dx' \right] \left\{ \int \left[ -i \frac{\partial}{\partial x} \psi(x) \right] e^{-ikx} dx \right\} dk, (12.25)$$

where in the last step we have used integration by parts and the boundary condition that  $\psi(x) \to 0$  when  $x \to \pm \infty$ . Since

$$\frac{1}{2\pi} \int e^{ik(x'-x)} dk = \delta(x'-x), \qquad (12.26)$$

we have

$$\overline{k} = \int \psi^*(x) \left[ -i \frac{\partial}{\partial x} \psi(x) \right] dx.$$
(12.27)

By the same procedure it can be shown that

$$\overline{k^2} = \int \phi^*(k) k^2 \phi(k) \, dk = \int \psi^*(x) \left(-i\frac{\partial}{\partial x}\right)^2 \psi(x) \, dx.$$
(12.28)

Define  $f_a(x)$  and  $f_b(x)$  by

$$f_a(x) = (x - \overline{x})\psi(x), \qquad (12.29)$$

$$f_b(x) = \left(-i\frac{\partial}{\partial x} - \overline{k}\right)\psi(x),$$
 (12.30)

we have

$$|f_{a}(x)|^{2} = \int \psi^{*}(x)(x-\overline{x})^{2}\psi(x) dx = (\Delta x)^{2}, \qquad (12.31)$$
  
$$|f_{b}(x)|^{2} = \int \left(i\frac{\partial}{\partial x}-\overline{k}\right)\psi^{*}(x)\left(-i\frac{\partial}{\partial x}-\overline{k}\right)\psi(x) dx \qquad = \int \psi^{*}(x)\left(-i\frac{\partial}{\partial x}-\overline{k}\right)^{2}\psi(x) dx, \qquad (12.32)$$

where in the last step we have used again integration by parts and the boundary condition that  $\psi(x) \to 0$  when  $x \to \pm \infty$ . Expressing  $\psi(x)$  in terms of  $\phi(k)$  by Eq. (12.22), we have

$$|f_b(x)|^2 = \frac{1}{2\pi} \int \left[ \int \phi^*(k') e^{-ik'x} dk' \right] \left( -i\frac{\partial}{\partial x} - \overline{k} \right)^2 \left[ \int \phi(k) e^{ikx} dk \right] dx$$
  
$$= \frac{1}{2\pi} \int \int \phi^*(k') (k - \overline{k})^2 \phi(k) \left[ \int e^{i(k-k')x} dx \right] dk' dk$$
  
$$= \int \phi^*(k) (k - \overline{k})^2 \phi(k) dk = (\Delta k)^2.$$
(12.33)

The inner product between  $f_b(x)$  and  $f_a(x)$  is defined by

$$\int f_b^*(x) f_a(x) dx$$

$$= \frac{1}{2} \left[ \int f_b^*(x) f_a(x) dx + \int f_a^*(x) f_b(x) dx \right]$$

$$+ \frac{1}{2} \left[ \int f_b^*(x) f_a(x) dx - \int f_a^*(x) f_b(x) dx \right]$$

$$= \frac{1}{2} \left[ \int f_b^*(x) f_a(x) dx + \int f_a^*(x) f_b(x) dx \right]$$

$$+ \frac{1}{2} \int \left( i \frac{\partial}{\partial x} - \overline{k} \right) \psi^*(x) (x - \overline{x}) \psi(x) dx$$

$$- \frac{1}{2} \int \psi^*(x) (x - \overline{x}) \left( -i \frac{\partial}{\partial x} - \overline{k} \right) \psi(x) dx. \quad (12.34)$$

The first term on the right-hand side is a real number, and let us denote it by F. Using integration by parts, the second and the third terms on the

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right-hand side can be reduced to

$$\frac{1}{2} \int \psi^*(x) \left[ \left( -i\frac{\partial}{\partial x} - \overline{k} \right) (x - \overline{x}) - (x - \overline{x}) \left( -i\frac{\partial}{\partial x} - \overline{k} \right) \right] \psi(x) dx$$

$$= -\frac{i}{2} \int \psi^*(x) \psi(x) dx$$

$$= -\frac{i}{2}.$$
(12.35)

By the Cauchy-Schwartz inequality, we have

$$|f_a(x)|^2 |f_b(x)|^2 \ge F^2 + \frac{1}{4}.$$
(12.36)

Since  $F^2 \ge 0$ , we have

$$(\Delta k)^2 (\Delta x)^2 \ge \frac{1}{4}.$$
 (12.37)

In other words,

$$\Delta p \Delta x \ge \frac{\hbar}{2}.\tag{12.38}$$

# Chapter 13

# Bound States in Quantum Models

#### **13.1** Method of Power Expansion

Power expansion is the most conventional method for solving the Schrödinger equation analytically. The basic idea of the power-expansion method is to assume that the solutions of the Schrödinger equation are of the following form:

$$\psi_n x = h_n(x)g(x),\tag{13.1}$$

where g(x) is the asymptotic solution of the Schrödinger equation at the boundaries that may include  $x \to \pm \infty$ , and  $h_n(x)$  is a polynomial of order n. The reason for this separation is that while g(x) is an asymptotic solution, it does not satisfy the Schrödinger equation except at the boundaries. Therefore we correct it with a polynomial. The order of the polynomial must be finite, otherwise it may change g(x) too much at the boundaries. By substituting  $\psi_n(x)$  into the Schrödinger equation, we obtain another equation for  $h_n(x)$ . In the solvable cases  $h_n(x)$  can be found for a particular energy  $E_n$ , then  $E_n$ is the quantized energy for the *n*th energy level. Otherwise  $\psi_n(x)$  diverges at the boundaries, then it is not an acceptable solution. For almost all the potential functions V(x), it is not possible to find such  $h_n(x)$  regardless of the choice of  $E_n$ . There are only a handful of V(x) for which analytical solutions in the form of power series have been found. These are known as the solvable models. Just like there are only a finite number of functions that can be integrated analytically, we must live with the fact that there are only a small number of V(x) for which the Schrödinger equation can be solved analytically.

In the following sections, we shall use the method of power expansion to obtain the solutions for four distinctive types of potential, namely the harmonic oscillator  $V(x) = kx^2/2$ , which has infinite walls on both sides, the Morse oscillator  $V(x) = A(e^{-2\alpha x} - 2e^{-\alpha x})$ , which has a finite wall on one side and an infinite wall on the other side, the Pöschl-Teller oscillator  $V(x) = -A \operatorname{sech}^2(\alpha x)$ , which has finite walls on both sides, and the Coulomb potential  $V(x) = -Ze^2/r$ , in which the wall is finite but there is an infinitely deep hole in the center. These potentials serve as illuminating models in atomic and molecular physics. Much insight can be gained by studying their solutions carefully. In the process of obtaining the solutions, one can also see clearly why energy is quantized for bound states.

### 13.2 Harmonic Oscillator

Any small-amplitude oscillation around a potential minimum can be approximated by a harmonic oscillator, because  $V(x) = kx^2/2$  is simply the first term in the Taylor expansion of the potential function around the equilibrium point. To solve the Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + \frac{1}{2}kx^2\psi(x) = E\psi(x), \qquad (13.2)$$

we first define the following parameters and change variables:

$$\alpha = \left(\frac{mk}{\hbar^2}\right)^{\frac{1}{4}}, \quad \lambda = \frac{2E}{\hbar}\sqrt{\frac{m}{k}}, \quad \xi = \alpha x.$$

Eq. (13.2) becomes

$$\frac{d^2\psi}{d\xi^2} + (\lambda - \xi^2)\psi = 0.$$
 (13.3)

To find the solutions, a standard approach is to factor out the asymptotic solutions before doing the power expansion. As  $\xi \to \pm \infty$ , Eq. (13.3) is no different from

$$\frac{d^2\psi}{d\xi^2} + (1-\xi^2)\psi = \left(\frac{d}{d\xi} - \xi\right)\left(\frac{d}{d\xi} + \xi\right)\psi = 0.$$
(13.4)

From

$$\left(\frac{d}{d\xi} + \xi\right)\psi = 0 \tag{13.5}$$

we find that the asymptotic solution is  $\psi(\xi) \approx e^{-\xi^2/2}$ . Then we can focus on the function  $v(\xi)$  defined by

$$\psi(\xi) = e^{-\xi^2/2} v(\xi). \tag{13.6}$$

The equation for  $v(\xi)$  is

$$\frac{d^2v}{d\xi^2} - 2\xi \frac{dv}{d\xi} + (\lambda - 1)v = 0.$$
(13.7)

Substitute  $\lambda = 2n + 1$  and  $v = \sum_{k=0}^{\infty} a_k \xi^k$  into Eq. (13.7), one obtains

$$\sum_{k=2}^{\infty} a_k k(k-1)\xi^{k-2} - \sum_{k=1}^{\infty} a_k(2k)\xi^k + \sum_{k=0}^{\infty} a_k(2n)\xi^k = 0,$$
(13.8)

or equivalently

$$\sum_{k=0}^{\infty} a_{k+2}(k+2)(k+1)\xi^k - \sum_{k=0}^{\infty} a_k(2k)\xi^k + \sum_{k=0}^{\infty} a_k(2n)\xi^k = 0.$$
(13.9)

The solution demands

$$a_{k+2} = -\frac{2(n-k)}{(k+2)(k+1)}a_k.$$
(13.10)

Namely

$$v(\xi) = a_0 \left[ 1 + \sum_{k=1}^{\infty} (-1)^k 2^k \frac{n(n-2)\cdots(n-2k+2)}{(2k)!} \xi^{2k} \right] \quad (13.11)$$
$$a_1 \left[ \xi + \sum_{k=1}^{\infty} (-1)^k 2^k \frac{(n-1)(n-3)\cdots(n-2k+1)}{(2k)!} \xi^{2k+1} \right] \quad (13.12)$$

+ 
$$a_1 \left[ \xi + \sum_{k=1}^{\infty} (-1)^k 2^k \frac{(n-1)(n-3) \cdots (n-2k+1)}{(2k+1)!} \xi^{2k+1} \right].$$
 (13.12)

Unless n is a nonnegative integer,  $a_{k+2}/a_k \rightarrow 2/k$  when k very large, then the first series is asymptotically  $\exp(2\xi^2)$  and the second series is asymptotically  $\xi \exp(2\xi^2)$ . These solutions of  $v(\xi)$  will make  $\psi(\xi)$  diverge as  $\xi \rightarrow \pm \infty$ , hence are not acceptable. Therefore n must be a nonnegative integer and  $a_1 = 0$  if n is even,  $a_0 = 0$  if n is odd.

$$v_n(\xi) = C \sum_{k=0}^{[n/2]} (-1)^k \frac{[n/2]!}{(n-2k)!k!} (2\xi)^{n-2k}.$$
 (13.13)

This is the Hermite polynomial  $v_n(\xi) = H_n(\xi)$ . In summary, the solutions are

$$\psi_n(\xi) = C \, e^{-\xi^2/2} H_n(\xi), \tag{13.14}$$

$$E_n = \frac{\hbar}{2} \sqrt{\frac{k}{m}} \left(2n+1\right) = \hbar \omega \left(n+\frac{1}{2}\right). \tag{13.15}$$

## 13.3 Morse Oscillator

When a chemical bond is weakly stretched or compressed, it behaves like a spring. However, if the bond is stretched too much, the restoring force becomes weaker and weaker. At a certain point the bond will break, then there is no more restoring force. On the contrary, when the bond is strongly compressed, the restoring force becomes larger and larger due to the strong repulsion between the nuclei. Such an asymmetric spring can be modeled by the Morse oscillator.

To solve the Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + A\left(e^{-2\alpha x} - 2e^{-\alpha x}\right)\psi(x) = E\psi(x), \qquad (13.16)$$

we first define the following parameters and change variables:

$$\epsilon = \frac{\sqrt{-2mE}}{\alpha\hbar}, \quad n = \frac{\sqrt{2mA}}{\alpha\hbar} - \left(\epsilon + \frac{1}{2}\right), \quad \xi = \frac{2\sqrt{2mA}}{\alpha\hbar}e^{-\alpha x}.$$
 (13.17)

Eq. (13.16) becomes

$$\frac{d^2\psi}{d\xi^2} + \frac{1}{\xi}\frac{d\psi}{d\xi} + \left(-\frac{1}{4} + \frac{n+\epsilon+1/2}{\xi} - \frac{\epsilon^2}{\xi^2}\right)\psi = 0.$$
 (13.18)

To find the solutions, a standard approach is to factor out the asymptotic solutions before doing the power expansion. Since  $\psi \approx e^{\pm \xi/2}$  as  $\xi \to \infty$ ,  $\psi \approx \xi^{\pm \epsilon}$  as  $\xi \to 0$ , and  $\psi$  must be finite as  $\xi \to 0$  and  $\infty$ , we can focus on the function  $v(\xi)$  defined by

$$\psi(\xi) = e^{-\xi/2} \xi^{\epsilon} v(\xi).$$
(13.19)

The equation for  $v(\xi)$  is

$$\xi \frac{d^2 v}{d\xi^2} + (2\epsilon + 1 - \xi) \frac{dv}{d\xi} + nv = 0.$$
(13.20)

 $\operatorname{Set}$ 

$$a = -n, \ c = 2\epsilon + 1,$$
 (13.21)

then

$$\xi \frac{d^2 v}{d\xi^2} + (c - \xi) \frac{dv}{d\xi} - av = 0.$$
(13.22)

Substitute  $v(\xi) = \sum_{k=0}^{\infty} a_k \xi^k$  into Eq. (13.22), one obtains

$$\sum_{k=2}^{\infty} a_k k(k-1)\xi^{k-1} + \sum_{k=1}^{\infty} a_k ck\xi^{k-1} - \sum_{k=1}^{\infty} a_k k\xi^k - \sum_{k=0}^{\infty} a_k a\xi^k = 0, \quad (13.23)$$

or equivalently

$$\sum_{k=0}^{\infty} a_{k+1}k(k+1)\xi^k + \sum_{k=0}^{\infty} a_{k+1}c(k+1)\xi^k - \sum_{k=0}^{\infty} a_kk\xi^k - \sum_{k=0}^{\infty} a_ka\xi^k = 0(13.24)$$

The solution demands

$$a_{k+1} = \frac{a+k}{(k+1)(c+k)}a_k.$$
(13.25)

Namely

$$v(\xi) = a_0 \left[ 1 + \frac{a}{c} \xi + \frac{a(a+1)}{2!c(c+1)} \xi^2 + \frac{a(a+1)(a+2)}{3!c(c+1)(c+2)} \xi^3 + \cdots \right] (13.26)$$

This is the confluent hypergeometric function  $v(\xi) = C_1 F_1(a, c; \xi)$ . Set

$$v(\xi) = \xi^{1-c} w(\xi), \tag{13.27}$$

then the equation for  $w(\xi)$  is

$$\xi \frac{d^2 w}{d\xi^2} + (2 - c - \xi) \frac{dw}{d\xi} - (a - c + 1)w = 0.$$
(13.28)

The solution is

$$w(\xi) = C_1 F_1(a - c + 1, 2 - c; \xi), \qquad (13.29)$$

or

$$v(\xi) = C \,\xi^{1-c}{}_1F_1(a-c+1,2-c\,;\,\xi). \tag{13.30}$$

This is another independent solution. If a is not zero or a negative integer,  $a_{k+1}/a_k \to 1/k$  when k very large, then the series  $v \propto e^{\xi}$ , hence  $\psi \propto e^{\xi/2}\xi^{\epsilon}$ . This divergence is not acceptable. Therefore a must be a nonpositive integer. In addition, c cannot be a nonpositive integer, otherwise the denominator of one of the terms in the series becomes zero. In summary,

$$v_n(\xi) = C_1 F_1(-n, 2\epsilon + 1; \xi),$$
  

$$\psi_n(\xi) = C e^{-\xi/2} \xi^{\epsilon_1} F_1(-n, 2\epsilon + 1; \xi).$$
(13.31)

