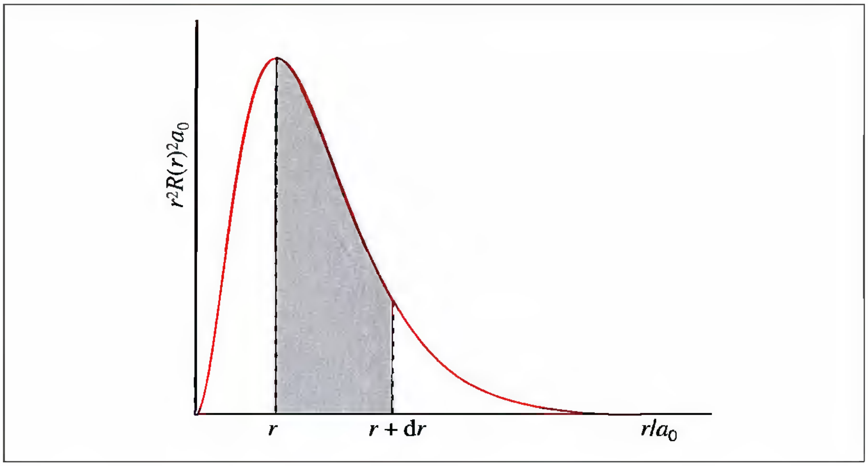

Figure 6.5 A plot of the radial probability density, $D(r) = Nr^2e^{-2r/a_0}$, for the 1s orbital of the hydrogen atom, where a_0 is the Bohr radius (units, m) and N has units of m^{-3}

6.3 The Indefinite Integral

The indefinite integral of a function $y = f(x)$ is usually written as:

$$\int f(x)\mathrm{d}x = F(x) + C \tag{6.9}$$

where:

- $f(x)$ is known as the **integrand**
- C is an arbitrary constant called the **constant of integration**
- $F(x) + C$ is known as the **indefinite integral**

The new function, $y = F(x) + C$, which we obtain after integration, must be such that its derivative is equal to $f(x)$, to ensure that the definition conforms with the requirement that integration is the reverse (or inverse) of differentiation. Thus, we must have:

$$\frac{\mathrm{d}}{\mathrm{d}x}(F(x) + C) = F'(x) = f(x) \tag{6.10}$$

The relation between the indefinite integral of $f(x)$ and $f(x)$ itself is shown schematically in Figure 6.6 for the functions $f(x) = 18x^2$ and $F(x) = 6x^3$.

So, to summarize: the indefinite integral is determined by finding a suitable function, $F(x)$, which, on differentiation, yields the function we are trying to integrate, and to which we then add a constant. In common with the strategies described in Chapter 4 for finding the derivative of a given function, an analogous set of strategies can be constructed for finding the indefinite integral of a function. For simple functions, a set of standard indefinite integrals can be constructed without too much difficulty, some of which are listed in Table 6.1.

