

# 4 Vector Analysis

## 4.1 INTRODUCTION

To provide a mathematical description of a particle in space it is essential to specify not only its mass, but also its position (perhaps with respect to an arbitrary origin), as well as its velocity (and hence its momentum). Its mass is constant and thus independent of its position and velocity, at least in the absence of relativistic effects. It is also independent of the system of coordinates used to locate it in space. Its position and velocity, on the other hand, which have direction as well as magnitude, are vector quantities. Their descriptions depend on the choice of coordinate system. In this chapter Heaviside's notation will be followed,\* *viz.* a scalar quantity is represented by a symbol in plain italics, while a vector is printed in bold-face italic type.

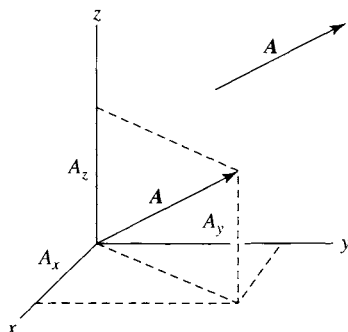
A useful image of a vector, which is independent of the notion of a coordinate system, is simply an arrow in space. The length of the arrow represents the magnitude of the vector, while its orientation in space specifies the direction of the vector. By convention the tail of the arrow is the origin of the (positive) vector and the head its terminus.

Although it is not at all necessary to describe a vector with reference to a system of coordinates, it is often useful to do so. The vector  $A$  shown in Fig. 1 represents the same quantity in either case. However, when attached to an origin (or any other given point) it can be expressed in terms of its components, which are its projections along a given set of coordinate axes. In the case of a Cartesian system<sup>†</sup> the magnitude of the vector  $A$ , the length of the arrow, is given by

$$A = \sqrt{A_x^2 + A_y^2 + A_z^2}. \quad (1)$$

\*Oliver Heaviside, British mathematician (1850–1925).

<sup>†</sup>René Descartes, French philosopher, mathematician (1596–1650).



**Fig. 1** A vector  $A$  in space and in a Cartesian coordinate system.

## 4.2 VECTOR ADDITION

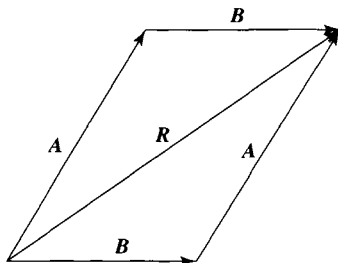
The basic algebra of vectors is formulated with the aid of geometrical arguments. Thus, the sum of two vectors  $A$  and  $B$ , can be obtained as shown in Fig. 2. To add  $B$  to  $A$ , the origin of  $B$  is placed at the head of  $A$  and the vector sum, represented by  $R$ , is constructed from the tail of  $A$  to the head of  $B$ . Clearly, the addition of  $A$  to  $B$  yields the same result (see Fig. 2); hence,

$$A + B = B + A = R \quad (2)$$

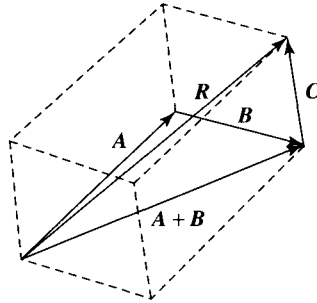
and vector addition is commutative.

When three vectors  $A$ ,  $B$  and  $C$  are added, the resultant  $R$  is the diagonal of the parallelepiped whose edges are the vectors, as shown in Fig. 3. The same result is obtained if any two of the vectors are combined and the sum is added to the third. Thus,

$$(A + B) + C = A + (B + C) = (C + A) + B = A + B + C = R, \quad (3)$$



**Fig. 2** The vector sum  $R = A + B$ .



**Fig. 3** The vector sum  $R = A + B + C$ .

and the associative law holds. Obviously, to subtract  $B$  from  $A$ , minus  $B$  is added to  $A$ , viz.

$$A - B = A + (-B). \quad (4)$$

It should be noted that in the above presentation of the combination of vectors by addition or subtraction, no reference has been made to their components, although this concept was introduced in the beginning of this chapter. It is, however, particularly useful in the definition of the product of vectors and can be further developed with the use of unit vectors. In the Cartesian system employed in Fig. 1 the unit vectors can be defined as shown in Fig. 4. It is apparent that

$$A = A_x \mathbf{i} + A_y \mathbf{j} + A_z \mathbf{k} \quad (5)$$

and similarly for another vector

$$B = B_x \mathbf{i} + B_y \mathbf{j} + B_z \mathbf{k}. \quad (6)$$

The sum of these vectors is then given by

$$A_x \mathbf{i} + B_x \mathbf{i} = (A_x + B_x) \mathbf{i} \quad (7)$$

*etc.* for the other components. Then,

$$A + B = (A_x + B_x) \mathbf{i} + (A_y + B_y) \mathbf{j} + (A_z + B_z) \mathbf{k}, \quad (8)$$

where the magnitudes of parallel vectors have been added as scalars. In other words the components of the vectors can be added to obtain the components of their sums.