This solution satisfies the boundary conditions

$$\lim_{x \to \infty} \psi_n = \lim_{\xi \to 0} \psi_n = 0, \tag{13.32}$$

$$\lim_{x \to -\infty} \psi_n = \lim_{\xi \to \infty} \psi_n = 0. \tag{13.33}$$

The other independent solution,

$$v_n(\xi) = C \,\xi^{-2\epsilon} {}_1F_1(-n - 2\epsilon, 1 - 2\epsilon; \,\xi),$$
  

$$\psi_n(\xi) = C \,e^{-\xi/2} \xi^{-\epsilon} {}_1F_1(-n - 2\epsilon, 1 - 2\epsilon; \,\xi),$$
(13.34)

does not satisfy Eq. (13.32), hence is excluded. From Eq. (13.17),

$$E_n = -A \left[ 1 - \frac{\alpha \hbar}{\sqrt{2mA}} \left( n + \frac{1}{2} \right) \right]^2.$$
(13.35)

### 13.4 Pöschl-Teller Oscillator

The Pöschl-Teller potential  $V(x) = -A \operatorname{sech}^2(\alpha x)$  represents a soft-edged quantum well with finite depth. Quantum wells can be made by sandwiching together semiconductors of different compositions. Unlike atoms, the energy levels of quantum wells can be engineered by adjusting the width and depth of the well. Therefore they are often considered as "artificial atoms". To solve the Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) - A\operatorname{sech}^2(\alpha x)\psi(x) = E\psi(x), \qquad (13.36)$$

we first define the following parameters

$$\epsilon = \frac{\sqrt{-2mE}}{\alpha\hbar}, \quad s = \frac{1}{2} \left( -1 + \sqrt{1 + \frac{8mA}{\alpha^2\hbar^2}} \right), \tag{13.37}$$

and change variable

$$\xi = \tanh(\alpha x). \tag{13.38}$$

Eq. (13.36) becomes

$$\frac{d}{d\xi}\left[(1-\xi^2)\frac{d\psi}{d\xi}\right] + \left[s(s+1) - \frac{\epsilon^2}{1-\xi^2}\right]\psi = 0.$$
(13.39)

Set

$$\psi = (1 - \xi^2)^{\epsilon/2} v(\xi), \qquad (13.40)$$

the equation for  $v(\xi)$  is

$$(1-\xi^2)\frac{d^2v}{d\xi^2} - 2(1+\epsilon)\,\xi\frac{dv}{d\xi} - (\epsilon-s)(\epsilon+s+1)v = 0. \tag{13.41}$$

Change the variable once again

$$u = \frac{1}{2}(1 - \xi), \tag{13.42}$$

Eq. (13.41) becomes

$$u(1-u)\frac{d^2v}{du^2} + (1+\epsilon)(1-2u)\frac{dv}{du} - (\epsilon-s)(\epsilon+s+1)v = 0.$$
(13.43)

Set

$$a = \epsilon - s, \ b = \epsilon + s + 1, \ c = 1 + \epsilon, \tag{13.44}$$

then

$$u(1-u)\frac{d^2v}{du^2} + [c - (a+b+1)u]\frac{dv}{du} - abv = 0.$$
(13.45)

Substitute  $v(u) = \sum_{k=0}^{\infty} a_k u^k$  into Eq. (13.45), one obtains

$$\sum_{k=2}^{\infty} a_k k(k-1) u^{k-1} - \sum_{k=2}^{\infty} a_k k(k-1) u^k + \sum_{k=1}^{\infty} a_k ck u^{k-1} - \sum_{k=1}^{\infty} a_k k(a+b+1) u^k - \sum_{k=0}^{\infty} a_k ab u^k = 0, \quad (13.46)$$

or equivalently

$$\sum_{k=0}^{\infty} a_{k+1}k(k+1)u^k - \sum_{k=0}^{\infty} a_kk(k-1)u^k + \sum_{k=0}^{\infty} a_{k+1}c(k+1)u^k - \sum_{k=0}^{\infty} a_kk(a+b+1)u^k - \sum_{k=0}^{\infty} a_kabu^k = 0.$$
 (13.47)

The solution demands

$$a_{k+1} = \frac{(a+k)(b+k)}{(k+1)(c+k)}a_k.$$
(13.48)

Namely

$$v(u) = a_0 \left[ 1 + \frac{ab}{c} \xi + \frac{a(a+1)b(b+1)}{2!c(c+1)} \xi^2 + \frac{a(a+1)(a+2)b(b+1)(b+2)}{3!c(c+1)(c+2)} \xi^3 + \cdots \right]$$
(13.49)

This is the hypergeometric function  $v(u) = C_2 F_1(a, b, c; u)$ . Set

$$v(u) = u^{1-c}w(u), (13.50)$$

then the equation for w(u) is

$$u(1-u)\frac{d^2w}{du^2} + (c-a-b+1)u\frac{dw}{du} - (a-c+1)(b-c+1)w = 0.$$
(13.51)

The solution is

$$w(u) = C_2 F_1(a - c + 1, b - c + 1, 2 - c; u),$$
(13.52)

or

$$v(u) = C u^{1-c} {}_2F_1(a-c+1, b-c+1, 2-c; u).$$
(13.53)

This is another independent solution. If c is not zero or a negative integer and a or b is a nonpositive integer, the series is finite. Since  $b = \epsilon + s + 1 > 0$ ,  $a = \epsilon - s$  must be a nonpositive integer. Let  $\epsilon - s = -n$ ,

$$v_n(u) = C_2 F_1(-n, \epsilon + s + 1, 1 + \epsilon; u), \qquad (13.54)$$

$$\psi_n(\xi) = C \left(1 - \xi^2\right)^{\epsilon/2} {}_2F_1\left[-n, \epsilon + s + 1, 1 + \epsilon; \frac{1}{2}(1 - \xi)\right]. (13.55)$$

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This solution satisfies the boundary conditions

$$\lim_{x \to \pm \infty} \psi_n = \lim_{\xi \to \pm 1} \psi_n = 0. \tag{13.56}$$

The other independent solution,

$$v_n(u) = C \, u^{-\epsilon} {}_2F_1(-s, s+1, 1-\epsilon; u), \tag{13.57}$$

$$\psi_n(\xi) = C \left(1+\xi\right)^{\epsilon/2} (1-\xi)^{-\epsilon/2} {}_2F_1\left[-s, s+1, 1-\epsilon; \frac{1}{2}(1-\xi)\right], (13.58)$$

does not satisfy Eq. (13.56), hence is excluded. From Eq. (13.37),

$$E_n = -\frac{\alpha^2 \hbar^2}{8m} \left[ -(1+2n) + \sqrt{1 + \frac{8mA}{\alpha^2 \hbar^2}} \right]^2.$$
(13.59)

## 13.5 Hydrogen Atom

As the simplest atom in the universe, the hydrogen atom is undoubtably the first step to understand atoms. Since the hydrogen atom has a spherical symmetric potential, the radial part of its solution can be separated with the angular part. Before we discuss specifically the Coulomb potential, we shall consider the general case of spherical symmetric potentials V = V(r), in which the angular part is the focus of our discussion.

The Schrödinger equation is

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V(r)\psi = E\psi.$$
(13.60)

In spherical coordinates it can be written as

$$-\frac{\hbar^2}{2m} \left[ \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial \psi}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial \psi}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 \psi}{\partial \phi^2} \right] + V\psi = E\psi. \quad (13.61)$$

Since

$$\mathbf{r} = r\hat{\mathbf{r}},\tag{13.62}$$

$$\nabla = \hat{\mathbf{r}}\frac{\partial}{\partial r} + \hat{\boldsymbol{\phi}}\frac{1}{r\sin\theta}\frac{\partial}{\partial\phi} + \hat{\boldsymbol{\theta}}\frac{1}{r}\frac{\partial}{\partial\theta}, \qquad (13.63)$$

we have

$$\mathbf{L} = -i\hbar\mathbf{r} \times \nabla = -i\hbar\left(-\hat{\boldsymbol{\theta}}\frac{1}{\sin\theta}\frac{\partial}{\partial\phi} + \hat{\boldsymbol{\phi}}\frac{\partial}{\partial\theta}\right).$$
(13.64)

From

$$\mathbf{r} = \sin\theta\cos\phi\hat{\mathbf{x}} + \sin\theta\sin\phi\hat{\mathbf{y}} + \cos\theta\hat{\mathbf{z}},\tag{13.65}$$

$$\boldsymbol{\phi} = -\sin\phi \hat{\mathbf{x}} + \cos\phi \hat{\mathbf{y}},\tag{13.66}$$

$$\hat{\boldsymbol{\phi}} = -\sin\phi\hat{\mathbf{x}} + \cos\phi\hat{\mathbf{y}}, \qquad (13.66)$$
$$\hat{\boldsymbol{\theta}} = \cos\theta\cos\phi\hat{\mathbf{x}} + \cos\theta\sin\phi\hat{\mathbf{y}} - \sin\theta\hat{\mathbf{z}}, \qquad (13.67)$$

we have

$$\frac{\partial \boldsymbol{\theta}}{\partial \theta} = -\hat{\mathbf{r}},\tag{13.68}$$

$$\frac{\partial \boldsymbol{\phi}}{\partial \theta} = 0, \tag{13.69}$$

$$\frac{\partial \boldsymbol{\theta}}{\partial \phi} = \cos \theta \hat{\boldsymbol{\phi}}, \qquad (13.70)$$

$$\frac{\partial \boldsymbol{\phi}}{\partial \phi} = -(\sin \theta \hat{\mathbf{r}} + \cos \theta \hat{\boldsymbol{\theta}}). \tag{13.71}$$

Therefore

$$L^{2} = -\hbar^{2} \left( -\hat{\theta} \frac{1}{\sin \theta} \frac{\partial}{\partial \phi} + \hat{\phi} \frac{\partial}{\partial \theta} \right) \cdot \left( -\hat{\theta} \frac{1}{\sin \theta} \frac{\partial}{\partial \phi} + \hat{\phi} \frac{\partial}{\partial \theta} \right)$$
$$= -\hbar^{2} \left( \frac{1}{\sin^{2} \theta} \frac{\partial^{2}}{\partial \phi^{2}} + \frac{\cos \theta}{\sin \theta} \frac{\partial}{\partial \theta} + \frac{\partial^{2}}{\partial \theta^{2}} \right)$$
(13.72)

$$= -\hbar^2 \left[ \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} + \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) \right], \qquad (13.73)$$

and Eq. (13.61) can be written as

$$-\frac{\hbar^2}{2mr^2} \left[ \frac{\partial}{\partial r} \left( r^2 \frac{\partial \psi}{\partial r} \right) - \frac{1}{\hbar^2} L^2 \psi \right] + V \psi = E \psi, \qquad (13.74)$$

Multiply both sides of Eq. (13.74) by  $-2mr^2/\hbar^2$ , it becomes

$$\frac{\partial}{\partial r} \left( r^2 \frac{\partial \psi}{\partial r} \right) - \frac{2mr^2}{\hbar^2} (V - E)\psi = \frac{1}{\hbar^2} L^2 \psi.$$
(13.75)

Substitute

$$\psi(r,\theta,\phi) = R(r)\Theta(\theta)\Phi(\phi) \tag{13.76}$$

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into Eq. (13.75), then divide both sides by  $R(r)\Theta(\theta)\Phi(\phi)$ , one has

$$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) - \frac{2mr^2}{\hbar^2}(V-E) = \frac{1}{\Theta\Phi}\frac{1}{\hbar^2}L^2(\Theta\Phi).$$
(13.77)

Note that the left hand side is a function of r, whereas the right hand side is a function of  $\theta$  and  $\phi$ , therefore both sides must be equal to a constant. Let the constant be  $\lambda$ , then

$$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) - \frac{2mr^2(V-E)}{\hbar^2} = \lambda,$$
(13.78)

and

$$\frac{1}{\Theta\Phi}\frac{1}{\hbar^2}L^2(\Theta\Phi) = \lambda. \tag{13.79}$$

We solve Eq. (13.79) first. From Eq. (13.73), Eq. (13.79) becomes

$$-\frac{1}{\Theta\Phi}\left\{\frac{1}{\sin^2\theta}\frac{\partial^2(\Theta\Phi)}{\partial\phi^2} + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left[\sin\theta\frac{\partial(\Theta\Phi)}{\partial\theta}\right]\right\} = \lambda.$$
 (13.80)

Multiply both sides by  $-\sin^2\theta$ , one obtains

$$\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2} = -\sin^2\theta \left[\lambda + \frac{1}{\Theta\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)\right].$$
 (13.81)

Again, the left hand side is a function of  $\phi$ , whereas the right hand side is a function of  $\theta$ , therefore both sides must be equal to a constant. Let the constant be  $-m^2$ , the left hand side is

$$\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2} = -m^2,\tag{13.82}$$

therefore

$$\Phi(\phi) = e^{\pm im\phi},\tag{13.83}$$

where m must be an integer to satisfy the periodic boundary condition  $\Phi(\phi) = \Phi(\phi + 2\pi)$ . The right hand side is

$$\lambda + \frac{1}{\Theta \sin \theta} \frac{d}{d\theta} \left( \sin \theta \frac{d\Theta}{d\theta} \right) - \frac{m^2}{\sin^2 \theta} = 0.$$
(13.84)

Set

$$x = \cos \theta, \tag{13.85}$$

Eq. (13.84) becomes

$$(1-x^2)\frac{d^2\Theta}{dx^2} - 2x\frac{d\Theta}{dx} + \left(\lambda - \frac{m^2}{1-x^2}\right)\Theta = 0.$$
(13.86)

This is the associated Legendre equation. Set

$$\Theta(x) = (1 - x^2)^{m/2} \frac{d^m v}{dx^m},$$
(13.87)

then v(x) satisfy the Legendre equation

$$(1-x^2)\frac{d^2v}{dx^2} - 2x\frac{dv}{dx} + \lambda v = 0.$$
 (13.88)

Substitute  $v(x) = \sum_{k=0}^{\infty} a_k x^k$  into Eq. (13.88), one obtains

$$\sum_{k=2}^{\infty} a_k k(k-1) x^{k-2} - \sum_{k=2}^{\infty} a_k k(k-1) x^k - \sum_{k=1}^{\infty} a_k (2k) x^k + \sum_{k=0}^{\infty} a_k \lambda x^k = 0, \quad (13.89)$$

or equivalently

$$\sum_{k=0}^{\infty} a_{k+2}(k+2)(k+1)x^k - \sum_{k=0}^{\infty} a_k k(k-1)x^k - \sum_{k=1}^{\infty} a_k (2k)x^k + \sum_{k=0}^{\infty} a_k \lambda x^k = 0.$$
 (13.90)

If  $\lambda = l(l+1)$ , the solution demands

$$a_{k+2} = -\frac{(l-k)(k+l+1)}{(k+2)(k+1)}a_k.$$
(13.91)

If l is not an integer,  $a_{k+2}/a_k \to 1$  when k very large, then the series diverges. This divergence is not acceptable, hence l must be an integer. Since change l = n to l = -n - 1,  $\lambda = l(l+1)$  will stay unchanged, we can assume  $l \ge 0$ . Eq. (13.87) then implies  $m \le l$ . Set  $a_1 = 0$  if l is even, and  $a_0 = 0$  if l is odd,

$$v_l(x) = C \sum_{k=0}^{\lfloor l/2 \rfloor} (-1)^k \frac{(2l-2k)!}{2^l k! (l-k)! (l-2k)!} x^{l-2k}.$$
 (13.92)