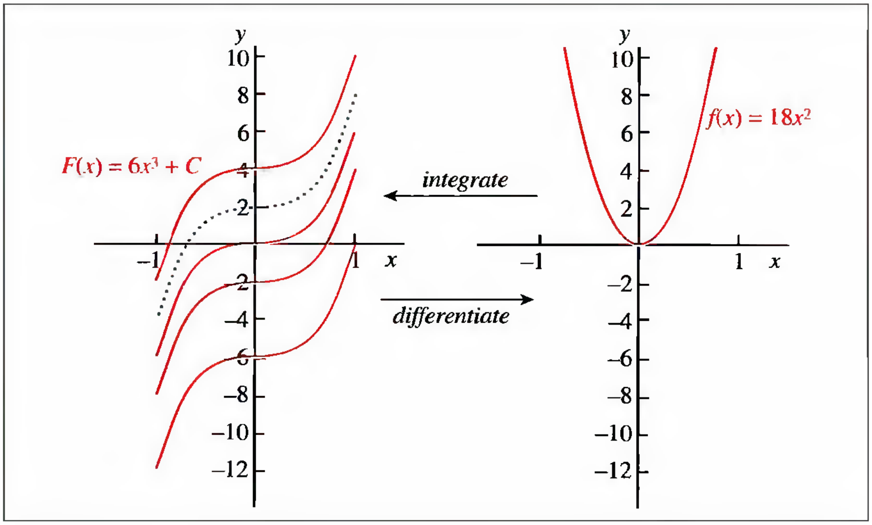

Figure 6.6 Integration of the function $f(x) = 18x^2$ (*right*) yields a family of functions given by the indefinite integral $F(x) = 6x^3+C$ (*left*), where C can take any value. Differentiation of $F(x)$ yields the original function, $f(x)$

Table 6.1 A selection of functions, $f(x)$, and their indefinite integrals, $F(x)+C$

$f(x)$	integrate →	$F(x)+C$
$x^a\ (a \neq -1)$		$\frac{x^{a+1}}{a+1}+C$
$\frac{1}{x}$		$\ln(x),+C$
$\frac{1}{x+a}$		$\ln(x+a)+C$
$\cos(ax)$		$\frac{1}{a}\sin(ax)+C$
$\sin(ax)$		$-\frac{1}{a}\cos(ax)+C$
e^{ax}		$\frac{1}{a}e^{ax}+C$
$\sec^2(x)$		$\tan(x)+C$
$f(x)$	← differentiate	$F(x)+C$

Worked Problem 6.1

Q (a) Show that: $\frac{d}{dx}\ln(1-2x) = -\frac{2}{1-2x}$.
(b) Deduce that: $\int \frac{1}{1-2x}dx = -\frac{1}{2}\ln(1-2x) + C$.

A (a) Since the first step involves establishing that the derivative of $y = \ln(1-2x)$ is $-\frac{2}{1-2x}$, it is simplest to use the chain rule (see Section 4.2.4). If $u = 1-2x$, then:

$$\frac{dy}{dx} = \frac{d}{dx}\ln(1-2x) = \frac{dy}{du}\frac{du}{dx} = \frac{1}{u}\times -2 = -\frac{2}{1-2x}$$

(b) Reversing the procedure by integration yields the following result, where B is the constant of integration:

$$-\int \frac{2}{1-2x}dx = \ln(1-2x) + B \Rightarrow \int \frac{1}{1-2x}dx = -\frac{1}{2}\ln(1-2x) + C$$

where $C = -B/2$.

Problem 6.1

(a) Evaluate $\frac{d}{dx}e^{2x}$ and hence deduce that $\int e^{2x}dx = \frac{1}{2}e^{2x} + C$.

(b) Show that $\frac{d}{dx}\left(\frac{1}{1+e^x}\right) = -\frac{e^x}{(1+e^x)^2}$ and hence find $\int \frac{e^x}{(1+e^x)^2}dx$.

6.4 General Strategies for Solving More Complicated Integrals

Integrals involving complicated forms for $f(x)$ require strategies for reducing the integral to one or more integrals of simpler (standard) form, thus making it possible to find $F(x)$. If all else fails, or we do not have an explicit form for $f(x)$, then numerical integration must be carried out, using methods described elsewhere.[1]

A chemical example of a function which does not have an explicit form can be found in thermodynamics, where the entropy is determined by integrating C_p/T, which may be known only at selected temperatures.

Some of the strategies involved in simplifying the form of an integral are quite straightforward. For example:

- If $f(x)$ is in the form of a linear combination of simpler functions, *e.g.*:

$$\int (3x^2 + 2x + 1)dx \quad (6.11)$$

then we may be able to rewrite such an integral as a sum of standard integrals that are immediately recognizable:

$$\int (3x^2 + 2x + 1)dx = \int 3x^2dx + \int 2xdx + \int 1dx \quad (6.12)$$

- Integrals can be simplified by placing constant terms outside the integral, *e.g.*:

$$\int (3x^2 + 2x + 1)dx = 3\int x^2dx + 2\int xdx + \int 1dx \quad (6.13)$$

Problem 6.2

Integrate the function $y = f(x) = 9x^2 + 2e^{2x} + \frac{1}{x}$.

