8 Partial differentials

If a function depends on more than one variable, its rate of change with respect to one of the variables can be determined keeping the others fixed. The differential is then a **partial differential**. The partial differential of $f(x, y, z)$ with respect x is denoted

$$\left(\frac{\partial f}{\partial x}\right)_{y,z},$$

the subscript y, z indicating that the variables y and z are kept constant. The second partial differential with respect to x is written

$$\left(\frac{\partial^2 f}{\partial x^2}\right)_{y,z}.$$

The subscripts are often omitted when it is obvious which variables are held fixed.

The partial differential of $(\partial f/\partial x)$ need not be with respect to x; it can be with respect to one of the other variables, say y, keeping x and z constant. It is written

$$\left(\frac{\partial^2 f}{\partial x \partial y}\right).$$

8.1 Functions of two variables

The formal definition of the partial derivative of a function $f(x, y)$ with respect to x with y constant is analogous to equation 2.3 for a function of one variable.

$$\left(\frac{\partial f}{\partial x}\right)_y = \frac{f(x + \partial x, y) - f(x, y)}{\partial x}, \tag{8.1}$$

where ∂x is the limit of a very small change in x as that change tends to zero. A similar equation holds for the partial derivative with respect to y with x constant and the infinitessimal change $\mathrm{d}f$ in the function f when both x and y change, by $\mathrm{d}x$ and $\mathrm{d}y$ respectively, is

$$\mathrm{d}f = \left(\frac{\partial f}{\partial x}\right)_y \mathrm{d}x + \left(\frac{\partial f}{\partial y}\right)_x \mathrm{d}y. \tag{8.2}$$

The last equation can be used to derive an identity which is often useful when dealing with functions of two variables. If we put $\mathrm{d}f = 0$ (f=const) the equation reduces

$$\left(\frac{\partial f}{\partial x}\right)_y \mathrm{d}x = -\left(\frac{\partial f}{\partial y}\right)_x \mathrm{d}y,$$

and hence

$$\left(\frac{\partial f}{\partial x}\right)_y \left(\frac{\partial x}{\partial y}\right)_f = -\left(\frac{\partial f}{\partial y}\right)_x. \tag{8.3}$$

For the smooth functions usually met in physics, which have no singularities where the function is double-valued,

$$\left(\frac{\partial f}{\partial y}\right)_x = 1/\left(\frac{\partial y}{\partial f}\right)_x,$$

and equation 8.3 can be written in its usual form

$$\left(\frac{\partial f}{\partial x}\right)_y \left(\frac{\partial x}{\partial y}\right)_f \left(\frac{\partial y}{\partial f}\right)_x = -1. \tag{8.4}$$

Example 8.1 Determine $(\partial f/\partial x)_y$ and $(\partial f/\partial y)_x$ for the function $f(x, y) = (x + y)^2$ and use equation 8.4 to deduce $(\partial x/\partial y)_f$. Verify the answer by expressing x as a function of f and y and determining $(\partial x/\partial y)_f$ directly.

Solution

$$(x + y)^2 = x^2 + 2xy + y^2.$$

$$\left(\frac{\partial f}{\partial x}\right)_y = 2x + 2y; \left(\frac{\partial f}{\partial y}\right)_x = 2x + 2y.$$

Hence

$$\left(\frac{\partial y}{\partial f}\right)_x = \frac{1}{(2x + 2y)},$$

and from equation 8.4

$$(\partial x/\partial y)_f = -1.$$

Expressing x as a function of f, the solution to the quadratic equation $x^2 + 2xy + y^2 - f = 0$ is

$$2x = -2y \pm \sqrt{4y^2 - 4(y^2 - f)},$$

or

$$x = -y \pm \sqrt{4f}$$

from which

$$(\partial x/\partial y)_f = -1.$$

Problem 8.1 For well-behaved functions,

$$\left(\frac{\partial^2 f}{\partial x \partial y}\right) = \left(\frac{\partial^2 f}{\partial y \partial x}\right).$$

Show this to be true for the function $f = (x + y)^3 - x^2$.

8.2 Functions of three variables

Space is three-dimensional, and functions of three variables are more often encountered in real situations than functions of two. The partial differentials of a function $f(x, y, z)$ with respect to one of the variables are now evaluated keeping the other two constant and for completeness two subscripts are needed on the derivative, although for first differentials it is easy to see that there is no ambiguity.