This is the Legendre polynomial  $v_l(x) = P_l(x)$ , and

$$\Theta(x) = (1 - x^2)^{m/2} \frac{d^m P_l(x)}{dx^m}.$$
(13.93)

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Now the only equation left to be solved is Eq. (13.78). From this point we specify the potential function to be  $V = -Ze^2/r$ . Eq. (13.78) becomes

$$\frac{d}{dr}\left(r^{2}\frac{dR}{dr}\right) + \frac{2mr^{2}Ze^{2}}{\hbar^{2}r}R + \frac{2mr^{2}E}{\hbar^{2}}R = l(l+1)R.$$
(13.94)

Set

$$R(r) = \frac{v(r)}{r},\tag{13.95}$$

the equation for v(r) is

$$\frac{d^2v}{dr^2} + \left[ -\frac{l(l+1)}{r^2} + \frac{2mZe^2}{\hbar^2 r} + \frac{2mE}{\hbar^2} \right] v = 0.$$
(13.96)

Since  $v(r) \to r^{l+1}$  or  $r^{-l}$  as  $r \to 0$ , and  $v(r) \to e^{\pm(\sqrt{-2mE}/\hbar)r}$  as  $r \to \infty$ , in addition R = v/r must at least be finite as  $r \to 0$  and  $\infty$ , we can set

$$v = \rho^{l+1} e^{-\rho} w(\rho),$$
 (13.97)

where

$$\rho = (\sqrt{-2mE}/\hbar)r. \tag{13.98}$$

The equation for  $w(\rho)$  is then

$$\rho \frac{d^2 w}{d\rho^2} + 2(l+1-\rho)\frac{dw}{d\rho} + [\rho_0 - 2(l+1)]w = 0, \qquad (13.99)$$

where

$$\rho_0 = \sqrt{\frac{2m}{-E}} \frac{Ze^2}{\hbar}.$$
(13.100)

Set

$$z = 2\rho, \tag{13.101}$$

Eq. (13.99) becomes

$$z\frac{d^2w}{dz^2} + (2l+2-z)\frac{dw}{dz} + \left[\frac{\rho_0}{2} - (l+1)\right]w = 0.$$
(13.102)

As shown in the case of Morse Oscillator, the solution for Eq. (13.102) is

$$w_N(z) = C_1 F_1(-N, 2l+2; z), \qquad (13.103)$$

therefore

$$R_N(\rho) = C \,\rho^l e^{-\rho_1} F_1(-N, 2l+2; 2\rho), \qquad (13.104)$$

where

$$N \equiv \frac{\rho_0}{2} - (l+1) \tag{13.105}$$

must be a nonnegative integer. This solution satisfies the boundary conditions

$$\lim_{r \to 0} R_N = \lim_{\rho \to 0} R_N = 0, \tag{13.106}$$

$$\lim_{r \to \infty} R_N = \lim_{\rho \to \infty} R_N = 0.$$
(13.107)

The other independent solution,

$$v_N(z) = C \, z^{-2l-1} {}_1F_1(-N-2l-1,-2l;z),$$
  

$$R_N(\rho) = C \, \rho^{-l-1} e^{-\rho} {}_1F_1(-N-2l-1,-2l;2\rho),$$
(13.108)

does not satisfy Eq. (13.106), hence is excluded. From Eqs. (13.100) and (13.105),

$$E_n = -\frac{mz^2 e^4}{2\hbar^2 n^2},\tag{13.109}$$

where  $n = \rho_0/2 = N + l + 1$ . Note that l can take values between 0 and n - 1, and m can take values between -l and l, therefore for each set of n and l there are m eigenstates of the same energy, and for each n there are  $\sum_{l=0}^{n-1}(2l+1) = n^2$  eigenstates of the same energy. Together with the fact that each eigenstate can accommodate two electrons of opposite spins, these levels of degeneracy form the basis of our understanding of the periodic table.

#### 13.6 Exercises

**Exercise 13.1.** Consider the Schrödinger equation for a spherical potential well of depth -V and radius R, as shown in Fig. 13.1. Calculate the energy level and the wavefunction of the ground state. You may assume the wavefunction  $\psi$  is only a function of r, namely  $\psi(\mathbf{r}) = \psi(r)$ . Hint: The Laplacian operator in the spherically symmetric case is

$$\nabla^2 u = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial u}{\partial r} \right). \tag{13.110}$$

The Schrödinger equation equation can be solved by changing variable to  $\phi(r) = \psi(r)/r$ . At the boundary r = R, the wavefunction and its derivative must be continuous.

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Fig. 13.1: A spherical potential well.

# Chapter 14

# **Operator Algebra in Quantum Mechanics**

# 14.1 Linear Space and Representation

Consider a general normalized matter wave u(x,t) which is a linear combination of monochromatic waves  $e^{ikx}$ . Each of the component waves has a definite wavenumber k.

$$u(x,t) = \frac{1}{\sqrt{2\pi}} \int \tilde{u}(k,t) e^{ikx} \, dk,$$
(14.1)

where

$$\int u^*(x,t)u(x,t)\,dx = \int \tilde{u}^*(k,t)\tilde{u}(k,t)dk = 1.$$
(14.2)

Because the relative strength of the wave component  $e^{ikx}$  is represented by  $|\tilde{u}(k,t)|^2$ , the expectation value of  $p = \hbar k$  is simply

$$\overline{p} = \int \hbar k \tilde{u}^*(k,t) \tilde{u}(k,t) \, dk.$$
(14.3)

If we write  $\overline{p}$  in terms of u(x, t),

$$\overline{p} = \int u^*(x,t)\hat{p}u(x,t)\,dx,\tag{14.4}$$

the following equations identify that  $\hat{p} = -i\hbar\partial/\partial x$ .

$$\int u^*(x,t) \left[ -i\hbar \frac{\partial}{\partial x} u(x,t) \right] dx$$

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$$= \frac{1}{2\pi} \int \left[ \int \tilde{u}^*(k,t) e^{-ikx} dk \right] \left[ \int \hbar k' \tilde{u}(k',t) e^{ik'x} dk' \right] dx$$
  
$$= \int \int \tilde{u}^*(k,t) \delta(k-k') \hbar k' \tilde{u}(k',t) dk dk'$$
  
$$= \int \hbar k \tilde{u}^*(k,t) \tilde{u}(k,t) dk.$$
(14.5)

By the symmetric roles of x and k in Fourier analysis, the expectation value of x is

$$\overline{x} = \int \tilde{u}^*(k,t) \frac{i\partial}{\partial k} \tilde{u}(k,t) dk$$
  

$$= \frac{1}{2\pi} \int \left[ \int u^*(x,t) e^{ikx} dx \right] \left[ \int x' u(x',t) e^{-ikx'} dx' \right] dk$$
  

$$= \int \int u^*(x,t) \delta(x-x') x' u(x',t) dx dx'$$
  

$$= \int u^*(x,t) x u(x,t) dx. \qquad (14.6)$$

Therefore if we agree that the probability distribution function of k is  $\tilde{u}^*(k)\tilde{u}(k)$ , then the probability distribution function of x is  $u^*(x,t)u(x,t)$ . Eqs. (14.3) and (14.6) point out a general rule: the expectation value of a physical quantity O(x, p) is

$$\overline{O} = \int u^*(x,t) \hat{O}u(x,t) \, dx, \qquad (14.7)$$

where  $\hat{O} = O(x, -i\hbar\partial/\partial x)$ . Alternatively, If we use  $\tilde{u}(k, t)$  to describe the matter wave, the expectation value of a physical quantity O(x, p) is

$$\overline{O} = \int \tilde{u}^*(k,t) \hat{O}\tilde{u}(k,t) \, dk, \qquad (14.8)$$

where  $\hat{O} = O(i\hbar\partial/\partial x, \hbar k)$ . If one expands u(x,t) with respect to an orthonormal basis set made of eigenfunctions of  $\hat{O}$ , *i.e.*  $u(x,t) = \sum_{i} a_i(t)s_i(x)$  and  $\hat{O}s_i(x) = O_i s_i(x)$ , then

$$\overline{O} = \sum_{i} O_i |a_i|^2. \tag{14.9}$$

Eq. (14.9) points out that the physical quantity O can have values  $O_1, O_2, O_3, \ldots$  with probability  $|a_1|^2, |a_2|^2, |a_3|^2, \ldots$  respectively. If a basis  $v_i(x)$  which is not a set of  $\hat{O}$ 's eigenfunctions is used,  $u(x,t) = \sum_i b_i(t)v_i(x)$ , the expectation value becomes

$$\overline{O} = \sum_{i,j} b_i^* b_j \int v_i^*(x) \hat{O} v_j(x) dx$$
$$\equiv \sum_{i,j} b_i^* O_{ij} b_j, \qquad (14.10)$$

#### 14.1. LINEAR SPACE AND REPRESENTATION

where  $O_{ij}$  is a matrix representation of the operator  $\hat{O}$  with respect to the basis  $v_i(x)$ . Because  $\overline{O}$  must be a real number, we have

$$\sum_{i,j} b_i^* O_{ij} b_j = \sum_{i,j} b_i O_{ij}^* b_j^*.$$
(14.11)

Interchanging the dummy index on the right-hand side, we have

$$\sum_{i,j} b_i^* (O_{ij} - O_{ji}^*) b_j = 0 \tag{14.12}$$

for any set of  $b_i$ . Therefore

$$O_{ij} = O_{ji}^*.$$
 (14.13)

An operator satisfying this condition is called a Hermitian operator. The requirement that the expectation value of a physical quantity must be a real number is equivalent to the requirement that the corresponding operator must be Hermitian.

Now it should be clear that in wave mechanics the state of a physical system is represented by the wavefunction u(x,t), which is a solution of the Schrödinger equation, and the value of a physical quantity is represented by its spectrum  $O_i$  and probability distribution  $|a_i|^2$ . The wavefunction can have different forms, such as u(x,t),  $\tilde{u}(k,t)$ ,  $a_i(t)$ , depending on which basis is used, so can physical quantities. For instance,  $\hat{p}$  can be written as  $\hbar k$  or  $-i\hbar\partial/\partial x$ , depending on whether  $\tilde{u}(k,t)$  or u(x,t) is used to describe the matter wave. Because in most cases of formal discussion it is not necessary to specify the basis, one can simply represent a wavefunction by  $|s\rangle$ , its complex conjugate by  $\langle s|$ , the expectation value of an operator by  $\langle s|\hat{O}|s\rangle$ , and the matrix element linking  $|s'\rangle$  and  $|s\rangle$  by  $\langle s'|\hat{O}|s\rangle$ . This is called the Dirac notation.

In the Dirac notation, the Schrödinger equation can be written as

$$i\hbar \frac{d}{dt}|t\rangle = \hat{H}|t\rangle,$$
 (14.14)

where  $|t\rangle$  represents the state at time t and

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{\mathbf{r}}) = -\frac{\hbar^2}{2m} \nabla^2 + V(\hat{\mathbf{r}})$$
(14.15)

is the energy operator. Obviously the the Schrödinger equation describes how a state evolves with time. In this picture the state changes with time, and the operators such as  $\hat{\mathbf{p}}$ ,  $\hat{\mathbf{r}}$  do not. This is called the Schrödinger representation. Alternatively, one can think the states are static, and instead the operators are changing with time. This is called the Heisenberg representation. In the Heisenberg representation the equation of motion for the operators is

$$i\hbar \frac{d\hat{O}(t)}{dt} = \left[\hat{O}, \hat{H}\right] + i\hbar \frac{\partial\hat{O}}{\partial t},\tag{14.16}$$

where  $[\hat{O}, \hat{H}] \equiv \hat{O}\hat{H} - \hat{H}\hat{O}$ . Eq. (14.16) can be obtained from Eq. (14.14) in the following way.

$$i\hbar \frac{d}{dt} \langle t|\hat{O}|t\rangle = \left(i\hbar \frac{d}{dt} \langle t|\right) \hat{O}|t\rangle + \langle t| \left(i\hbar \frac{\partial}{\partial t} \hat{O}\right) |t\rangle + \langle t|\hat{O}\left(i\hbar \frac{d}{dt}|t\rangle\right)$$
$$= \langle t| \left[\hat{O}, \hat{H}\right] + i\hbar \frac{\partial \hat{O}}{\partial t} |t\rangle.$$
(14.17)

It does not matter which representation we choose to describe the motion of the quantum systems, because what is important are the matrix elements  $\langle s'|\hat{O}|s \rangle$  that represent the probability of states. Whether we attribute the time evolution to the operators or the states does not change the time evolution of the matrix elements.

#### 14.2 Uncertainty Principle

In linear algebra it is known that if two operators A and B do not commute, they do not share the same set of eigenvectors. Therefore if  $|s\rangle$  is an eigenstate of A, it cannot be an eigenstate of B. This means if a state corresponds a precise value of A, its value of B must be a probability distribution with some uncertainty. In other words, A and B cannot both have precise values. This is known as the **uncertainty principle**.

To derive a precise mathematical expression of the uncertainty principle, consider three Hermitian operators A, B, and C that satisfy the relation

$$[A,B] \equiv AB - BA = iC. \tag{14.18}$$

Let  $|a\rangle = (A - \overline{A})|s\rangle$ ,  $|b\rangle = (B - \overline{B})|s\rangle$ . We have

$$\begin{aligned} \langle a|a\rangle &= \langle s|(A-A)^2|s\rangle = (\Delta A)^2, \\ \langle b|b\rangle &= \langle s|(B-\overline{B})^2|s\rangle = (\Delta B)^2, \\ \langle a|b\rangle &= \langle s|(A-\overline{A})(B-\overline{B})|s\rangle. \end{aligned}$$
(14.19)

#### 14.3. Eigenvalues of the Angular Momentum

By the Cauchy-Schwartz inequality, we have

$$(\Delta A)^2 (\Delta B)^2 \ge |\langle s|(A - \overline{A})(B - \overline{B})|s\rangle|^2.$$
(14.20)

We may rewrite  $(A - \overline{A})(B - \overline{B})$  as

$$(A - \overline{A})(B - \overline{B}) = \frac{1}{2}[(A - \overline{A})(B - \overline{B}) + (B - \overline{B})(A - \overline{A})] + \frac{i}{2}C$$
$$\equiv F + \frac{i}{2}C.$$
(14.21)

Since both F and C are Hermitian,  $\langle s|F|s\rangle$  and  $\langle s|C|s\rangle$  are real numbers. This means

$$(\Delta A)^2 (\Delta B)^2 \ge \overline{F}^2 + \frac{1}{4}\overline{C}^2 \ge \frac{1}{4}\overline{C}^2.$$
(14.22)

Namely

$$(\Delta A)(\Delta B) \ge \frac{1}{2}\overline{C}.$$
(14.23)

# 14.3 Eigenvalues of the Angular Momentum

The commutator between operators A and B is defined by AB - BA and denoted by [A, B]. Some commonly used rules for commutators are:

$$[A, B + C] = [A, B] + [A, C], \qquad (14.24)$$

$$[A + B, C] = [A, C] + [B, C],$$
(14.25)

$$[A, BC] = [A, B]C + B[A, C], (14.26)$$

$$[AB, C] = A[B, C] + [A, C]B, \qquad (14.27)$$

$$[A, [B, C]] + [B, [C, A]] + [C, [A, B]] = 0.$$
(14.28)

From the following relation,

$$\mathbf{p} = -i\hbar\nabla,\tag{14.29}$$

we have

$$[p_i, r_j] = -i\hbar\delta_{ij},\tag{14.30}$$

$$[p_i, p_j] = 0, (14.31)$$

$$[r_i, r_j] = 0, \tag{14.32}$$

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where  $\mathbf{p} = (p_1, p_2, p_3)$  and  $\mathbf{r} = (r_1, r_2, r_3)$ .