In practice, we may find ourselves faced with more complicated functions, the solutions to which require us to use methods involving adaptation of some of the rules for differentiation. The choice of method more often than not involves some guesswork, but coming up with the correct guesses is all part of the fun! In addition, it may be necessary to use a combination of several methods. In the following two sections, we discuss **integration by parts** and the **substitution method**

6.4.1 Integration by Parts

This method starts from the familiar product rule, used in differential calculus (equation 4.9):

$$\frac{d}{dx}(uv) = v\frac{du}{dx} + u\frac{dv}{dx}$$

Integration over x yields:

$$\int \frac{d}{dx}(uv)dx = \int v\frac{du}{dx}dx + \int u\frac{dv}{dx}dx \tag{6.14}$$

and, on using the properties of differentials, the left side $\int \frac{d}{dx}(uv)dx$ becomes $\int d(uv) = uv$. It follows that rearrangement of the above expression yields:

$$\int u\frac{dv}{dx}dx = uv - \int v\frac{du}{dx}dx \tag{6.15}$$

Equation (6.15) shows that the integral on the left side, which is the one sought, is replaced by two terms, one of which is another integral which we hope is more tractable than the initial integral. This method of integral evaluation is appropriate for integrands of product form. The success of the method relies on making the right choices for u and dv/dx. The term identified as u is differentiated to form part of the integrand on the right side of equation (6.15); the other part of the integrand is formed by integrating the term identified as dv/dx.

Worked Problem 6.2

Q Given the integrand $f(x) = x \cos x$, find the indefinite integral.

A The integrand is the product of x and $\cos x$, and in this case we identify x with u and dv/dx with $\cos x$ in equation (6.15): $u = x$ and

$dv/dx = \cos x$. Thus, $du/dx = 1$ and $v = \sin x$, and so equation (6.15) becomes:

$$\int x \cos x \, dx = x \sin x - \int \sin x \, dx.$$

The final step simply requires us to evaluate $\int \sin x \, dx$, which we know by reference to Table 6.1 to be $-\cos x + C$. Thus:

$$\int x \cos x \, dx = x \sin x + \cos x + D$$

where $D = -C$. If, on the other hand, we had identified u and dv/dx the other way round, we end up with a more complicated integral to evaluate:

$$\int x \cos x \, dx = x^2 \cos x + \int \frac{x^2}{2} \sin x \, dx$$

Clearly, some practice is required in identifying u and dv/dx for use in equation (6.15), when it seems that integration by parts is appropriate.

Problem 6.3

Use the method of integration by parts to evaluate $\int xe^{-x} dx$, assuming:

(a) $u = x$ and $dv/dx = e^{-x}$; (b) $u = e^{-x}$ and $dv/dx = x$.

Comment on which choice you think is the most appropriate for this integral.

6.4.2 Integration Using the Substitution Method

The second integration technique, known as the substitution method, derives from the inversion of the chain rule for differentiation described in Chapter 4. The objective here, once again, is to transform the integrand into a simpler or, preferably, a standard form. However, just like the integration by parts method, there is usually a choice of substitutions and although, in some cases, different substitutions yield different answers, these answers must only differ by a constant (remember that, for an indefinite integral, the answer is determined by inclusion of a constant). The substitution method is best illustrated using a worked problem.

Worked Problem 6.3

Q Evaluate $\int xe^{ax^2}dx$.