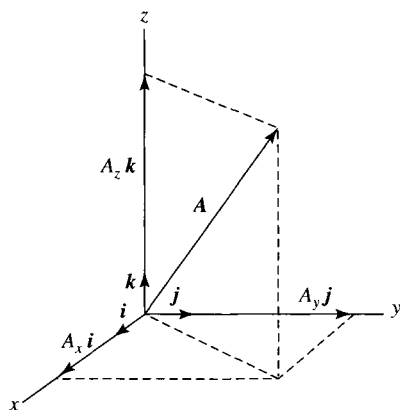


Fig. 4 Definition of the unit vectors  $i, j, k$ .

### 4.3 SCALAR PRODUCT

The scalar (or inner) product of two vectors is defined by the relation

$$\mathbf{A} \cdot \mathbf{B} = AB \cos \theta, \quad (9)$$

where  $\theta$  is the angle between the vectors  $\mathbf{A}$  and  $\mathbf{B}$ . Therefore, the scalar product of two perpendicular vectors must vanish, as  $\theta = \pi/2$  and  $\cos \theta = 0$ . Similarly, the scalar product of any unit vector with itself must be equal to unity, as  $\theta = 0$  and, hence,  $\cos \theta = 1$ . In terms of the unit vectors shown in Fig. 4,

$$\mathbf{i} \cdot \mathbf{j} = \mathbf{j} \cdot \mathbf{k} = \mathbf{k} \cdot \mathbf{i} = 0 \quad (10)$$

and

$$\mathbf{i} \cdot \mathbf{i} = \mathbf{j} \cdot \mathbf{j} = \mathbf{k} \cdot \mathbf{k} = i^2 = j^2 = k^2 = 1. \quad (11)$$

From Eqs. (9) and (11) it is evident that

$$\mathbf{A} \cdot \mathbf{B} = A_x B_x + A_y B_y + A_z B_z \quad (12)$$

in a Cartesian coordinate system.

The scalar product, often called the “dot product”, obeys the commutative and distributive laws of ordinary multiplication, *viz.*

$$\mathbf{A} \cdot \mathbf{B} = \mathbf{B} \cdot \mathbf{A} \quad (13)$$

and

$$\mathbf{A} \cdot (\mathbf{B} + \mathbf{C}) = (\mathbf{A} \cdot \mathbf{B}) + (\mathbf{A} \cdot \mathbf{C}). \quad (14)$$

Furthermore, it is seen from Eq. (9) that any relation involving the cosine of an included angle may be written in terms of the scalar product of the vectors which define it. Finally, the reader is warned that a relation such as  $A \cdot B = A \cdot C$  does not imply that  $B = C$ , as

$$A \cdot B - A \cdot C = A \cdot (B - C) = 0. \tag{15}$$

Thus, the correct conclusion is that  $A$  is perpendicular to the vector  $B - C$ .

### 4.4 VECTOR PRODUCT

Another way of combining two vectors is with the use of the vector (or outer) product. A description of this product can be developed with reference to Fig. 5. If  $A$  and  $B$  are two arbitrary vectors drawn from a common origin, they define a plane, providing of course that  $\theta$ , the angle between them, lies in the range  $0 < \theta < \pi$ . If a vector  $C$  is constructed at the same origin and perpendicular to the plane, Eq. (12) leads to

$$C \cdot A = C_x A_x + C_y A_y + C_z A_z = 0, \tag{16}$$

and

$$C \cdot B = C_x B_x + C_y B_y + C_z B_z = 0. \tag{17}$$

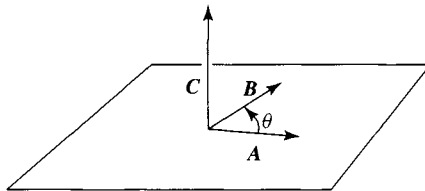
Equations (16) and (17) form a pair of simultaneous, homogeneous equations. They cannot be solved uniquely for the components of  $C$ . However, their solution can be found in terms of a parameter  $a$ . The result, which can be easily verified (problem 1), is