The angular momentum operator is defined by

$$\mathbf{L} = (yp_z - zp_y, zp_x - xp_z, xp_y - yp_x).$$

From the definition we have

$$[L_x, y] = [yp_z - zp_y, y] = -z[p_y, y] = i\hbar z.$$
(14.33)

$$[L_x, p_y] = [yp_z - zp_y, p_y] = [y, p_y]p_z = i\hbar p_z.$$
(14.34)

$$[L_x, x] = 0. (14.35)$$

$$[L_x, p_x] = 0. (14.36)$$

From these commutation relations we can derive the commutation relations between components of  $\mathbf{L}$ .

$$[L_x, L_y] = [L_x, zp_x - xp_z] = [L_x, z]p_x - x[L_x, p_z]$$
  
=  $-i\hbar yp_x + i\hbar xp_y = i\hbar L_z,$  (14.37)

and similarly

$$[L_y, L_z] = i\hbar L_x,\tag{14.38}$$

$$[L_z, L_x] = i\hbar L_y. \tag{14.39}$$

Let us define

$$L_{+} = L_{x} + iL_{y}, \tag{14.40}$$

$$L_{-} = L_{x} - iL_{y}, (14.41)$$

$$L^2 = L_x^2 + L_y^2 + L_z^2. (14.42)$$

These operators satisfy the following commutation relations:

$$[L_z, L_+] = \hbar L_+, \tag{14.43}$$

$$[L_{-}, L_{z}] = \hbar L_{-}, \tag{14.44}$$

$$[L_+, L_-] = 2\hbar L_z, \tag{14.45}$$

$$[L^2, \mathbf{L}] = 0. \tag{14.46}$$

Let us denote the eigenvalues of  $L^2$  by  $\lambda \hbar^2$  and the eigenvalues of  $L_z$  by  $m\hbar$ . Because  $L^2$  and **L** commute, they have a common set of eigenvectors  $|\lambda m\rangle$ . Namely

$$L_z |\lambda m\rangle = m\hbar |\lambda m\rangle, \tag{14.47}$$

$$L^2 |\lambda m\rangle = \lambda \hbar^2 |\lambda m\rangle. \tag{14.48}$$

The fact  $\langle \lambda m | L_x^2 + L_y^2 | \lambda m \rangle \ge 0$  implies

$$\lambda \ge m^2. \tag{14.49}$$

Multiplying Eq. (14.47) by  $L_+$  and  $L_-$  and using Eqs. (14.43) and (14.44), we have

$$L_z L_+ |\lambda m\rangle = (m+1)\hbar L_+ |\lambda m\rangle, \qquad (14.50)$$

$$L_z L_- |\lambda m\rangle = (m-1)\hbar L_- |\lambda m\rangle. \tag{14.51}$$

From Eq. (14.48) we have

$$L^{2}L_{+}|\lambda m\rangle = \lambda \hbar^{2}L_{+}|\lambda m\rangle, \qquad (14.52)$$

$$L^{2}L_{+}|\lambda m\rangle = \lambda \hbar^{2}L_{+}|\lambda m\rangle, \qquad (14.52)$$

$$L^{2}L_{-}|\lambda m\rangle = \lambda \hbar^{2}L_{-}|\lambda m\rangle.$$
(14.53)

These four equations show that if  $|\lambda m\rangle$  is an eigenvector of  $L^2$  and  $L_z$  with eigenvalues  $\lambda \hbar^2$  and  $m\hbar$  respectively, then  $L_{\pm}|\lambda m\rangle$  is also an eigenvector of  $L^2$  and  $L_z$  with eigenvalues  $\lambda \hbar^2$  and  $(m \pm 1)\hbar$  respectively. Therefore we have

$$L_+|\lambda m\rangle \propto |\lambda m+1\rangle,$$
 (14.54)

$$L_{-}|\lambda m\rangle \propto |\lambda m - 1\rangle.$$
 (14.55)

Because m can never be larger than  $\sqrt{\lambda}$  or smaller than  $-\sqrt{\lambda}$ , we may denote l the maximum value of m. Then we must have

$$L_{+}|\lambda l\rangle = 0, \tag{14.56}$$

otherwise  $L_{+}|\lambda l\rangle$  will be an eigenvector of  $L_{z}$  with a larger eigenvalue than  $l\hbar$ . This will lead to a contradiction. Multiplying by  $L_{-}$ , we have

$$L_{-}L_{+}|\lambda l\rangle = (L^{2} - L_{z}^{2} - \hbar L_{z})|\lambda l\rangle = (\lambda - l^{2} - l)\hbar|\lambda l\rangle = 0.$$
(14.57)

This gives

$$\lambda = l(l+1). \tag{14.58}$$

Similarly, if l' is the minimum value of m, we have

$$L_{-}|\lambda l'\rangle = 0, \tag{14.59}$$

and

$$L_{+}L_{-}|\lambda l\rangle = (L^{2} - L_{z}^{2} + \hbar L_{z})|\lambda l\rangle = (\lambda - l'^{2} + l')\hbar|\lambda l\rangle = 0.$$
(14.60)

This gives

$$\lambda = l'(l' - 1). \tag{14.61}$$

Comparing with Eq. (14.58), we have l' = -l. Because we may start with a state represented by  $|\lambda l\rangle$  and after multiplying it by  $L_{-}$  a number of times to obtain a state represented by  $|\lambda l'\rangle$ , l - l' must be an integer. This leads to the conclusion that l must be a half-integer or an integer.

Now we may summarize the result. The eigenvectors of  $L^2$  and  $L_z$  can be labeled by l and m, where both of them are either integers or half-integers and  $|m| \leq |l|$ , such that

$$L^2|lm\rangle = l(l+1)\hbar^2|lm\rangle, \qquad (14.62)$$

$$L_z |lm\rangle = m\hbar |lm\rangle. \tag{14.63}$$

## 14.4 Operator Algebra of the Harmonic Oscillator

The Hamiltonian function of a simple harmonic oscillator is

$$H = \frac{p^2}{2m} + \frac{m\omega^2 q^2}{2},$$
 (14.64)

where p is the momentum and q is the coordinate. Define the annihilation operator a and the creation operator  $a^{\dagger}$  by

$$a \equiv \sqrt{\frac{m\omega}{2\hbar}} \left( q + i \frac{p}{m\omega} \right), \qquad a^{\dagger} \equiv \sqrt{\frac{m\omega}{2\hbar}} \left( q - i \frac{p}{m\omega} \right),$$
(14.65)

then

$$aa^{\dagger} - a^{\dagger}a = 1, \tag{14.66}$$

and

$$H = \hbar\omega \left( a^{\dagger}a + \frac{1}{2} \right). \tag{14.67}$$

Let us label the eigenvalues of the operator  $a^{\dagger}a$  by  $\lambda_n$ , and the corresponding eigenvector by  $|n\rangle$ , that is

$$a^{\dagger}a|n\rangle = \lambda_n|n\rangle. \tag{14.68}$$

Since  $\langle n|a^{\dagger}a|n\rangle$  is the norm of  $a|n\rangle$ , it follows  $\lambda_n \geq 0$ . If  $|n\rangle$  is an eigenvector of  $a^{\dagger}a$ , then  $a|n\rangle$  and  $a^{\dagger}|n\rangle$  are also eigenvectors, as can be seen from the following equations.

$$(a^{\dagger}a) a|n\rangle = (aa^{\dagger} - 1) a|n\rangle = (\lambda_n - 1) a|n\rangle, \qquad (14.69)$$

#### 14.4. Operator Algebra of the Harmonic Oscillator

and similarly,

$$(a^{\dagger}a) a^{\dagger}|n\rangle = (\lambda_n + 1) a^{\dagger}|n\rangle.$$
(14.70)

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By applying a successively, new eigenvectors with smaller and smaller eigenvalues can be derived. However, since the eigenvalues can not be smaller than zero, this process must stop at some eigenvector which has the lowest possible eigenvalue. This particular eigenvector is called the ground state  $|0\rangle$ . Since there can be no eigenvector with smaller eigenvalue,  $a|0\rangle$  must not be another eigenvector. The only choice is then  $a|0\rangle = 0$  and thus  $\lambda_0 = 0$ . It follows from Eq. (14.70) that  $\lambda_n = n$ , and the eigenvalues of the Hamiltonian are  $E_n = \hbar \omega (n + 1/2)$ .

In the Schrödinger representation,

$$i\hbar \frac{d}{dt}|n\rangle = H|n\rangle = \hbar\omega\left(n + \frac{1}{2}\right)|n\rangle.$$
 (14.71)

The solution is

$$|n\rangle = e^{-i\omega(n+1/2)t}|n\rangle_0, \qquad (14.72)$$

where  $|n\rangle_0$  is the *n*th state at time t = 0. In the Heisenberg representation,

$$i\hbar \frac{da}{dt} = [a, H] = \left[a, \hbar\omega \left(a^{\dagger}a + \frac{1}{2}\right)\right] = \hbar\omega a.$$
 (14.73)

The solution is

$$a = a(0)e^{-i\omega t},$$
 (14.74)

and similarly

$$a^{\dagger} = a^{\dagger}(0)e^{i\omega t}.$$
 (14.75)

We have shown  $a^{\dagger}a|n\rangle = n|n\rangle$ ,  $a|n\rangle = c_d|n-1\rangle$ , and  $a^{\dagger}|n\rangle = c_u|n+1\rangle$ . The constants  $c_d$  and  $c_u$  can be determined by the following equations:

$$\langle n|a^{\dagger}a|n\rangle = \langle n|n|n\rangle = n,$$
 (14.76)

$$\langle n|a^{\dagger}a|n\rangle = \langle n-1|c_d^*c_d|n-1\rangle = |c_d|^2, \qquad (14.77)$$

hence  $|c_d| = \sqrt{n}$ .

$$\langle n|aa^{\dagger}|n\rangle = \langle n|a^{\dagger}a+1|n\rangle = n+1, \qquad (14.78)$$

$$\langle n|aa^{\dagger}|n\rangle = \langle n+1|c_u^*c_u|n+1\rangle = |c_u|^2, \qquad (14.79)$$

hence  $|c_u| = \sqrt{n+1}$ . From Eqs. (14.74) and (14.75),  $c_d = |c_d|e^{-i(\omega t - \phi)}$  and  $c_u = |c_u|e^{i(\omega t - \phi)}$ , where  $\phi$  is a constant phase. The relative phase between  $|n\rangle$  and  $|n+1\rangle$  can be chosen to be 0, then at t = 0

$$a|n\rangle = \sqrt{n}|n-1\rangle, \qquad a^{\dagger}|n\rangle = \sqrt{n+1}|n+1\rangle.$$
 (14.80)

The wavefunction of the ground state can be determined by  $a|0\rangle = 0$ . Change variable to

$$\xi = \sqrt{\frac{m\omega}{\hbar}}q,\tag{14.81}$$

 $a|0\rangle = 0$  becomes

$$\left(\frac{\partial}{\partial\xi} + \xi\right)\psi_0(\xi) = 0. \tag{14.82}$$

The solution is

$$\psi_0(\xi) = e^{-\xi^2/2}.\tag{14.83}$$

From the ground-state wavefunction we can construct the wavefunction of the first excited state by using the relation  $a^{\dagger}|0\rangle = |1\rangle$ .

$$\psi_1(\xi) = \left(-\frac{\partial}{\partial\xi} + \xi\right) e^{-\xi^2/2} = 2\xi e^{-\xi^2/2}.$$
 (14.84)

We may continue this process to obtain the wavefunction of the *n*th state by using the relation  $a^{\dagger}|n\rangle = \sqrt{n+1}|n+1\rangle$ .

## 14.5 Quantization of Mechanical Waves

One of the simplest phenomena in systems of many degrees of freedom is mechanical waves. To illustrate how to quantize a mechanical wave, we now consider a thin string of uniform mass and tension distribution. Both ends of the string are fixed, and the length of the string is L. Let us model the string by a sequence of massive beads linked by ideal springs, and denote the displacement of the *m*th bead from its equilibrium position  $u_m(t)$ . Assume each bead-spring unit occupies a length *a* in space. The mass of the bead can be written as  $\rho a$ , where  $\rho$  is the mass density. Similarly, the spring constant can be written as  $\tau/a$ , where  $\tau$  is the tension of the string. The Hamiltonian function is just the sum of the kinetic energy of the beads and the potential energy of the springs.

$$H = \frac{\rho}{2} \sum_{m=1}^{N} a \left(\frac{du_m}{dt}\right)^2 + \frac{\tau}{2} \sum_{m=1}^{N} a \left(\frac{u_{m+1} - u_m}{a}\right)^2.$$
(14.85)

Now let  $a \to 0$  while keeping  $\rho$  and  $\tau$  constant, we obtain

$$H = \int_{L} \frac{\rho}{2} \left(\frac{\partial u}{\partial t}\right)^{2} + \frac{\tau}{2} \left(\frac{\partial u}{\partial x}\right)^{2} dx, \qquad (14.86)$$

where we have replaced  $u_m(t)$  by u(x,t), the displacement of the string at x. To reduce the Hamiltonian to a much simpler form, we first decompose u(x,t) into Fourier components.

$$u(x,t) = \sqrt{\frac{2}{\rho L}} \sum_{m} q_m(t) \sin(k_m x),$$
 (14.87)

where  $k_m = n\pi/L$ . Then we substitute Eq. (14.87) into Eq. (14.86). The result is

$$H = \frac{1}{2} \sum_{m} \left( \dot{q}_m^2 + \omega_m^2 q_m^2 \right),$$
 (14.88)

where  $\omega_m \equiv k_m \sqrt{\tau/\rho}$ . We see that the Hamiltonian has the same form as a group of independent simple harmonic oscillators, and  $q_i$ ,  $p_j \equiv \dot{q}_j$ , are canonical variables. Set

$$a_m \equiv \sqrt{\frac{\omega_m}{2\hbar}} \left( q_m + i \frac{p_m}{\omega_m} \right), \qquad a_m^{\dagger} \equiv \sqrt{\frac{\omega_m}{2\hbar}} \left( q_m - i \frac{p_m}{\omega_m} \right), \tag{14.89}$$

the Hamiltonian function can be written as

$$H = \sum_{m} \hbar \omega_m \left( a_m^{\dagger} a_m + \frac{1}{2} \right), \qquad (14.90)$$

where the physical meaning of  $a_m$  is the complex amplitude of the *m*th wave component.