A Here $f(x) = xe^{ax^2}$. Let us try the substitution $u = ax^2$ in order to transform the integral over x to an integral over u. From the properties of differentials we know that:

$$du = \frac{du}{dx}dx = 2ax\,dx$$

This result enables us to express dx in terms of du, according to $dx = \frac{1}{2ax}du$, thus transforming the integral into:

$$\int xe^u \frac{du}{2ax} = \frac{1}{2a}\int e^u du = \frac{1}{2a}e^u + C$$

We now express the result in terms of the original variable, x, by substituting back for u:

$$\int xe^{ax^2}dx = \frac{1}{2a}e^{ax^2} + C$$

At this point, it is good practice to check the result by differentiating the function $F(x) = \frac{1}{2a}e^{ax^2}$, to ensure that the original integrand $f(x)$ is regenerated (see equation 6.10):

$$F'(x) = \frac{d}{dx}\left(\frac{1}{2a}e^{ax^2}\right) = \frac{2ax}{2a}e^{ax^2} = xe^{ax^2}$$

as required.

Problem 6.4

Repeat Worked Problem 6.3, using the substitution $u = x^2$.

Worked Problem 6.4

Q Evaluate

$$\int \frac{x}{(1-x)^{1/2}}dx.$$

A A possible substitution is given by $u=(1-x)^{1/2}$, from which it follows that:

$$u^2 = 1 - x \Rightarrow x = 1 - u^2$$

Differentiating the last equation with respect to u gives:

$$\frac{\mathrm{d}x}{\mathrm{d}u} = -2u \Rightarrow \mathrm{d}x = -2u\,\mathrm{d}u$$

Hence:

$$\begin{aligned}\int \frac{x}{(1-x)^{1/2}}\mathrm{d}x &= \int \frac{1-u^2}{u} \times -2u\,\mathrm{d}u \\ &= -2\int (1-u^2)\,\mathrm{d}u = -2u + \frac{2}{3}u^3 + C \\ \Rightarrow \int \frac{x}{(1-x)^{1/2}}\mathrm{d}x &= -\frac{2}{3}(1-x)^{1/2}(2+x) + C\end{aligned}$$

Problem 6.5

Evaluate the indefinite integral $\int \frac{x}{(1-x)^{1/2}}\mathrm{d}x$, using the substitution $u=1-x^2$.

Problem 6.6

(a) Find $\int x(x^2+4)^{1/2}\mathrm{d}x$, using the substitution $u=x^2 + 4$.

(b) Show that $\int \frac{1}{x \ln x}\,\mathrm{d}x = \ln(\ln x) + C$, using the substitution $u=\ln x$.

Use of Trigonometrical Substitutions

The integrand in Problem 6.5 is of a form which suggests that a trigonometrical substitution might be appropriate. Bearing in mind the key identity $\cos^2 u + \sin^2 u = 1$, the appearance of a factor like $(1-x^2)^{1/2}$ in the integrand suggests the substitutions $x=\cos u$ or $x=\sin u$. Thus, for the substitution $x=\cos u$, the factor $(1-x^2)^{1/2}$ becomes $(1-\cos^2 u)^{1/2}=\sin u$.

Problem 6.7

(a) Repeat Problem 6.5, using the trigonometrical substitution $x = \cos u$.
Hint. You will need to remember that $\sin^2 u = 1 - \cos^2 u$ and consequently that $\sin u = (1 - \cos^2 u)^{1/2}$ for the final step of your integration. You should have obtained the same result as your answer to Problem 6.5.

(b) Show that $\int \frac{\cos x}{\sin x} \mathrm{d}x = \ln(\sin x) + C$ using the substitution $u = \sin x$.

General Comment

The choice of method for evaluating indefinite integrals relies on experience to a large extent. Sometimes, integration by parts and the substitution methods are equally applicable; however, in many cases they are not. For example, the integration by parts method is much more suited to finding the integral of the function $f(x) = x \cos x$, described in Worked Problem 6.2, than the substitution method (which would prove frustrating and fruitless in this case). It may also be necessary to use several applications of one or both methods before the answer is accessible. However, whichever method is used, the answer may always be checked by verifying that $F'(x) = f(x)$.