$$C_x = a(A_y B_z - A_z B_y), \tag{18}$$

$$C_y = a(A_z B_x - A_x B_z) \tag{19}$$

and

$$C_z = a(A_x B_y - A_y B_x). \tag{20}$$



**Fig. 5** The vector product  $C = A \times B$ .

The parameter  $a$  is arbitrary and, for convenience, can be chosen equal to plus one. Then, from Eq. (1) and Eqs. (18) to (20),

$$\begin{aligned} C^2 &= C_x^2 + C_y^2 + C_z^2 = (A_x^2 + A_y^2 + A_z^2)(B_x^2 + B_y^2 + B_z^2) \\ &\quad - (A_x B_x + A_y B_y + A_z B_z)^2 \\ &= A^2 B^2 - A^2 B^2 \cos^2 \theta \\ &= (AB \sin \theta)^2 \end{aligned} \quad (21)$$

Thus, the vector  $\mathbf{C}$  represents the product of the vectors  $\mathbf{A}$  and  $\mathbf{B}$  such that its length is given by  $C = AB \sin \theta$ . In the usual notation  $\mathbf{C} = \mathbf{A} \times \mathbf{B}$ .<sup>\*</sup> This operation is referred to as the vector product of the two vectors and in the jargon used in this application it is called the “cross product”. It must then be carefully distinguished from the dot product defined by Eq. (9).

With the use of Eqs. (18) to (20) the vector product can be written in the form

$$\mathbf{C} = \mathbf{A} \times \mathbf{B} = (A_y B_z - A_z B_y)\mathbf{i} + (A_z B_x - A_x B_z)\mathbf{j} + (A_x B_y - A_y B_x)\mathbf{k}, \quad (22)$$

which is represented by

$$\mathbf{A} \times \mathbf{B} = \mathbf{i} \begin{vmatrix} A_y & A_z \\ B_y & B_z \end{vmatrix} + \mathbf{j} \begin{vmatrix} A_x & A_z \\ B_x & B_z \end{vmatrix} + \mathbf{k} \begin{vmatrix} A_x & A_y \\ B_x & B_y \end{vmatrix}, \quad (23)$$

or more conveniently by the single determinant

$$\mathbf{A} \times \mathbf{B} = \begin{vmatrix} A_x & A_y & A_z \\ B_x & B_y & B_z \\ \mathbf{i} & \mathbf{j} & \mathbf{k} \end{vmatrix}. \quad (24)$$

Following the general rules for the development of determinants (see Section 7.4), it is apparent that vector multiplication is not commutative, as  $\mathbf{A} \times \mathbf{B} = -\mathbf{B} \times \mathbf{A}$ . However, the normal distributive law still applies, as, for example,

$$\mathbf{A} \times (\mathbf{B} + \mathbf{C}) = \mathbf{A} \times \mathbf{B} + \mathbf{A} \times \mathbf{C}. \quad (25)$$

From the definition of the vector product given above, it is clear that the magnitude of the vector  $\mathbf{C}$  in Eq. (22) is equal to the area of the parallelogram defined by the vectors  $\mathbf{A}$  and  $\mathbf{B}$  which describe its sides. However, there are two problems associated with this definition. First of all, the direction of the vector  $\mathbf{C}$  is ambiguous in the absence of a convention. It is usually assumed, however, that the “right-hand rule” applies. Thus, if the first finger of the right

<sup>\*</sup>The notation  $\mathbf{C} = \mathbf{A} \wedge \mathbf{B}$  is used for the vector product in most texts in French.

hand is directed along  $A$  and the second along  $B$ , the direction of the vector  $C$  is indicated by the thumb.

A second question arises for those who understand the importance of dimensional analysis, a subject that is treated briefly in Appendix II. If  $A$  and  $B$  are both vector quantities with, say, dimensions of length, how can their cross product result in a vector  $C$ , presumably with dimensions of length? The answer is hidden in the homogeneous equations developed above [Eqs. (18) to (20)]. The constant  $a$  was set equal to unity. However, in this case it has the dimension of reciprocal length. In other words,  $C = aAB \sin \theta$  is the length of the vector  $C$ . In general, a vector such as  $C$  which represents the cross product of two "ordinary" vectors is an areal vector with different symmetry properties from those of  $A$  and  $B$ .