#### 14.6 Quantization of Electromagnetic Waves

The quantization of electromagnetic waves is similar to that of mechanical waves. Consider a region of volume V which contains no charge or

electric current. The electromagnetic fields can be expressed as superpositions of orthonormal spatial modes. Let us denote  $\mathbf{E}_m(\mathbf{r}) \exp(-i\omega_m t)$ ,  $\mathbf{B}_m(\mathbf{r}) \exp(-i\omega_m t)$  the fields of the *m*th spatial mode, where the complex functions  $\mathbf{E}_m(\mathbf{r})$  satisfies the orthonormal condition.

$$\int \mathbf{E}_m^*(\mathbf{r}) \cdot \mathbf{E}_n(\mathbf{r}) \, d^3 r = \delta_{mn}. \tag{14.91}$$

From the Maxwell equations

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t},\tag{14.92}$$

$$\nabla \times \mathbf{B} = \frac{1}{c^2} \frac{\partial \mathbf{E}}{\partial t},\tag{14.93}$$

one has

$$\nabla \times \mathbf{E}_m = i\omega_m \mathbf{B}_m,\tag{14.94}$$

$$\nabla \times \mathbf{B}_m = -\frac{\imath \omega_m}{c^2} \mathbf{E}_m. \tag{14.95}$$

From Eq. (14.95) we have

$$\int (\nabla \times \mathbf{B}_m^*) \cdot (\nabla \times \mathbf{B}_n) \, d^3 \mathbf{r} = \frac{\omega_m^2}{c^4} \int \mathbf{E}_m^*(\mathbf{r}) \cdot \mathbf{E}_n(\mathbf{r}) \, d^3 \mathbf{r} = \frac{\omega_m^2}{c^4} \delta_{mn}.$$
(14.96)

Because

$$\int (\nabla \times \mathbf{B}_{m}^{*}) \cdot (\nabla \times \mathbf{B}_{n}) d^{3}\mathbf{r}$$

$$= -\int \mathbf{B}_{m}^{*} \cdot (\nabla \times \nabla \times \mathbf{B}_{n}) d^{3}\mathbf{r}$$

$$= \int \mathbf{B}_{m}^{*} \cdot (\nabla^{2}\mathbf{B}_{n}) d^{3}\mathbf{r}$$

$$= \frac{\omega_{m}^{2}}{c^{2}} \int \mathbf{B}_{m}^{*}(\mathbf{r}) \cdot \mathbf{B}_{n}(\mathbf{r}) d^{3}\mathbf{r}, \qquad (14.97)$$

we have

$$\int \mathbf{B}_m^*(\mathbf{r}) \cdot \mathbf{B}_n(\mathbf{r}) \, d^3 \mathbf{r} = \frac{\delta_{mn}}{c^2}.$$
(14.98)

Let us expand an arbitrary electromagnetic field as

$$\mathbf{E}(\mathbf{r},t) = \frac{1}{2} \sum_{m} \left[ v_m(t) \mathbf{E}_m(\mathbf{r}) + v_m^*(t) \mathbf{E}_m^*(\mathbf{r}) \right], \qquad (14.99)$$

$$\mathbf{B}(\mathbf{r},t) = \frac{1}{2} \sum_{m} \left[ u_m(t) \mathbf{B}_m(\mathbf{r}) + u_m^*(t) \mathbf{B}_m^*(\mathbf{r}) \right], \qquad (14.100)$$
where  $v_m(t)$  and  $u_m(t)$  are complex functions. From Eqs. (14.92)–(14.95), we have

$$\dot{u}_m(t) = -i\omega_m v_m(t),$$
 (14.101)

$$\dot{v}_m(t) = -i\omega_m u_m(t). \tag{14.102}$$

Thus

$$u_m(t) = v_m(t) = c_m e^{-i\omega t},$$
 (14.103)

where  $c_m$  is an integration constant.

Let us define

$$a_m(t) = \sqrt{\frac{\epsilon_0}{2\hbar\omega_m}} u_m(t) \tag{14.104}$$

and substitute Eqs. (14.99) and (14.100) into the Hamiltonian function

$$H = \int_{V} \frac{\epsilon_0 \mathbf{E} \cdot \mathbf{E}}{2} + \frac{\mathbf{B} \cdot \mathbf{B}}{2\mu_0} d^3 r.$$
(14.105)

Averaging over time we obtain

$$H = \sum_{m} \hbar \omega_m a_m^* a_m. \tag{14.106}$$

Let

$$q_m = \sqrt{\frac{\hbar}{2\omega_m}} (a_m + a_m^*), \qquad p_m = -i\sqrt{\frac{\hbar\omega_m}{2}} (a_m - a_m^*), \qquad (14.107)$$

we have

$$p_m(t) = \dot{q}_m(t),$$
 (14.108)

$$\dot{p}_m(t) = -\omega^2 q_m(t),$$
 (14.109)

and the time averaged Hamiltonian function becomes

$$H = \frac{1}{2} \sum_{m} \left( p_m^2 + \omega_m^2 q_m^2 \right).$$
 (14.110)

The equation of motion and the Hamiltonian function have the same form as a group of independent simple harmonic oscillators, and the amplitude of each mode corresponds to an independent simple harmonic oscillator, just like mechanical waves. Therefore we may quantize the system the same way as quantizing harmonic oscillators. After quantization,  $p_m$  and  $q_m$  becomes operators with the commutation relation

$$[q_m, p_m] = -i\hbar. (14.111)$$

Correspondingly, we should change notation from  $a_m^*$  to  $a_m^{\dagger}$  so that it properly represents an operator. In terms of the two operators  $a_m$  and  $a_m^{\dagger}$ , after quantization the Hamiltonian function becomes

$$H = \sum_{m} \hbar \omega_m \left( a_m^{\dagger} a_m + \frac{1}{2} \right), \qquad (14.112)$$

where the extra 1/2 comes from the commutator  $[a_m, a_m^{\dagger}] = 1$ .

Now we can quantize Eqs. (14.99) and (14.100) by replacing  $v_m(t)$  and  $u_m(t)$  with  $a_m$  and  $a_m^{\dagger}$ .

$$\hat{\mathbf{E}}(\mathbf{r},t) = \sum_{m} \sqrt{\frac{\hbar\omega_m}{2\epsilon_0}} \left[ a_m \mathbf{E}_m(\mathbf{r}) + a_m^{\dagger} \mathbf{E}_m^*(\mathbf{r}) \right], \qquad (14.113)$$

$$\hat{\mathbf{B}}(\mathbf{r},t) = \sum_{m} \sqrt{\frac{\hbar\omega_m}{2\epsilon_0}} \left[ a_m \mathbf{B}_m(\mathbf{r}) + a_m^{\dagger} \mathbf{B}_m^*(\mathbf{r}) \right].$$
(14.114)

After this quantization procedure,  $\mathbf{E}(\mathbf{r}, t)$  and  $\mathbf{B}(\mathbf{r}, t)$  are no longer classical variables. They become operators since they are linear combinations of  $a_m$  and  $a_m^{\dagger}$ . The mode functions  $\mathbf{E}_m(\mathbf{r})$  and  $\mathbf{B}_m(\mathbf{r})$  play the role of the linear-combination coefficients. To distinguish from the classical fields, we write them as  $\hat{\mathbf{E}}(\mathbf{r}, t)$  and  $\hat{\mathbf{B}}(\mathbf{r}, t)$  in Eqs. (14.113) and (14.114).

#### 14.7 Coherent States

Since  $\langle n|a|n\rangle = \langle n|a^{\dagger}|n\rangle = 0$ , the expectation values of the field operators in a pure *n*-photon state  $|n\rangle$  are always zero. Hence pure *n*-photon states are not states which correspond to classical electromagnetic waves. It is nature to ask which states give nonzero expectation values of the field operators. A good guess is the eigenstate of *a*. If  $|\alpha_m\rangle$  is an eigenstate of  $a_m$ , Eqs. (14.113) and (14.114) imply

$$\langle \alpha_m | \hat{\mathbf{E}} | \alpha_m \rangle = \sum_m \sqrt{\frac{\hbar \omega_m}{2\epsilon_0}} \left[ \langle \alpha_m | a_m | \alpha_m \rangle \mathbf{E}_m(\mathbf{r}) + \langle \alpha_m | a_m^{\dagger} | \alpha_m \rangle \mathbf{E}_m^*(\mathbf{r}) \right]$$

$$= \sum_m \sqrt{\frac{\hbar \omega_m}{2\epsilon_0}} \left[ \alpha_m \mathbf{E}_m(\mathbf{r}) + \alpha_m^* \mathbf{E}_m^*(\mathbf{r}) \right],$$
(14.115)

#### 14.7. Coherent States

$$\langle \alpha_m | \hat{\mathbf{B}} | \alpha_m \rangle = \sum_m \sqrt{\frac{\hbar \omega_m}{2\epsilon_0}} \left[ \langle \alpha_m | a_m | \alpha_m \rangle \mathbf{B}_m(\mathbf{r}) + \langle \alpha_m | a_m^{\dagger} | \alpha_m \rangle \mathbf{B}_m^*(\mathbf{r}) \right]$$

$$= \sum_m \sqrt{\frac{\hbar \omega_m}{2\epsilon_0}} \left[ \alpha_m \mathbf{B}_m(\mathbf{r}) + \alpha_m^* \mathbf{B}_m^*(\mathbf{r}) \right].$$
(14.116)

The expectation value is indeed the classical mode expansion. Eqs. (14.115) and (14.116) show that coherent states provide the connection between classical and quantum mechanical descriptions of electromagnetic fields.

Similarly, for a simple harmonic oscillator in a coherent state the expectation values of p and q follow their classical trajectory.

$$\langle \alpha | p | \alpha \rangle = -i \sqrt{\frac{\hbar m \omega}{2}} \langle \alpha | a - a^{\dagger} | \alpha \rangle = -\sqrt{2\hbar m \omega} |\alpha| \sin(\omega t + \phi),$$
 (14.117)

$$\langle \alpha | q | \alpha \rangle = \sqrt{\frac{\hbar}{2m\omega}} \langle \alpha | a + a^{\dagger} | \alpha \rangle = \sqrt{\frac{2\hbar}{m\omega}} |\alpha| \cos(\omega t + \phi),$$
 (14.118)

where  $\phi = \arg(\alpha)$ . Again it is seen the coherent state provides the connection between classical and quantum mechanical descriptions.

To find what  $|\alpha\rangle$  is, we expand  $|\alpha\rangle$  in a series of  $|n\rangle$ ,

$$|\alpha\rangle = \sum_{n} c_n |n\rangle. \tag{14.119}$$

At t = 0,

$$\alpha |\alpha\rangle = a |\alpha\rangle = \sum_{n} c_n \sqrt{n} |n-1\rangle.$$
 (14.120)

On the other hand,

$$\alpha |\alpha\rangle = \sum_{n} \alpha c_{n} |n\rangle = \sum_{n} \alpha c_{n-1} |n-1\rangle.$$
(14.121)

Comparing the two equations, one obtains  $c_n = (\alpha/\sqrt{n})c_{n-1}$ . By induction,  $c_n = (\alpha^n/\sqrt{n!})c_0$ . Now all the expansion coefficients have been determined except  $c_0$ , which can be fixed by the normalization condition  $\langle \alpha | \alpha \rangle = |c_0|^2 \exp(|\alpha|^2) = 1$ . Hence

$$|\alpha\rangle = \exp\left(-\frac{1}{2}|\alpha|^2\right)\sum_n \frac{\alpha^n}{\sqrt{n!}}|n\rangle.$$
(14.122)

The state  $|\alpha\rangle$  is called the coherent state.

For a coherent state, the probability of finding n quanta in the harmonic oscillator is

$$P(n) = \frac{|\alpha|^{2n} e^{-|\alpha|^2}}{n!}.$$
(14.123)

This is the well-known Poisson distribution. The average number of quanta is  $\overline{n} = |\alpha|^2$ , and the standard deviation is  $\Delta n = |\alpha|$ . For a classical state  $|\alpha| \gg 1$ , we have

$$\frac{\Delta n}{\overline{n}} \ll 1. \tag{14.124}$$

This means the peak of P(n) centered at  $\overline{n}$  becomes increasingly sharp as  $\overline{n}$  increases. However, this does not mean the state  $|\alpha\rangle$  approaches the eigenstate  $|\overline{n}\rangle$ . No matter how large  $\overline{n}$  is,  $\langle \overline{n}|p|\overline{n}\rangle = \langle \overline{n}|q|\overline{n}\rangle = 0$ , whereas  $\langle \alpha|p|\alpha\rangle$  and  $\langle \alpha|p|\alpha\rangle$  follow Eqs. (14.117) and (14.118).

### 14.8 Quantum Fluctuation of Electromagnetic Waves

The fractional uncertainty of the electric field for a coherent state is defined by

$$\frac{\Delta E}{E} = \sqrt{\frac{\left|\langle \alpha | \hat{\mathbf{E}} \cdot \hat{\mathbf{E}} | \alpha \rangle \right| - \left|\langle \alpha | \hat{\mathbf{E}} | \alpha \rangle \right|^2}{\left|\langle \alpha | \hat{\mathbf{E}} | \alpha \rangle\right|^2}},\tag{14.125}$$

According to Eqs. (14.113), (14.115), if we define

$$\mathbf{C}_m(\mathbf{r}) = \sqrt{\frac{\hbar\omega_m}{2\epsilon_0}} \mathbf{E}_m(\mathbf{r}),$$

for a single mode we have

$$\hat{\mathbf{E}} = a_m \mathbf{C}_m + a_m^{\dagger} \mathbf{C}^*,$$

$$\begin{split} |\langle \alpha | \hat{\mathbf{E}} | \alpha \rangle|^2 &= \alpha^2 \mathbf{C}_m \cdot \mathbf{C}_m + 2 |\mathbf{C}_m|^2 \alpha|^2 + \alpha^{*2} \mathbf{C}_m^* \cdot \mathbf{C}_m^*, \\ \hat{\mathbf{E}} \cdot \hat{\mathbf{E}} &= a_m^2 \mathbf{C}_m \cdot \mathbf{C}_m + a_m^{\dagger 2} \mathbf{C}_m^* \cdot \mathbf{C}_m^* + a_m a_m^{\dagger} \mathbf{C}_m \cdot \mathbf{C}_m^* + a_m^{\dagger} a_m \mathbf{C}_m \cdot \mathbf{C}_m^*, \\ \langle \alpha | \hat{\mathbf{E}} \cdot \hat{\mathbf{E}} | \alpha \rangle &= \alpha^2 \mathbf{C}_m \cdot \mathbf{C}_m + \alpha^{*2} \mathbf{C}_m^* \cdot \mathbf{C}_m^* + |\mathbf{C}_m|^2 (1+2|\alpha|^2). \end{split}$$

After time averaging, we obtain

$$\left| \langle \alpha | \hat{\mathbf{E}} | \alpha \rangle \right|^2 = 2 \left| \mathbf{C}_m \right|^2 \left| \alpha \right|^2,$$

 $\left| \langle \alpha | \hat{\mathbf{E}} \cdot \hat{\mathbf{E}} | \alpha \rangle \right| = |\mathbf{C}_m|^2 \left( 1 + 2 |\alpha|^2 \right).$ 

Therefore

$$\left| \langle \alpha | \hat{\mathbf{E}} \cdot \hat{\mathbf{E}} | \alpha \rangle \right| - \left| \langle \alpha | \hat{\mathbf{E}} | \alpha \rangle \right|^2 = |\mathbf{C}_m|^2 \,,$$

and

$$\frac{\Delta E}{E} = \frac{1}{\sqrt{2}\left|\alpha\right|}.\tag{14.126}$$

For the single-mode plane wave, we have

$$\mathbf{E}_m(\mathbf{r}) = \frac{e^{i\mathbf{k}_m \cdot \mathbf{r}}}{\sqrt{V}}.$$
(14.127)

The energy of the field is

$$\mathcal{E} = \epsilon_0 \int_V \left| \langle \alpha | \hat{\mathbf{E}} | \alpha \rangle \right|^2 d^3 \mathbf{r}$$
  

$$= \epsilon_0 \int_V 2 |\mathbf{C}_m|^2 |\alpha|^2 d^3 \mathbf{r}$$
  

$$= \epsilon_0 \int_V \hbar \omega_m |\alpha|^2 \mathbf{E}_m^*(\mathbf{r}) \cdot \mathbf{E}_m(\mathbf{r}) d^3 \mathbf{r}$$
  

$$= \hbar \omega_m |\alpha|^2. \qquad (14.128)$$

Hence

$$\frac{\Delta E}{E} = \sqrt{\frac{\hbar\omega}{2\mathcal{E}}} = \frac{1}{\sqrt{2n}},\tag{14.129}$$

where  $n = \hbar \omega / \mathcal{E}$  is number of photons in V.