6.5 The Connection Between the Definite and Indefinite Integral

As we saw in Section 6.2.1, the concept of integration emerged from attempts to determine the area bounded by a plot of a function $f(x)$ and the x-axis, within some interval $[a,b]$. This area is given by the definite integral, the definition of which derives from numerical methods involving limits (see Section 6.2.1). Such numerical methods can be tedious to apply in practice (although instructive!) but, fortunately, there is a direct link between the indefinite integral, $F(x) + C$, of a function, $f(x)$, and the definite integral, in which x is constrained to the interval $[a,b]$. The relationship between the two forms of integration is provided by the fundamental theorem of calculus:

$$\int_a^b f(x)\mathrm{d}x = (F(b) + C) - (F(a) + C) = F(b) - F(a) \tag{6.16}$$

where $F(a)$ is the value of $F(x)$ at $x = a$ and $F(b)$ is the value of $F(x)$ at $x = b$. In other words, the definite integral over the interval $[a,b]$ is obtained by subtracting the indefinite integral at the point $x=a$ from that at $x=b$. Furthermore, we see that the constant of integration, which appears in the indefinite integral, does not appear in the final result (see equation 6.16).

Worked Problem 6.5

Q Evaluate $\int_0^1 \frac{x}{1+x}\mathrm{d}x$.

A The first step requires us to find the indefinite integral $\int \frac{x}{1+x}\mathrm{d}x$. Using the substitution $u=1+x$, the integral becomes:

$$\int \frac{u-1}{u}\mathrm{d}u = \int\left(1-\frac{1}{u}\right)\mathrm{d}u = u - \ln u + C = (1+x) - \ln(1+x) + C$$

Thus identifying $F(x)$ with $(1 + x)-\ln(1 + x)$, the definite integral can be evaluated from:

$$\int_0^1 \frac{x}{1+x}\mathrm{d}x = F(1) - F(0) = 2 - \ln 2 - 1 - 0 = 1 - \ln 2$$

Problem 6.8

(a) Evaluate (i) $\int_1^2 \frac{1}{x^3}\mathrm{d}x$; (ii) $\int_0^2 x(x^2+4)^{1/2}\mathrm{d}x$ (see Problem 6.6a).

(b) Show that $\int_0^2 \frac{x}{(x^2+4)}\mathrm{d}x = \frac{1}{2}\ln 2$, using an appropriate substitution.

Problem 6.9

For the expansion of a perfect gas at constant temperature, the reversible work is given by the expression:

$$W = \int_{V_a}^{V_b} p\,\mathrm{d}V$$

where $p=nRT/V$ and V_a and V_b are the initial and final volumes, respectively. Derive an expression for the work done by evaluating the integral between the limits V_a and V_b.

Problem 6.10

Let K be the equilibrium constant for the formation of CO_2 and H_2 from CO and H_2O at a given temperature T. From thermodynamics, we know that:

$$\frac{d}{dT}\ln K = \Delta H^{\circ}/RT^2 \tag{6.17}$$

(a) Assuming that ΔH° is independent of temperature, integrate equation (6.17) to find how ln K varies with T.

(b) Given $\Delta H^{\circ} = 42.3$ kJ mol^{-1}, find the change in ln K as the temperature is raised from 500 K to 600 K.

Summary of Key Points

This chapter provides an introduction to integral calculus, together with examples set in a chemical context. However, as we shall see in the following chapter, we need integral calculus to solve the differential equations which appear in chemical kinetics, quantum mechanics, spectroscopy and other areas of chemistry. The key points discussed in this chapter include:

1. The definition of integration as the inverse of differentiation, yielding the indefinite integral.
2. The definition of integration as a means of evaluating the area bounded by a plot of a function over a given interval and the x-axis, yielding the definite integral.
3. The use of integration by parts method for integrating products of functions.
4. The use of the substitution method for reducing more complicated functions to a simpler or standard form.
5. The use of trigonometric substitutions in the substitution method.

Reference

1. See, for example, M. J. Englefield, *Mathematical Methods for Engineering and Science Students*, Arnold, London, 1987, chap. 15.