The infinitesimal change in f when the variables are changed infinitesimally is

$$\mathrm{d}f = \left(\frac{\partial f}{\partial x}\right)_{y,z} \mathrm{d}x + \left(\frac{\partial f}{\partial y}\right)_{z,x} \mathrm{d}y + \left(\frac{\partial f}{\partial z}\right)_{x,y} \mathrm{d}z. \tag{8.5}$$

Example 8.2

Show that for the function $f = \ln(x^3 + y^2 + z)$

$$\frac{\partial^3 f}{\partial x \partial y \partial z} = \frac{\partial^3 f}{\partial z \partial x \partial y}.$$

Solution

$$\frac{\partial f}{\partial x} = \frac{1}{(x^3 + y^2 + z)} 3x^2,$$

$$\frac{\partial^2 f}{\partial x \partial y} = -\frac{1}{(x^3 + y^2 + z)^2} 6x^2 y,$$

and

$$\frac{\partial^3 f}{\partial x \partial y \partial z} = \frac{1}{(x^3 + y^2 + z)^3} 12x^2 y.$$

Similar differentiation in the order of first z then x then y gives the same answer.

Problem 8.2 For the function f of Example 8.2 prove that

$$\frac{\partial^2 f}{\partial x \partial y} = \left(\frac{\partial}{\partial x}\right) \left[-\left(\frac{\partial f}{\partial z}\right) \left(\frac{\partial z}{\partial y}\right) \right].$$

8.3 Partial differential equations

Much of theoretical physics is formulated in terms of partial differential equations, that is, equations involving the partial derivatives of functions of several variables. The equations may be first- or second-order and may be linear or non-linear. However, those susceptible to solution in closed form, that is, solved without recourse to numerical solution using computers, are usually linear and of these those usually met are second-order.

An example involving two variables is the wave equation for a particle of mass m moving under the influence of a time-dependent force which can be represented by a potential $V(x, y, z, t)$. The partial differential equation for the wave function ϕ is

$$-\frac{\hbar^2}{2m} \left(\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} + \frac{\partial^2 \phi}{\partial z^2} \right) + V(x, y, z, t)\phi = j\hbar \frac{\partial \phi}{\partial t}, \tag{8.6}$$

where $\hbar$ is a constant and $j = \sqrt{-1}$.

If the potential is independent of time, the physical interpretation of ϕ requires that the equation simplifies to

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2\phi}{\partial x^2}+\frac{\partial^2\phi}{\partial y^2}+\frac{\partial^2\phi}{\partial z^2}\right)+V(x,y,z)\phi=E\phi, \tag{8.7}$$

where E is a constant. If $V=(1/2)k(x^2+y^2+z^2)$, the differential equation to be solved for ϕ is

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2\phi}{\partial x^2}+\frac{\partial^2\phi}{\partial y^2}+\frac{\partial^2\phi}{\partial z^2}\right)+\frac{1}{2}k(x^2+y^2+z^2)\phi=E\phi. \tag{8.8}$$

A method which may be successful for the solution of partial differential equations and which can be used to help solve the above is the **separation of variables**. Assume a form of the solution and see if, by substitution in the equation, it results in a new equation in which one side contains all the references to one of the variables. Since both sides are now independent of each other they must both be equal to a constant and we have an equation involving one variable only. That variable is said to be separated.

Example 8.3 In trying to solve equation 8.8 assume a solution of the form $\phi=X(x)Y(y)Z(z)$ and separate the variables.

Solution

$$\frac{\partial^2\phi}{\partial x^2}=Y(y)Z(z)\frac{\partial^2 X}{\partial x^2},$$

and similarly

$$\frac{\partial^2\phi}{\partial y^2}=X(x)Z(z)\frac{\partial^2 Y}{\partial y^2}$$

$$\frac{\partial^2\phi}{\partial z^2}=X(x)Y(y)\frac{\partial^2 Z}{\partial z^2}.$$

Substitution in equation 8.8 gives

$$-\frac{\hbar^2}{2m}\left(YZ\frac{\partial^2 X}{\partial x^2}+XZ\frac{\partial^2 Y}{\partial y^2}+XY\frac{\partial^2 Z}{\partial z^2}\right)+\frac{1}{2}k(x^2+y^2+z^2)XYZ=E\ XYZ,$$

and dividing both sides by XYZ leads to

$$-\frac{\hbar^2}{2m}\left(\frac{1}{X}\frac{\partial^2 X}{\partial x^2}+\frac{1}{Y}\frac{\partial^2 Y}{\partial y^2}+\frac{1}{Z}\frac{\partial^2 Z}{\partial z^2}\right)+\frac{1}{2}k(x^2+y^2+z^2)=E.$$

All three variables are now separable resulting in equations of the form

$$\frac{1}{X}\left(\frac{\partial^2 X}{\partial x^2}\right)+Ax^2=B,$$

with A and B constants.

Problem 8.3 A quantum mechanical particle is constrained to move in a square box of side a. Its wave functions are given by the solutions of equation 8.7 and their energies are given by different possibilities for the the number E. The potential V is zero inside the box but infinite outside so that the particle's wave function must be zero at the walls of the box. Show that the smallest value of the energy E is

$$\frac{3\pi^2\hbar^2}{2ma^2}.$$

Choose one of the bottom corners of the square to be at $x = y = z = 0$ and remember that since the potential is zero in the box all possible energies E are greater than zero.