Let us calculate the quantum fluctuation in the electromagnetic wave radiated by an FM radio station. Assume the frequency is 100 MHz, the total radiating power of the station is 10 kW, and we measure the field at a distance of 10 km from the station. For dipole radiation in the direction perpendicular to the dipole, the energy density  $\rho$  of the wave is

$$\rho = \frac{\text{power}}{\frac{4\pi}{3}r^2c} = \frac{3 \times 10^5}{4\pi \times 10^8 \times 3 \times 10^8} \text{ Jm}^{-3}.$$

We are interested in the noise integrated over a duration of 0.1 ms, which corresponds to the upper portion of the music spectrum. Assuming the cross section of the antenna is  $(\lambda/2)^2$ , the volume of integration is

$$V = \left(\frac{\lambda}{2}\right)^2 \times 0.0001 \times 3 \times 10^8 = (1.5)^2 \times 0.0001 \times 3 \times 10^8 \text{ m}^3.$$

The number of photons in this volume is

$$n = 8.1 \times 10^{16},$$

and

$$\frac{\Delta E}{E} = 2.5 \times 10^{-9}$$

This is much smaller than the thermal noise and the shot noise of electrons in the amplifier. Therefore we do not need to worry the quantum fluctuation when we listen to the FM broadcasting.

As a comparison, let us also calculate  $\Delta E/E$  for a pixel on a CCD camera irradiated by a 100-W light bulb at a distance of 1 km. Assume the wavelength is 600 nm and the efficiency of the light bulb is 15%. The area of the pixel is 10  $\mu$ m×10  $\mu$ m, and the integration time is 1 ms. The energy density is

$$\rho = \frac{\text{power}}{4\pi r^2 c} = \frac{15}{4\pi \times 10^6 \times 3 \times 10^8} \text{ Jm}^{-3}.$$

The volume of integration is  $10^{-10} \times 0.001 \times 3 \times 10^8$  m<sup>3</sup>. The photon number is

n = 0.36,

and

$$\frac{\Delta E}{E} = 1.2.$$

This presents a significant quantum noise on the CCD pixel. In reality, in front of the CCD sensor there is a focusing lens. Assume the aperture of the lens is  $1 \text{ cm}^2$ . The number of photons becomes  $3.6 \times 10^5$ , and  $\Delta E/E$  becomes  $1.2 \times 10^{-3}$ .

#### 14.9 Exercises

**Exercise 14.1.** In quantum mechanics, if the expectation value of some Hermitian operator  $\hat{O}$  is independent of time, we say  $\hat{O}$  is a conserved physical quantity. From the Schrödinger equation

$$i\hbar \frac{\partial \psi(\mathbf{r},t)}{\partial t} = H\psi(\mathbf{r},t),$$

we have

$$\frac{d}{dt}\int\psi^*(\mathbf{r},t)\hat{O}\psi(\mathbf{r},t)\,d^3\mathbf{r} = \frac{1}{i\hbar}\int\psi^*(\mathbf{r},t)[\hat{O}\hat{H}-\hat{H}\hat{O}]\psi(\mathbf{r},t)\,d^3\mathbf{r}$$

#### 14.9. EXERCISES

for any state  $\psi(\mathbf{r}, t)$ . Therefore the necessary and sufficient condition for  $\hat{O}$  to be a conserved quantity is  $\hat{O}\hat{H} - \hat{H}\hat{O} = 0$ . If the Hamiltonian function has the following form

$$H = \frac{p^2}{2m} + V(r),$$

namely the potential function V(r) is only a function of r, not  $\theta$  or  $\phi$ , we know in classical mechanics the angular momentum **L** is conserved, because

$$\frac{d\mathbf{L}}{dt} = \frac{d}{dt}(\mathbf{r} \times \mathbf{p}) = \mathbf{r} \times \dot{\mathbf{p}} = \mathbf{r} \times [-\nabla V(r)] = 0.$$

In quantum mechanics, we have

$$\hat{\mathbf{L}} = \mathbf{r} \times \frac{\hbar}{i} \nabla.$$

Prove that  $\hat{\mathbf{L}}$  is a conserved quantity by showing  $\hat{\mathbf{L}}\hat{H} - \hat{H}\hat{\mathbf{L}} = 0$ .

**Exercise 14.2.** If  $\psi_n(x,t)$  is the wavefunction of the *n*th eigenstate of a quantum harmonic oscillator. Show that

$$\overline{x}(t) = \int \psi_n^*(x,t) x \psi_n(x,t) dx = 0,$$

and

$$\overline{p}(t) = \int \psi_n^*(x,t) \left( -i\hbar \frac{\partial}{\partial x} \right) \psi_n(x,t) dx = 0,$$

for every n. These results means even for large n, the expectation values of position and momentum are both zero. However, for a classical harmonic oscillator we have

$$x = a\cos(\omega t) \neq 0,$$

and

$$p = -m\omega a \sin(\omega t) \neq 0.$$

If we claim the expectation value of a physical quantity in quantum mechanics is equal to the classical value of the same quantity, how would you resolve the above discrepancy?

**Exercise 14.3.** Consider the Schrödinger equation for a two-dimensional harmonic oscillator.

$$\left[-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) + V(x,y)\right]\psi(x,y) = E\psi(x,y),$$

where

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$$V(x,y) = \frac{1}{2}k(x^2 + y^2).$$

Within all the solutions of this equation, what is the minimum-energy quantum state which is the eigenstate of  $L_z = xp_y - yp_x$  with eigenvalue equal to  $\hbar$ ? You do not need to write out the wavefunctions explicitly. You can use the Dirac notation  $|n\rangle|m\rangle$  to represent the product of wavefunctions of the *n*th state in the *x*-axis and the *m*th state in the *y*-axis.

# Appendix A

## Theory of Measurement Uncertainty

## A.1 Variance of Arithmetic Means

In any measurement, there is always uncertainty in the result. It is only a matter of degree. There are many causes of the uncertainty, such as vibration of the floor, power fluctuation of the electricity, temperature and pressure change of the surrounding, or even the quantization error of digital recording instruments. These causes are mostly uncorrelated, therefore the measurement result can be treated as random variables. The simplest way to describe a random variable x is by its expectation value E(x) and its variance V(x).

$$E(x) \equiv \alpha \equiv \int x P(x) \, dx,$$
 (A.1)

$$V(x) \equiv \sigma_x^2 \equiv E(x - \alpha)^2$$
  
=  $\int (x - \alpha)^2 P(x) dx$ ,  
=  $E(x^2) - E(x)^2$ , (A.2)

where P(x) is the probability distribution of x. The uncertainty of measurement can be reduced by taking the average of many measurements, because the deviation from the true result which can only be obtained with perfect instruments in an ideal environment tends to cancel partially for each other. It is possible to estimate how much the uncertainty is reduced. Let

 $x_1, x_2, \ldots, x_n$  be the results of n measurements and y the average result.

$$y = \frac{1}{n} \sum_{i} x_i. \tag{A.3}$$

Since the sum of random variables is also a random variable, one can ask what the expectation value and the variance of y are.

$$E(y) = \frac{1}{n} \sum_{i} E(x_i) = \alpha, \qquad (A.4)$$

$$V(y) = E(y - \alpha)^{2}$$

$$= \frac{1}{n^{2}} E\left(\sum_{i} x_{i} - n\alpha\right)^{2}$$

$$= \frac{1}{n^{2}} E\left[\sum_{i} (x_{i} - \alpha)^{2} + \sum_{i \neq j} (x_{i} - \alpha)(x_{j} - \alpha)\right]$$

$$= \frac{\sigma_{x}^{2}}{n}.$$
(A.5)

In the above equation, because  $x_i$  and  $x_j$  are independent random variables,

$$E\left[\sum_{i\neq j} (x_i - \alpha)(x_j - \alpha)\right] = \sum_{i\neq j} E(x_i - \alpha)E(x_j - \alpha) = 0.$$
(A.6)

It is seen that the average measurement result has a much smaller variance when n is large. This is how averaging works.

## A.2 Sample Variance

A subtle question is: how can one know  $\sigma_x^2$  in the first place? To determine, one needs to know P(x) precisely, which is possible only with an infinite number of measurements. However, one can still estimate  $\sigma_x^2$  from the finite (but large) number of measurement results available. Let us define the sample variance  $s_x^2$  by

$$s_x^2 \equiv \frac{1}{n} \sum_i (x_i - y)^2.$$
 (A.7)

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Note that the definition of  $s_x^2$  does not involve P(x). In fact,  $s_x^2$  itself is a random variable whose expectation value we would like to know.

$$E(ns_x^2) = \sum_i E(x_i - y)^2$$
  
=  $\sum_i E[(x_i - \alpha) - (y - \alpha)]^2$   
=  $\sum_i E[(x_i - \alpha)^2 - 2(x_i - \alpha)(y - \alpha) + (y - \alpha)^2]$   
=  $\sum_i E(x_i - \alpha)^2 - \frac{2}{n} \sum_i E[(x_i - \alpha)(x_i - \alpha)]$   
 $-\frac{2}{n} \sum_{i \neq j} E[(x_i - \alpha)(x_j - \alpha)] + \sum_i E(y - \alpha)^2.$  (A.8)

The first two terms combines to be  $(n-2)\sigma_x^2$ , the third term is zero because  $x_i$  and  $x_j$  are independent, and the last term is  $\sigma_x^2$  according to Eq. (A.5). Therefore one has

$$E(s_x^2) = \frac{n-1}{n}\sigma_x^2. \tag{A.9}$$

If we are lucky enough that the  $s_x^2$  we get from our random samples of measurement is close to  $E(s_x^2)$ , then we may replace  $E(s_x^2)$  by  $s_x^2$  in Eq. (A.9). The result is

$$V(y) = \frac{\sigma_x^2}{n} \approx \frac{s_x^2}{n-1}.$$
 (A.10)

Eq. (A.10) tells us how to plot the error bar in our presentation of measurement data.

### A.3 Central Limit Theorem

In Sec. A.1, we showed how to estimate the uncertainty of the average measurement result. One can push much further to show that the probability distribution of y is a Gaussian function regardless of the shape of P(x). This is known as the central limit theorem.

For simplicity let us change variable x to  $x - \alpha$  such that the expectation value of x is zero. Let us also define the characteristic function C(k) to be the Fourier transformation of P(x),

$$C(k) = \frac{1}{\sqrt{2\pi}} \int P(x)e^{ikx} dx.$$
 (A.11)

By Taylor expansion

$$C(k) = b_0 + b_1 k + b_2 k^2 + b_3 k^3 + \cdots,$$
 (A.12)

where

$$b_{0} = \frac{1}{\sqrt{2\pi}} \int P(x) \, dx = \frac{1}{\sqrt{2\pi}}$$
$$b_{1} = \frac{1}{\sqrt{2\pi}} \int P(x)(ix) \, dx = 0$$
$$b_{2} = \frac{1}{\sqrt{2\pi}} \int P(x) \frac{(ix)^{2}}{2} \, dx = -\frac{\sigma_{x}^{2}}{2\sqrt{2\pi}},$$
(A.13)

and in general

$$b_n = \frac{1}{\sqrt{2\pi}} \int P(x) \frac{(ix)^n}{n!} \, dx = \frac{(i)^n M_n}{n! \sqrt{2\pi}}.$$
 (A.14)

 $M_n$  is the *n*th moment of P(x). Consider the probability distribution of  $z = x_1 + x_2$ ,

$$P_2(z) = \int P(x_1)P(z - x_1)dx_1.$$
 (A.15)

By the Fourier convolution theorem, the characteristic function of  $P_2(z)$  is simply  $C_2(k) = \sqrt{2\pi}C(k)^2$ . Consider in general the probability distribution of  $z = x_1 + x_2 + \cdots + x_n$ .

$$P_{n}(z) = \int P(x_{n})P_{n-1}(z - x_{n})dx_{n}.$$
 (A.16)

Again by the Fourier convolution theorem, the characteristic function of  $P_n(z)$  is simply  $C_n(k) = \sqrt{2\pi}C(k)C_{n-1}(k)$ . Clearly, by mathematical induction,  $C_n(k) = (\sqrt{2\pi})^{n-1}C(k)^n$ . Let the probability distribution of y = z/n be  $P_y(y)$ . Because  $P_y(y)dy = P_n(z)dz$ ,  $P_y(y) = nP_n(ny)$  and the corresponding characteristic function is

$$C_n\left(\frac{k}{n}\right) = \frac{1}{\sqrt{2\pi}} \left[1 - \frac{\sigma_x^2 k^2}{2n^2} + o\left(\frac{1}{n^2}\right)\right]^n.$$
(A.17)

Since

$$\left(1 + \frac{c}{n^2}\right)^n = \exp\left[n\ln\left(1 + \frac{c}{n^2}\right)\right] = \exp\left[\frac{c}{n} + o\left(\frac{1}{n}\right)\right], \qquad (A.18)$$

$$C_n\left(\frac{k}{n}\right) = \frac{1}{\sqrt{2\pi}} \exp\left[\frac{-\sigma_x^2 k^2}{2n} + o\left(\frac{1}{n}\right)\right] \to \frac{1}{\sqrt{2\pi}} \exp\left(\frac{-\sigma_x^2 k^2}{2n}\right). \quad (A.19)$$

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By inverse Fourier transformation,

$$P_y(y) \to \sqrt{\frac{n}{2\pi}} \frac{1}{\sigma_x} \exp\left(\frac{-ny^2}{2\sigma_x^2}\right).$$
 (A.20)

Eq. (A.20) shows the probability distribution of the average measurement result is a Gaussian distribution with a variance  $\sigma_x^2/n$ . Note that we did not assume x has a Gaussian distribution. The central limit theorem tells us that for any reasonable distribution, the average result is a Gaussian distribution with a variance n-fold smaller than that of P(x).

#### A.4 Curve Fitting as an Indirect Measurement

Consider a set of measurement data  $y_i$  associated with a set of variables  $x_i$ . Each measurement is carried out by setting the variable to x, and the measured data is y. A plot of  $y_i$  with respect to  $x_i$  will show how y changes with x. By curve fitting, the set  $\{x_i, y_i\}$  can be used to construct a function that best describe the relation between y and x.

By physical arguments, one may anticipate a functional form  $y = f(x; a_i)$ where  $a_i$  is a set of parameters to be determined from the data set  $\{x_i, y_i\}$ . For example, for a pendulum one already knows the angular frequency of oscillation  $\omega$  is related to the pendulum length l by  $\omega^2 = l/q$ . A data set  $\{\omega_i, l_i\}$  will help us to determine the gravitational acceleration g. Intuitively, one may determine g for each measurement by  $g_i = l_i/\omega_i^2$ , and then take the average of  $g_i$  as the best estimate of g and the standard deviation of  $g_i$  as the best estimate of its uncertainty. But how rigorous statistically is such a procedure? In particular, because the measurements are affected by noise and fluctuation,  $\omega$  may be modelled as a random variable with a distribution function  $P(\omega|l)$  which represents the probability of  $\omega$  under the condition that the length of the pendulum is l. Can one obtain information about  $P(\omega|l)$  from the data set  $\{\omega_i, l_i\}$ ? Given  $\{\omega_i, l_i\}$ , what are the best estimates of the expectation value and the standard deviation of q? Using curve fitting to determine  $a_i$  from experimental data can be considered as an indirect measurement. Therefore, it is important to know the uncertainty of such measurements.