#### 4.5 TRIPLE PRODUCTS

Triple products involving vectors arise often in physical problems. One such product is  $(A \times B) \times C$ , which is clearly represented by a vector. It is therefore called the vector triple product, whose development can be made as follows. If, in a Cartesian system, the vector  $A$  is chosen to be collinear with the  $x$  direction,  $A = A_x i$ . The vector  $B$  can, without loss of generality, be placed in the  $x,y$  plane. It is then given by  $B = B_x i + B_y j$ . The vector  $C$  is then in a general direction, as given by  $C = C_x i + C_y j + C_z k$ , as shown in Fig. 6. Then, the cross products can be easily developed in the form  $A \times B = A_x B_y k$  and

$$(A \times B) \times C = -A_x B_y C_y i + A_x B_y C_x j. \quad (26)$$

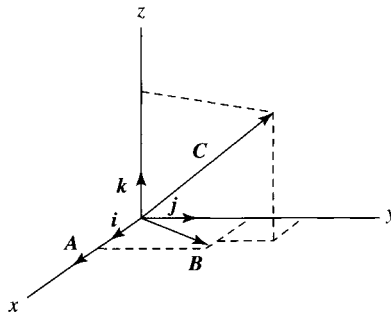


Fig. 6 Development of the triple product  $(A \times B) \times C$ .

The evaluation of the scalar products  $\mathbf{A} \cdot \mathbf{C}$  and  $\mathbf{B} \cdot \mathbf{C}$  and substitution into Eq. (26) leads to the relation

$$(\mathbf{A} \times \mathbf{B}) \times \mathbf{C} = (\mathbf{A} \cdot \mathbf{C})\mathbf{B} - (\mathbf{B} \cdot \mathbf{C})\mathbf{A}. \quad (27)$$

An analogous derivation can be carried out to obtain

$$\mathbf{C} \times (\mathbf{A} \times \mathbf{B}) = (\mathbf{C} \cdot \mathbf{B})\mathbf{A} - (\mathbf{C} \cdot \mathbf{A})\mathbf{B} \quad (28)$$

(problem 4). The two expansions of the triple vector products given by Eqs. (27) and (28) are very useful in the manipulation of vector relations. Furthermore, vector multiplication is not associative. In general,

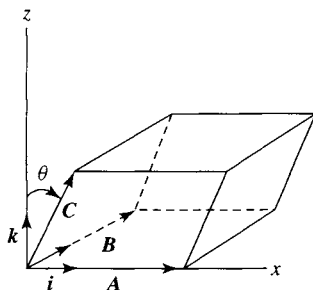
$$(\mathbf{A} \times \mathbf{B}) \times \mathbf{C} \neq \mathbf{A} \times (\mathbf{B} \times \mathbf{C}), \quad (29)$$

as can be shown by developing Eqs. (27) and (28).

Consider now the vector product  $\mathbf{A} \times \mathbf{B}$ , where these vectors are shown in Fig. 7. It is perpendicular to the  $x, y$  plane and has a magnitude equal to  $A_x B_y$ , the area of the base of the parallelepiped. The height of the parallelepiped is given by  $C_z = C \cos \theta$ . Therefore, the volume of the parallelepiped is equal to  $(\mathbf{A} \times \mathbf{B}) \cdot \mathbf{C} = \mathbf{A} \cdot \mathbf{B} \times \mathbf{C}$ , which can also be written in the form of a determinant of the components, *viz.*

$$\mathbf{A} \cdot \mathbf{B} \times \mathbf{C} = \begin{vmatrix} A_x & A_y & A_z \\ B_x & B_y & B_z \\ C_x & C_y & C_z \end{vmatrix}. \quad (30)$$

It should be noted that the positive sign of this result depends on the choice of a right-handed coordinate system in which the angle  $\theta$  is acute. The relation developed here for the volume of a parallelepiped is often employed in crystallography to calculate the volume of a unit cell, as shown in the following section.



**Fig. 7** Calculation of the volume of a parallelepiped.



An important symmetry property of the scalar triple product can be illustrated by the relations

$$(\mathbf{A} \times \mathbf{B}) \cdot \mathbf{C} = (\mathbf{B} \times \mathbf{C}) \cdot \mathbf{A} = (\mathbf{C} \times \mathbf{A}) \cdot \mathbf{B}, \quad (31)$$

that is, successive cyclic permutation. However, it changes sign upon interchange of any two vectors. These results follow directly from the properties of the determinant, Eq. (30). Furthermore, the value of the triple scalar product is not altered by the exchange of the symbols “dot” and “cross”; thus,

$$\mathbf{A} \times \mathbf{B} \cdot \mathbf{C} = \mathbf{B} \times \mathbf{C} \cdot \mathbf{A} = \mathbf{A} \cdot \mathbf{B} \times \mathbf{C}, \quad (32)$$

nor are the parentheses necessary in this case.