7

Differential Equations

In Chapter 2 we explored some of the methods used for finding the roots of algebraic equations in the form $y = f(x)$. In all of the examples given we were seeking to determine the value of an unknown (typically the value of the independent variable, x) that resulted in a particular value for y, the dependent variable. In general, the methods discussed can be used to solve algebraic equations where the dependent variable takes a value other than zero, because the equation can always be rearranged into a form in which $y = 0$. For example, if we seek the solution to the equation:

$$4 = x^2 - 5$$

then we can rearrange it to:

$$0 = x^2 - 9$$

by subtracting 4 from both sides. The problem now boils down to one in which we search for the two roots of the equation which, in this case, are $x = \pm 3$.

In this chapter we are concerned with equations containing derivatives of functions. Such equations are termed **differential equations**, and arise in the derivation of model equations describing processes involving rates of change, as in, for example:

- Chemical kinetics (concentrations changing with time).
- Quantum chemical descriptions of bonding (probability density changing with position).
- Vibrational spectroscopy (atomic positional coordinates changing with time).

In these three, as well as in other, examples we are trying to determine how the chosen property (such as concentration, probability density or atomic position) varies with respect to time, position or some other variable. This is a problem which requires the solution of one or more differential equations in a procedure that is made possible by using the tools of differentiation and integration discussed in Chapters 4 and 6, respectively.

Aims

This chapter builds on the content of earlier chapters to develop techniques for solving equations associated with processes involving rates of change. By the end of this chapter you should be able to:

- Identify a differential equation and classify it according to its order
- Use simple examples to demonstrate the origin and nature of differential equations
- Identify the key areas of chemistry where differential equations most often appear
- Use the separation of variables method to find the general solutions to first-order differential equations of the form $\frac{dy}{dx} = f(x)g(y)$
- Use the integrating factor method to find the general solutions to first-order differential equations linear in y
- Find the general solutions to linear second-order differential equations with constant coefficients by substitution of trial functions
- Apply constraints (boundary conditions) to the solution(s) of differential equations

7.1 Using the Derivative of a Function to Create a Differential Equation

Consider the function:

$$y = Be^{-2x} \tag{7.1}$$

where B is a constant. The first derivative of this function takes the form:

$$\frac{dy}{dx} = -2Be^{-2x} \tag{7.2}$$

If we now substitute for y, using equation (7.1), we obtain the **first-order** differential equation:

$$\frac{dy}{dx} = -2y \tag{7.3}$$

A first-order differential equation is so called because the highest order derivative is one.

which must be solved for y as a function of x. In other words, the solution to this problem will provide us with an equation which shows quantitatively how y varies as a function of x. The solution is, of course, provided by the original equation (7.1), but the purpose here is to explore the means by which we find that out for ourselves!

If we now differentiate equation (7.2) with respect to x, and substitute for dy/dx using equation (7.3), we obtain the second-order differential equation (7.4):

$$\frac{d^2y}{dx^2} = 4y \tag{7.4}$$

This differential equation is of **second order**, simply because the *highest* order derivative is two.

Problem 7.1

(a) Express the first and second derivatives of the function $y = 1/x$ in the form of differential equations, and give their orders.
(b) Express the second derivative of the function $y = \cos ax$ in the form of a differential equation.
(c) Show that the function $y = Ae^{4x}$ is a solution of the differential equations $\frac{dy}{dx} - 4y = 0$ and $\frac{d^2y}{dx^2} - 5\frac{dy}{dx} + 4y = 0$

The last part of Problem 7.1 demonstrates that a given function does not necessarily correspond to the solution of only one differential equation. In later sections we shall address the question of how to determine the number of different functions (where each function differs from another by more than simply multiplication by a constant) that are solutions of a given differential equation.

If the function $y = Ae^{4x}$ is a solution to Problem 7.1(c), then so is ky, where k is a constant.