## A.5 Linear Regression

Consider the simplest case where  $y = \alpha + \beta x$ . If  $P(y_i|x_i)$  is modelled as

$$P(y_i|x_i) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left\{-\frac{1}{2}\left[\frac{y_i - (\alpha + \beta x_i)}{\sigma}\right]^2\right\},\tag{A.21}$$

one can find  $\alpha$ ,  $\beta$ , and  $\sigma$  by the method of maximum likelihood:

$$\frac{\partial \ln L}{\partial \alpha} = \frac{1}{\sigma^2} \sum_{i=1}^{n} [y_i - (\alpha + \beta x_i)] = 0, \qquad (A.22)$$

$$\frac{\partial \ln L}{\partial \beta} = \frac{1}{\sigma^2} \sum_{i=1}^n x_i [y_i - (\alpha + \beta x_i)] = 0, \qquad (A.23)$$

$$\frac{\partial \ln L}{\partial \sigma} = -\frac{n}{\sigma} + \frac{1}{\sigma^3} \sum_{i=1}^{n} [y_i - (\alpha + \beta x_i)]^2 = 0, \qquad (A.24)$$

where  $L = \prod_i P(y_i|x_i)$  is the total probability. The solution of these equations gives us the maximum likelihood estimates of  $\alpha$ ,  $\beta$ , and  $\sigma$ .

$$\hat{\beta} = \frac{n \sum x_i y_i - (\sum x_i)(\sum y_i)}{n \sum x_i^2 - (\sum x_i)^2},$$
(A.25)

$$\hat{\alpha} = \frac{\sum y_i - \beta \sum x_i}{n}, \qquad (A.26)$$

$$\hat{\sigma} = \sqrt{\frac{1}{n} \sum [y_i - (\hat{\alpha} + \hat{\beta} x_i)]^2}.$$
(A.27)

Define

$$S_{xx} \equiv \sum (x_i - \bar{x})^2 = \sum x_i^2 - \frac{1}{n} \left( \sum x_i \right)^2,$$
(A.28)

$$S_{yy} \equiv \sum (y_i - \bar{y})^2 = \sum y_i^2 - \frac{1}{n} \left( \sum y_i \right)^2, \qquad (A.29)$$

$$S_{xy} \equiv \sum (x_i - \bar{x})(y_i - \bar{y}) = \sum x_i y_i - \frac{1}{n} \left( \sum x_i \right) \left( \sum y_i \right), \quad (A.30)$$

we have

$$\hat{\beta} = \frac{S_{xy}}{S_{xx}},\tag{A.31}$$

$$\hat{\alpha} = \bar{y} - \hat{\beta}\bar{x}, \tag{A.32}$$

$$\hat{\sigma} = \sqrt{\frac{1}{n}} (S_{yy} - \hat{\beta} S_{xy}). \tag{A.33}$$

#### A.5. LINEAR REGRESSION

Now we have the maximum likelihood estimates of  $\alpha$  and  $\beta$ , but what are the uncertainties of them? Note that  $y_i$  are actually random variables. If we do the same measurement again, we are likely to get a different set of  $y_i$ . If we express  $\hat{\alpha}$  and  $\hat{\beta}$  in terms of  $y_i$ , we can calculate their expectation values and variances.

$$\hat{\beta} = \frac{\sum (x_i - \bar{x})(y_i - \bar{y})}{S_{xx}} = \sum \left(\frac{x_i - \bar{x}}{S_{xx}}\right) y_i, \tag{A.34}$$

$$\hat{\alpha} = \frac{\sum y_i - \hat{\beta} \sum x_i}{n} = \sum \left( \frac{S_{xx} + n\bar{x}^2 - n\bar{x}x_i}{nS_{xx}} \right) y_i.$$
(A.35)

$$E(\hat{\beta}) = \sum \left(\frac{x_i - \bar{x}}{S_{xx}}\right) E(y_i | x_i)$$
  
= 
$$\sum \left(\frac{x_i - \bar{x}}{S_{xx}}\right) (\alpha + \beta x_i)$$
  
= 
$$\beta, \qquad (A.36)$$

$$V(\hat{\beta}) = \sum \left(\frac{x_i - \bar{x}}{S_{xx}}\right)^2 V(y_i|x_i)$$
  
= 
$$\sum \left(\frac{x_i - \bar{x}}{S_{xx}}\right)^2 \sigma^2$$
  
= 
$$\frac{\sigma^2}{S_{xx}}.$$
 (A.37)

$$E(\hat{\alpha}) = \left(\frac{S_{xx} + n\bar{x}^2 - n\bar{x}x_i}{nS_{xx}}\right) E(y_i|x_i)$$
  
=  $\left(\frac{S_{xx} + n\bar{x}^2 - n\bar{x}x_i}{nS_{xx}}\right) (\alpha + \beta x_i)$   
=  $\alpha$ , (A.38)

$$V(\hat{\alpha}) = \sum \left(\frac{S_{xx} + n\bar{x}^2 - n\bar{x}x_i}{nS_{xx}}\right)^2 V(y_i|x_i)$$
  
$$= \sum \left(\frac{S_{xx} + n\bar{x}^2 - n\bar{x}x_i}{nS_{xx}}\right)^2 \sigma^2$$
  
$$= \frac{\sigma^2}{S_{xx}}.$$
 (A.39)

#### A.6 Multivalue fitting with unknown error bars

Consider the case in which  $y = \sum_{k=1}^{m} a_k X_k(x)$ , where *m* is the number of parameters to be fit,  $a_k$  are the parameters, and  $X_k(x)$  are a set of functions of *x*. By changing variables, many curve fitting problems can be reduced to this form. For example, if the model function is

$$y = a_1 \exp\left[-\left(\frac{x - a_2}{a_3}\right)^2\right],\tag{A.40}$$

one may transform it into

$$\ln y = \left(\ln a_1 - \frac{a_2^2}{a_3^2}\right) + \frac{2a_2}{a_3^2}x - \frac{1}{a_3^2}x^2.$$
(A.41)

The crucial point is to make y linear in all the fitting parameters. Let us simplify the notation  $X_k(x_i)$  to  $X_{ik}$ . The equations for maximum likelihood estimates of  $a_i$  and  $\sigma$  are:

$$\frac{\partial \ln L}{\partial a_j} = \frac{1}{\sigma^2} \sum_{i=1}^n X_{ij} \left( y_i - \sum_{k=1}^m a_k X_{ik} \right) = 0, \qquad (A.42)$$

$$\frac{\partial \ln L}{\partial \sigma} = -\frac{n}{\sigma} + \frac{1}{\sigma^3} \sum_{i=1}^n \left( y_i - \sum_{k=1}^m a_k X_{ik} \right)^2 = 0.$$
 (A.43)

In the matrix notation  $\mathbf{X} \equiv X_{ij}$ ,  $\mathbf{a} \equiv a_i$ , and  $\mathbf{y} \equiv y_i$ , the solution of Eqs. (A.42) and (A.43) can be written as

$$\hat{\mathbf{a}} = \left(\mathbf{X}^{\mathrm{T}}\mathbf{X}\right)^{-1}\mathbf{X}^{\mathrm{T}}\mathbf{y},\tag{A.44}$$

$$\hat{\sigma} = \sqrt{\frac{\mathbf{y}^{\mathrm{T}}\mathbf{y} - \hat{\mathbf{a}}^{\mathrm{T}}\mathbf{X}^{\mathrm{T}}\mathbf{y}}{n}}.$$
(A.45)

where  $\mathbf{X}^{\mathrm{T}}$  is the transpose of  $\mathbf{X}$ , and  $\hat{\mathbf{a}}, \hat{\sigma}$  are the maximum likelihood estimates of  $\mathbf{a}$  and  $\sigma$ . Let us write  $(\mathbf{X}^{\mathrm{T}}\mathbf{X})^{-1}$  as  $C_{ij}$ ,

$$\hat{a}_{j} = \sum_{k=1}^{m} C_{jk} \sum_{i=1}^{n} X_{ik} y_{i} = \sum_{i=1}^{n} \left( \sum_{k=1}^{m} C_{jk} X_{ik} \right) y_{i}.$$
(A.46)  
$$E(\hat{a}_{j}) = \left( \sum_{k=1}^{m} C_{jk} \sum_{i=1}^{n} X_{ik} \right) \sum_{l=1}^{m} X_{il} a_{l}$$
$$= \sum_{l=1}^{m} \sum_{k=1}^{m} C_{jk} \left( \sum_{i=1}^{n} X_{ik} X_{il} \right) a_{l}$$
$$= \sum_{l=1}^{m} \sum_{k=1}^{m} C_{jk} (C_{kl})^{-1} a_{l} = a_{j},$$
(A.47)

$$V(\hat{a}_{j}) = \sum_{i=1}^{n} \left( \sum_{k=1}^{m} C_{jk} X_{ik} \right) \left( \sum_{l=1}^{m} C_{jl} X_{il} \right) \sigma^{2}$$
  
$$= \sum_{l=1}^{m} \sum_{k=1}^{m} C_{jl} C_{jk} \left( \sum_{i=1}^{n} X_{ik} X_{il} \right) \sigma^{2}$$
  
$$= \sum_{l=1}^{m} \sum_{k=1}^{m} C_{jl} C_{jk} (C_{kl})^{-1} \sigma^{2} = C_{jj} \sigma^{2}.$$
(A.48)

## A.7 Multivalue fitting with known error bars

To improve the signal-to-noise ratio, it is a common practice to take  $y_i$  as the average of a large number of repeated measurements. In such cases, we would already have a good estimate of the variance  $\sigma_i^2$  of  $y_i$ . The equations for maximum likelihood estimates of  $a_i$  become

$$\frac{\partial \ln L}{\partial a_j} = \sum_{i=1}^n \frac{X_{ij}}{\sigma_i^2} \left( y_i - \sum_{k=1}^m a_k X_{ik} \right) = 0.$$
(A.49)

By a change of variables  $A_{ij} = X_{ij}/\sigma_i$  and  $u_i = y_i/\sigma_i$ , Eq. (A.49) is reduced to Eq. (A.42). From the result of previous section it can be seen immediately that if  $C_{ij} \equiv (\mathbf{A}^{\mathrm{T}} \mathbf{A})^{-1}$ , we have

$$\hat{\mathbf{a}} = \left(\mathbf{A}^{\mathrm{T}}\mathbf{A}\right)^{-1}\mathbf{A}^{\mathrm{T}}\mathbf{u},\tag{A.50}$$

$$E(\hat{a_{j}}) = \left(\sum_{k=1}^{m} C_{jk} \sum_{i=1}^{n} A_{ik}\right) \sum_{l=1}^{m} A_{il} a_{l}$$
  
$$= \sum_{l=1}^{m} \sum_{k=1}^{m} C_{jk} \left(\sum_{i=1}^{n} A_{ik} A_{il}\right) a_{l}$$
  
$$= \sum_{l=1}^{m} \sum_{k=1}^{m} C_{jk} (C_{kl})^{-1} a_{l} = a_{j}, \qquad (A.51)$$

$$V(\hat{a}_{j}) = \sum_{i=1}^{n} \left( \sum_{k=1}^{m} C_{jk} A_{ik} \right) \left( \sum_{l=1}^{m} C_{jl} A_{il} \right)$$
  
$$= \sum_{l=1}^{m} \sum_{k=1}^{m} C_{jl} C_{jk} \left( \sum_{i=1}^{n} A_{ik} A_{il} \right)$$
  
$$= \sum_{l=1}^{m} \sum_{k=1}^{m} C_{jl} C_{jk} (C_{kl})^{-1} = C_{jj}.$$
 (A.52)

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# Appendix B

## Hints of Selected Exercises

### Chapter 2

**Hint 2.11**. Assume the position vector of the car is  $\mathbf{r}(t) = [x(t), z(t)]$ . Then one has  $\mathbf{v}(t) = [\dot{x}(t), \dot{z}(t)]$ . The condition of constant speed is

$$v = \sqrt{\dot{x}^2(t) + \dot{z}^2(t)} = \sqrt{1 + \left(\frac{dz}{dx}\right)^2} \left(\frac{dx}{dt}\right),$$

hence

$$\dot{x}(t) = \frac{v}{\sqrt{1 + \left(\frac{dz}{dx}\right)^2}},$$
$$\dot{z}(t) = \frac{v\left(\frac{dz}{dx}\right)}{\sqrt{1 + \left(\frac{dz}{dx}\right)^2}}.$$

Hint 2.16. As the train accelerates on the surface of the Earth, the angular velocity of the Earth must change because angular momentum is conserved. Therefore the rotational energy of the Earth must also change.

**Hint 2.25.** Calculate the gravitational potential as a function of d, where d is the distance from the wire. Alternatively, you may calculate the gravitational force at a distance d and integrate the force to obtain the potential. To escape, the kinetic energy must be larger than the potential energy. Note

that only the difference of potential energy for two positions is meaningful. The absolute value of potential energy has no physical meaning.

Hint 2.26. Patch up the opening and use the shell theorem. What is the contribution of the patch to the gravitational force?

Hint 2.32. From the initial energy E and the initial angular momentum L the trajectory of the satellite can be determined. See Eqs. (2.88)–(2.91) in the lecture note. However, since the Earth is not a point mass, one must make sure the trajectory of the satellite does not cross the surface of the Earth. This means the ratio between the long axis and the short axis must not be too large.

**Hint 2.33.** From the initial energy E and the initial angular momentum L the trajectory of the alpha particle can be determined. It is a hyperbola. The angle  $\theta$  is just the angle between the two asymptotes of the hyperbola.

#### Chapter 3

**Hint 3.5.** Write down the equation of motion along the curve, and show that it is equivalent to the simple harmonic oscillator. If the curve is described by  $\mathbf{r} = [x(\theta), y(\theta)]$ , where  $\theta = 0$  represents the bottom of the curve, then the length of the curve from the bottom is

$$l(\theta) = \int_0^\theta \sqrt{dx^2 + dy^2} = \int_0^\theta \sqrt{x'^2(\phi) + y'^2(\phi)} \, d\phi.$$

**Hint 3.6.** If the potential function is V(x), one has

$$\frac{mv^2}{2} = E - V(x),$$

where v is the velocity of the ball and E is the total energy. Hence

$$\frac{dx}{dt} = \pm \sqrt{\frac{2E - 2V(x)}{m}}.$$

The oscillation period can be calculated from the following integral,

$$\int_{x_0}^0 -\sqrt{\frac{m}{2E - 2V(x)}} \, dx = \int_0^{t_c} \, dt = \frac{T}{4},$$

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where  $x_0$  is the initial displacement and  $t_c$  is the time when the ball passes the point x = 0.