## 4.6 RECIPROCAL BASES

A set of three noncoplanar vectors forms a basis in a three-dimensional space. Any vector in this space can be represented by these three basis vectors. In certain applications, particularly in crystallography, it is convenient to define a second basis, in reciprocal space. Thus, if the vectors  $\mathbf{t}_1, \mathbf{t}_2$  and  $\mathbf{t}_3$  form a basis, in which  $\mathbf{t}_1 \times \mathbf{t}_2 \cdot \mathbf{t}_3 \neq 0$ , another basis can be defined by the vectors  $\mathbf{b}_1, \mathbf{b}_2$  and  $\mathbf{b}_3$ . The two bases are said to be reciprocal if

$$\mathbf{t}_i \cdot \mathbf{b}_j = \delta_{i,j}, \quad (33)$$

where  $i, j = 1, 2, 3$  and  $\delta_{i,j}$  is the Kronecker delta.\* Thus, for example,  $\mathbf{t}_1 \cdot \mathbf{b}_1 = 1, \mathbf{t}_1 \cdot \mathbf{b}_2 = 0$  and  $\mathbf{t}_1 \cdot \mathbf{b}_3 = 0$ . These relations show that  $\mathbf{b}_1$  is perpendicular to both  $\mathbf{t}_2$  and  $\mathbf{t}_3$ ; it is therefore parallel to  $\mathbf{t}_2 \times \mathbf{t}_3$ . Then,  $\mathbf{b}_1 = c \mathbf{t}_2 \times \mathbf{t}_3$ , where  $c$  is a constant. Scalar multiplication by  $\mathbf{t}_1$  then gives  $\mathbf{t}_1 \cdot \mathbf{b}_1 = c \mathbf{t}_1 \cdot \mathbf{t}_2 \times \mathbf{t}_3 = 1$ . These relations then lead to the expression

$$\mathbf{b}_1 = \frac{\mathbf{t}_2 \times \mathbf{t}_3}{\mathbf{t}_1 \cdot \mathbf{t}_2 \times \mathbf{t}_3}. \quad (34)$$

The corresponding relations for  $\mathbf{b}_2$  and  $\mathbf{b}_3$  follow by cyclic permutations of the subscripts (see Chapter 8).

An infinite three-dimensional crystal lattice is described by a primitive unit cell which generates the lattice by simple translations. The primitive cell can be represented by three basic lattice vectors such as  $\mathbf{t}_1, \mathbf{t}_2$  and  $\mathbf{t}_3$  defined above. They may or may not be mutually perpendicular, depending on the crystal

\*Leopold Kronecker, German mathematician (1823–1891).

system. The volume of the primitive cell is equal to  $\mathbf{t}_1 \times \mathbf{t}_2 \cdot \mathbf{t}_3$  and the position of each lattice point is specified by a vector

$$\boldsymbol{\tau}_n = n_1 \mathbf{t}_1 + n_2 \mathbf{t}_2 + n_3 \mathbf{t}_3, \quad (35)$$

where  $n_1, n_2$  and  $n_3$  are integers.

The vectors which define the so-called reciprocal lattice are given by

$$\mathbf{k}_h = h_1 \mathbf{b}_1 + h_2 \mathbf{b}_2 + h_3 \mathbf{b}_3, \quad (36)$$

where  $h_1, h_2$  and  $h_3$  are integers. The analog of the primitive cell in reciprocal space is known as the first Brillouin zone.\* Its volume is given by

$$\mathbf{b}_1 \cdot \mathbf{b}_2 \times \mathbf{b}_3 = \frac{(\mathbf{t}_2 \times \mathbf{t}_3) \cdot [(\mathbf{t}_3 \times \mathbf{t}_1) \times (\mathbf{t}_1 \times \mathbf{t}_2)]}{(\mathbf{t}_1 \cdot \mathbf{t}_2 \times \mathbf{t}_3)^3} = \frac{1}{\mathbf{t}_1 \cdot \mathbf{t}_2 \times \mathbf{t}_3}. \quad (37)$$

The conclusion to be drawn from Eq. (37) is that the volume of the first Brillouin zone is equal to the reciprocal of the volume of the primitive cell. It should be noted that the scalar product

$$\boldsymbol{\tau}_n \cdot \mathbf{k}_h = n_1 h_1 + n_2 h_2 + n_3 h_3 \quad (38)$$

is an integer.