7.2 Some Examples of Differential Equations Arising in Classical and Chemical Contexts

One of the principal motivations for the development of calculus by Newton and Leibnitz in the 18th century came from the need to solve physical problems. Examples of such problems include:

- The description of a body falling under the influence of the force of gravity:

$$\frac{d^2h}{dt^2} = -g \tag{7.5}$$

If a body is falling in a viscous medium, then the body is under the influence of both gravity and the drag forces exerted by the medium.

- The motion of a pendulum, which is an example of simple harmonic motion, described by the equation:

$$\frac{d^2x}{dt^2} = -\omega^2 x \tag{7.6}$$

If we extend this last example to the modelling of molecular vibrations, we need to include additional terms in the differential equation to account for non-harmonic (anharmonic) forces.

In these last two examples of equations of motion, the objective is to determine functions of the form $h = f(t)$ or $x = g(t)$, respectively, which satisfy the appropriate differential equation. For example, the solution of the classical harmonic motion equation is an oscillatory function, $x = g(t)$, where $g(t) = \cos \omega t$, and ω defines the frequency of oscillation. This function is represented schematically in Figure 7.1 (see also Worked Problem 4.4).

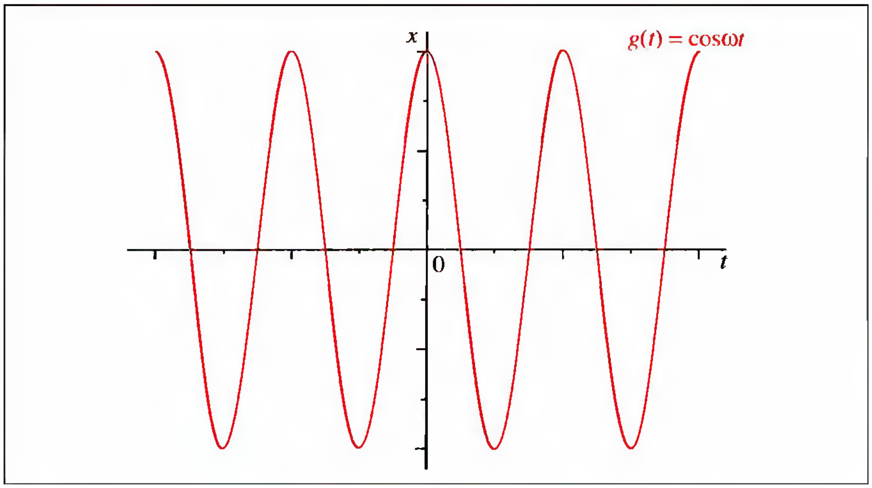

Figure 7.1 A plot of the function $g(t) = \cos \omega t$, describing simple harmonic motion

In chemistry, we are mostly concerned with changing quantities. For example:

- In kinetics, the concentration of a species A may change with time in a manner described by the solution of the differential equation:

$$-\frac{d[A]}{dt} = k[A] \tag{7.7}$$

- In quantum mechanics, the value of a wave function, ψ, changes with the position. For a single particle system, ψ is obtained as the solution of the Schrödinger equation:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi \tag{7.8}$$

where the **Hamiltonian** operator, $\hat{H}$, given by $-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$, is associated with the total energy, E, and $V(x)$ is the potential energy of the particle; m is the mass of the particle and $\hbar$ is the Planck constant divided by 2π.

- In spectroscopy, the response of a molecule to an oscillating electromagnetic field leads to absorption of energy, the details of which are revealed after solving an equation of the form:

$$i\hbar\frac{d\psi}{dt} = \left\{\hat{H} + \hat{H}'(t)\right\}\psi \qquad (7.9)$$

i is the imaginary number $\sqrt{-1}$ (see Chapter 2, Volume 2).