Hint 3.11. The equation of motion for the two masses can be written in the following form:

$$m\ddot{x}_1 = k_{11}x_1 + k_{12}x_2$$
$$m\ddot{x}_2 = k_{21}x_1 + k_{22}x_2.$$

Change the coordinate to

$$y_1 = a_{11}x_1 + a_{12}x_2$$
$$y_2 = a_{21}x_1 + a_{22}x_2.$$

Find a suitable set of  $(a_{11}, a_{12}, a_{21}, a_{22})$  such that

$$m\ddot{y}_1 = \lambda_1 y_1$$
$$m\ddot{y}_2 = \lambda_2 y_2.$$

Hint 3.12. In general, the period of an oscillator can be calculated from the following equation.

$$\frac{dx}{dt} = \sqrt{\frac{2[E - V(x)]}{m}},$$

or

$$\frac{T}{2} = \int_{x_{\min}}^{x_{\max}} dt = \sqrt{\frac{m}{2}} \int_{x_{\min}}^{x_{\max}} \frac{dx}{\sqrt{E - V(x)}}.$$

For this particular oscillator we have

$$\frac{T}{2} = \int_{x_{\min}}^{x_{\max}} dt = \sqrt{\frac{m}{2(a+E)}} \int_{x_{\min}}^{x_{\max}} \frac{dx}{\sqrt{1 - \frac{a}{a+E}(e^{-\alpha x} - 1)^2}}.$$

The integration can be simplified by a change of variable  $\sin u = \sqrt{a/(a+E)(1-e^{-\alpha x})}$ . Note that  $x_{\min}$  and  $x_{\max}$  occur at zero kinetic energy. You should be able to figure out the upper bound and the lower bound for the integration with respect to u.

$$\frac{T}{2} = \int_{x_{\min}}^{x_{\max}} dt = \sqrt{\frac{m}{2(a+E)}} \int_{u_{\min}}^{u_{\max}} \frac{du}{\alpha \left(\sqrt{\frac{a}{a+E}} - \sin u\right)}.$$

#### Chapter 4

**Hint 4.4.** Assume the radius of the chicken is  $r_c$  and that of the elephant is  $r_e$ , and the defrosting time for the chicken is  $t_c$  and that for the elephant is  $t_e$ . Rewrite the diffusion equation in the dimensionless form, then the ratio  $t_c/t_e$  becomes clear when it is required that the two dimensionless equations have the same solution.

**Hint 4.12.** Assume the concentration is x at  $r = \infty$  and  $x_0$  at r = R in the steady state. Use the continuity equation to find the flux of water molecules **J** as a function of r. To completely determine **J**, you will need the equation  $\mathbf{J} = -D\nabla\rho$  to impose the boundary conditions. From **J** you may calculate the evaporation rate as a function of x,  $x_0$ ,  $\rho_w$ ,  $\rho_v$ , R, and D.

**Hint 4.13.** The first law of thermodynamics is TdS = dU + Vdq, where q is the amount of charge that flows through the battery. The Helmholtz free energy is defined by A = U - TS. Consider the second derivatives of A with respect to q and T.

#### Chapter 6

Hint 6.8. Use  $J = \sigma E$ , the Gauss' law, and the continuity equation.

Hint 6.9. To make an ion trap using only static electric field, one must construct a three-dimensional electric potential well. Apply Gauss' law at the bottom of the potential well.

#### Chapter 8

Hint 8.8. The cable can be thought as a series of inductors and capacitors connected in a way shown by Fig. B.1. The *i*th capacitor is charged by two neighboring inductors. The equation is

$$\frac{dq_i}{dt} = I_{i-1} - I_{i+1}.$$

At the same time the current in the ith inductor is driven by the voltage of two neighboring capacitors. The equation is

$$L\frac{dI_i}{dt} = \frac{1}{C}(q_{i-1} - q_{i+1}).$$

In the continuum limit we change the index from integer i to the position x, and these two equations can be combined into a wave equation.

Hint 8.9. The cable can be thought as a series of inductors and capacitors connected in a way shown by Fig. B.1. Assume the impedance of the cable is Z, then one can cut out a small piece of the cable without changing the impedance. The small piece of cable can be represented by a voltage divider made of a small inductor and a small capacitor. Let L and C represent the inductance and capacitance per unit length respectively, then the cut-out inductance and capacitance are  $\epsilon L$  and  $\epsilon C$  respectively, where  $\epsilon$  is an arbitrarily small number. The impedance Z satisfies the following equation:

$$Z = Z_L + (Z_C \parallel Z),$$

where  $Z_L$  is the impedance of  $\epsilon L$ ,  $Z_C$  is the impedance of  $\epsilon C$ , and the binary operator  $\parallel$  means the two elements are connected in parallel.

**Hint 8.10.** If you remember that the electric field produced by a line charge is proportional to 1/r, then it is easy to obtain that the electric potential  $\phi(r)$  is proportional to  $\ln(r/d)$ . Then you can compare

$$U_e = \frac{1}{2} \int \rho(\mathbf{r}) \phi(\mathbf{r}) \, d^3 \mathbf{r}$$

and

$$U_e = \frac{Q^2}{2C}$$

to obtain the capacitor per unit length. Similarly you can compare

$$U_m = \frac{1}{2} \int \mathbf{J}(\mathbf{r}) \cdot \mathbf{A}(\mathbf{r}) \, d^3 \mathbf{r}$$

and

$$U_m = \frac{LI^2}{2}$$

to obtain the inductance per unit length. Because

$$\nabla^2 \phi(\mathbf{r}) = -\frac{\rho}{\epsilon_0},$$



Fig. B.1: Equivalent circuit of a coaxial cable.

$$abla^2 \mathbf{A}(\mathbf{r}) = -\mu_0 \mathbf{J}_2$$

the dependence of **A** on **J** is the same as that of  $\phi$  on  $\rho$ . Hence it is pretty easy to make the same comparison to obtain the inductance per unit length.

Hint 8.14. If the motion of the electron is a linear harmonic oscillator, you may use the standard formula of dipole radiation. However, a circular motion is simply the superposition of two perpendicular linear harmonic oscillators with a phase difference of  $\pi/2$ .

#### Chapter 9

**Hint 9.6.** Is magnetic force the only force the particle experiences in frame B? The wire is neutral in frame A, is it still neutral in frame B? Solve this exercise in two ways, one by the transformation of  $\rho$  and  $\mathbf{J}$ , and the other by the transformation of  $\mathbf{E}$  and  $\mathbf{B}$ .

Hint 9.7. Because  $(\mathbf{p}, E/c)$  is a four-vector, we have

$$dp'_{x} = \gamma \left( dp_{x} - \frac{\beta}{c} dE \right),$$
$$dp'_{y} = dp_{y},$$
$$dp'_{z} = dp_{z}.$$

Using the relation

$$dt' = \gamma \left( dt - \frac{\beta}{c} dx \right)$$

we have

$$\frac{dp'_x}{dt'} = \frac{dp_x - \frac{\beta}{c}dE}{dt - \frac{\beta}{c}dx} = \frac{\frac{dp_x}{dt} - \frac{\beta dE}{cdt}}{1 - \beta^2} = \gamma^2 \left(\frac{dp_x}{dt} - \frac{\beta dE}{cdt}\right),$$

$$\frac{dp'_y}{dt'} = \frac{dp_y}{\gamma\left(dt - \frac{\beta}{c}dx\right)} = \frac{\frac{dp_y}{dt}}{\gamma(1 - \beta^2)} = \gamma \frac{dp_y}{dt},$$

and similarly

$$\frac{dp'_z}{dt'} = \gamma \frac{dp_z}{dt}.$$

Therefore

$$\frac{d\mathbf{p}}{dt} = \frac{dE}{dt} = 0$$

implies

$$\frac{d\mathbf{p}'}{dt'} = 0$$

#### Chapter 10

**Hint 10.1.** In a conventional positive lens, light is delayed more at the center, because the lens is thicker at the center. In a graded-index lens, light is also delayed more at the center, because the index of refraction is larger at the center even though the thickness is the same. If the two devices have the same optical delay as a function of r, they have the same focal length.

**Hint 10.3.** One must consider the relative phase of the waves. The power reflectivity is related to amplitude reflectivity by  $R = |\mathcal{R}|^2$  and similarly  $T = |\mathcal{T}|^2$ . What is the relation between the phase angles of  $\mathcal{R}$  and  $\mathcal{T}$  in order to meet the energy conservation law? The result of Exercise 10.2 should help.

**Hint 10.6.** Use Fourier transform to inspect the plane-wave components of  $\mathbf{E}(\mathbf{r}, t)$ .

Hint 10.8. When we deal with evanescent waves across the surface of total reflection, we usually choose

$$\mathbf{k}_t = (k_{xi}, k_{yi}, ik_0 \sqrt{n_i^2 \sin^2 \theta_i - n_t^2})$$

instead of

$$\mathbf{k}_t = (k_{xi}, k_{yi}, -ik_0\sqrt{n_i^2\sin^2\theta_i - n_t^2})$$

even though both satisfy the condition

$$k_{\perp t}^{2} = k_{0}^{2} (n_{t}^{2} - n_{i}^{2} \sin^{2} \theta_{i})$$

when  $\sin \theta_i > n_t/n_i$ . This is because if there is only one surface, the second choice will lead to an exponential growth of the wave amplitude, which is not possible. However, if there is another parallel surface beyond which the wave can revert to a traveling wave, one cannot rule out the second choice.

#### Chapter 11

Hint 11.5. In exercise 11.4 the angular momentum cannot be zero even for the ground state.

Hint 11.7. Since  $d\mathbf{r} = dr\hat{\mathbf{r}} + rd\theta\hat{\boldsymbol{\theta}}$  and  $\mathbf{p} = p_r\hat{\mathbf{r}} + r\dot{\theta}\hat{\boldsymbol{\theta}}$ , we have

$$\oint \mathbf{p} \cdot d\mathbf{r} = \oint m\dot{r} \, dr + \oint m(r\dot{\theta})(rd\theta) = nh.$$

Consider the quantity

$$\frac{d}{dt}(\mathbf{p}\cdot\mathbf{r}) = \frac{d\mathbf{p}}{dt}\cdot\mathbf{r} + \mathbf{p}\cdot\frac{d\mathbf{r}}{dt}.$$

For the hydrogen atom the first term on the right-hand side is the potential energy V and the second term on the right-hand side is 2T, where T is the kinetic energy. Since the motion is periodic, if we take the time average of the above equation over the period  $\tau$ , we get

$$\frac{1}{\tau} \int_0^\tau \frac{d}{dt} (\mathbf{p} \cdot \mathbf{r}) \, dt = \frac{1}{\tau} [\mathbf{p}(\tau) \cdot \mathbf{r}(\tau) - \mathbf{p}(\mathbf{0}) \cdot \mathbf{r}(0)] = 0 = \frac{1}{\tau} \int_0^\tau V \, dt + \frac{1}{\tau} \int_0^\tau 2T \, dt.$$

Note that

$$\oint \mathbf{p} \cdot d\mathbf{r} = \oint \mathbf{p} \cdot \frac{d\mathbf{r}}{dt} \, dt = \int_0^\tau 2T \, dt.$$

Using the results derived in Section 2.13, you have all the equations needed to express the energy as a function of n.

Hint 11.8. For each polarization of lattice vibration (two transverse and one longitudinal), the internal energy as a function of T can be written as

$$U_{i} = \int_{0}^{\nu_{\max}} P(\nu) d\nu = \int_{0}^{\nu_{\max}} \frac{4\pi\nu^{2}}{v_{i}^{3}} \frac{h\nu}{\exp\left(\frac{h\nu}{kT}\right) - 1} d\nu$$

where  $v_i$  is the propagation speed of lattice vibration for the *i*th polarization, and  $\nu_{\text{max}}$  is determined by the number of modes (atoms).

#### Chapter 14

**Hint 14.1.** (1) Show that

$$\int \psi^*(\mathbf{r}) \left[ \hat{\mathbf{L}} V(r) - V(r) \hat{\mathbf{L}} \right] \psi(\mathbf{r}) \, d^3 \mathbf{r} = 0.$$

(2) Using  $[r_i, p_j] = r_i p_j - p_j r_i = i\hbar \delta_{ij}$ , show that

$$\int \psi^*(\mathbf{r}) \left[ \hat{\mathbf{L}} p^2 - p^2 \hat{\mathbf{L}} \right] \psi(\mathbf{r}) \, d^3 \mathbf{r} = 0.$$

Combining (1) and (2), you have the answer.

Hint 14.2. Since in the classical harmonic oscillator the position and momentum change with time, it cannot be the corresponding state of a stationary state. Instead it must be the corresponding state of a superposition of eigenstates. You should find the right superposition to answer this problem.

**Hint 14.3.** (1) Since  $[L_z, H] = 0$ , one can find wavefunctions that are simultaneously the eigenfunction of H and  $L_z$ . (2) In classical mechanics, a rotation can be thought of as a superposition of two vibrations, one in the x-axis and the other in the y-axis with a phase shift of  $\pi/2$ . It is similar in quantum mechanics.

# Appendix C

## Topics to be added

- 1. calculus of complex functions
- 2. Rutherford scattering
- 3. small oscillation
- 4. Lagrangian and Hamiltonian mechanics
- 5. wave propagation in a periodic medium
- 6. nucleation
- 7. Maxwell daemon
- 8. coarse graining
- 9. phasor and AC impedance
- 10. transmission lines
- 11. Bose-Einstein distribution
- 12. Fermi-Dirac distribution
- 13. quantum tunneling
- 14. scattering in quantum mechanics
- 15. Kramers-Kronig relations

- 16. Fermi's golden rule
- 17. quantum version of the interaction between light and matter
- 18. semiconductor band gap
- 19. Gaussian beam
- 20. lasers
- 21. fast light and slow light
- 22. Rabi oscillation
- 23. laser cooling
- 24. nonlinear optics
- 25. chaos and fractal
- 26. relativity in accelerated frame
- 27. simple version of general relativity
- 28. Bell's inequality
- 29. quantum computation

# Appendix D

# **ASCII** and Greek Characters

## D.1 ASCII Characters

	space, blank	!	exclamation point, exclamation (mark)
п	quotation mark, (double) quote	#	crosshatch, pound, pound sign
\$	dollar sign, dollar	%	percent sign, percent
&	ampersand, and	-	apostrophe, (single) quote
*	asterisk, star	()	parentheses
)	right parentheses	+	plus sign, plus
,	comma	-	hyphen, minus (sign)
	period, dot	/	slash
:	colon	;	semicolon
<>	angle brackets	=	equal sign
?	question mark	0	at sign
[]	brackets, square brackets	]	right bracket
	backslash	^	circumflex, caret
_	underscore, underline	-	grave, (grave/acute) accent
{}	braces	{	left brace, brace
}	right brace, unbrace		vertical bar
~	tilde		

$\alpha$	alpha	$\beta$	beta	$\gamma, \Gamma$	gamma	$\delta, \Delta$	delta	$\epsilon$	epsilon
ε	varepsilon	$\zeta$	zeta	$\eta$	eta	$\theta, \Theta$	theta	$\vartheta$	vartheta
ι	iota	$\kappa$	kappa	$\lambda, \Lambda$	lambda	$\mid \mu$	mu	$\nu$	nu
$\xi, \Xi$	xi	0	0	$\pi, \Pi$	pi	$\overline{\omega}$	varpi	$\rho$	rho
$\varrho$	varrho	5	varsigma	$\tau$	tau	$v, \Upsilon$	upsilon	$\phi, \Phi$	phi
$\varphi$	varphi	$\chi$	chi	$\psi, \Psi$	psi	$\omega, \Omega$	omega		

## D.2 Greek Characters

# D.3 Military Phonetic Alphabet

Α	Alfa	В	Bravo	C	Charlie	D	Delta	E	Echo
F	Foxtrot	G	Golf	H	Hotel	Ι	India	J	Juliett
K	Kilo	L	Lima	M	Mike	Ν	November	Ο	Oscar
Р	Papa	Q	Quebec	R	Romeo	S	Sierra	Т	Tango
U	Uniform	V	Victor	W	Whiskey	X	X-ray	Y	Yankee
Z	Zulu				-		-		

0	Zeero	1	Wun	2	Too	3	Tree/Thr-ree	4	Fower
5	Fife	6	Siks	7	Seven	8	Ate	9	Niner

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