- In vibrational spectroscopy, where the treatment of molecular vibrations is based on the differential equation for an harmonic oscillator:

$$\frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \tfrac{1}{2}kx^2\psi = E\psi \qquad (7.10)$$

In all of the examples given above, we are faced with having to deal with the relationship between some property and its rate of change. The differential equations that describe such relationships contain first-, second- or even higher-order derivatives. Most examples of this type of equation that we meet in chemistry are either of the first or second order, and so this is where we shall concentrate our efforts.

7.3 First-order Differential Equations

As already indicated, a *first-order* differential equation involves the *first* derivative of a function, and takes the general form:

$$\frac{dy}{dx} = F(x, y) \qquad (7.11)$$

where y is a function of x, and $F(x,y)$ is, in general, a function of *both* x and y. The method used to solve equation (7.11) depends upon the form of $F(x,y)$.

7.3.1 *F(x,y)* is Independent of *y*

In this simplest example, where $F(x,y) = f(x)$, the general solution is found by a simple one-step integration:

$$\frac{dy}{dx} = f(x) \Rightarrow y = \int f(x)dx = F(x) + C \qquad (7.12)$$

where $F(x) + C$ is the indefinite integral and C is the constant of integration (see Chapter 6), which can, in principle, take any value. It is important to note that the solution to a *first-order* equation involves:

- *One* step of integration.
- *One* constant of integration.

The solution of an nth order differential equation involves n steps of integration and yields n constants of integration.

Worked Problem 7.1

Q Solve $\frac{dy}{dx} = x^2 + 1$.

A Simple integration yields the general solution:

$$y = \frac{x^3}{3} + x + C$$

which can be described in terms of a family of cubic functions, each with a different value of C (see Figure 7.2). In this example, $F(x) = \frac{x^3}{3} + x$.

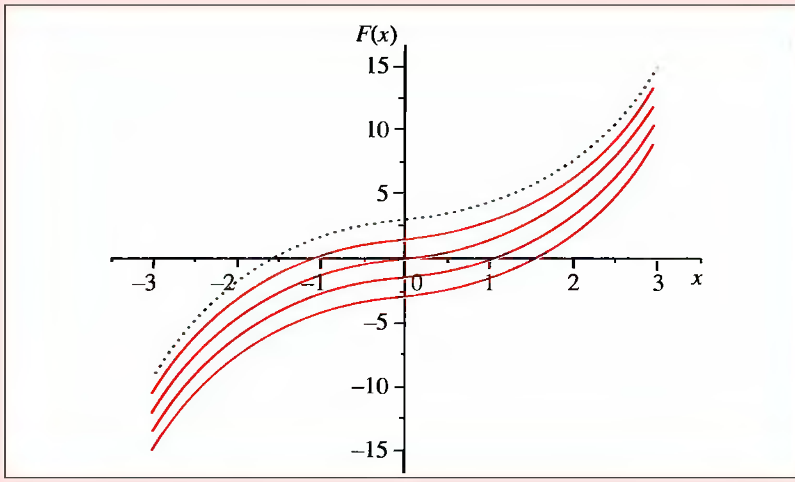

Figure 7.2 The family of solutions $y = \frac{x^3}{3} + x + C$ (for $C = \ldots, 3, 1.5, 0, -1.5, -3, \ldots$) to the differential equation $\frac{dy}{dx} = x^2+1$. Note that $F(x) = \frac{x^3}{3}+x$. The *dashed line* is the solution satisfying the boundary condition $y=0$, $x=3$

7.3.2 Boundary Conditions

In the case of a first-order differential equation, the constant of integration is usually determined by a **boundary condition**, or constraint on the solution. For example, if y is known at $x=0$, then this boundary condition is sufficient to determine the constant of integration, C. Thus, out of the family of possible solutions, only one solution is acceptable and this is the one satisfying the boundary condition.

For example, if the boundary condition for the solution of the differential equation in Worked Problem 7.1 is such that $y=3$ at $x=0$, then the solution is constrained to take the form:

$$y = F(x) + 3 = \frac{x^3}{3} + x + 3$$

since $F(0) = 0 \Rightarrow C = 3$ (see the dashed-line solution in Figure 7.2).