## 4.7 DIFFERENTIATION OF VECTORS

If a vector  $\mathbf{R}$  is a function of a single scalar quantity  $s$ , the curve traced as a function of  $s$  by its terminus, with respect to a fixed origin, can be represented as shown in Fig. 8. Within the interval  $\Delta s$  the vector  $\Delta \mathbf{R} = \mathbf{R}_2 - \mathbf{R}_1$  is in the direction of the secant to the curve, which approaches the tangent in the limit as  $\Delta s \rightarrow 0$ . This argument corresponds to that presented in Section 2.3 and illustrated in Fig. 4 of that section. In terms of unit vectors in a Cartesian coordinate system

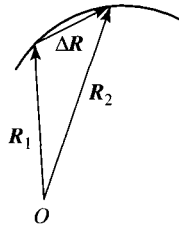
$$\mathbf{R} = i R_x + j R_y + k R_z, \quad (39)$$

and

$$\frac{d\mathbf{R}}{dt} = i \frac{dR_x}{dt} + j \frac{dR_y}{dt} + k \frac{dR_z}{dt}. \quad (40)$$

Clearly, Eq. (40) includes variations in both the magnitude and direction of the vector  $\mathbf{R}$ . It is easily generalized to represent higher derivatives. For a function

\*Léon Brillouin, French-American physicist (1889–1969).



**Fig. 8** Increment of a vector  $R$ .

of two or more vectors, each of which depends on the single scalar parameter  $s$ , the usual rules of differentiation hold, as summarized in Section 2.3 for scalar quantities. However, the order of the vectors must not be changed in cases involving the vector product. Specifically, if  $R(s)$  and  $S(s)$  are differentiable vector functions,

$$\frac{d(\mathbf{R} \times \mathbf{S})}{dt} = \mathbf{R} \times \frac{d\mathbf{S}}{dt} + \frac{d\mathbf{R}}{dt} \times \mathbf{S}, \quad (41)$$

where it is essential to preserve the order of the factors in each term on the right-hand side of Eq. (41).

## 4.8 SCALAR AND VECTOR FIELDS

The term scalar field is used to describe a region of space in which a scalar function is associated with each point. If there is a vector quantity specified at each point, the points and vectors constitute a vector field.

Suppose that  $\phi(x, y, z)$  is a scalar point function, that is, a scalar function that is uniquely defined in a given region. Under a change of coordinate system to, say,  $x', y', z'$ , it will take on another form, although its value at any point remains the same. Applying the chain rule (Section 2.12),

$$\frac{\partial \phi}{\partial x'} = \frac{\partial x}{\partial x'} \frac{\partial \phi}{\partial x} + \frac{\partial y}{\partial x'} \frac{\partial \phi}{\partial y} + \frac{\partial z}{\partial x'} \frac{\partial \phi}{\partial z} = a_{11} \frac{\partial \phi}{\partial x} + a_{12} \frac{\partial \phi}{\partial y} + a_{13} \frac{\partial \phi}{\partial z}, \quad (42)$$

$$\frac{\partial \phi}{\partial y'} = a_{21} \frac{\partial \phi}{\partial x} + a_{22} \frac{\partial \phi}{\partial y} + a_{23} \frac{\partial \phi}{\partial z} \quad (43)$$

and

$$\frac{\partial \phi}{\partial z'} = a_{31} \frac{\partial \phi}{\partial x} + a_{32} \frac{\partial \phi}{\partial y} + a_{33} \frac{\partial \phi}{\partial z}. \quad (44)$$

The quantities  $\partial\phi/\partial x$ ,  $\partial\phi/\partial y$  and  $\partial\phi/\partial z$  are components of a vector,

$$\nabla\phi = \mathbf{i} \frac{\partial\phi}{\partial x} + \mathbf{j} \frac{\partial\phi}{\partial y} + \mathbf{k} \frac{\partial\phi}{\partial z}, \quad (45)$$

which has been transformed from one coordinate system to another. This operation can be written in more compact form with the use of matrix algebra, a subject that is developed in Chapter 7.

Equation (44) suggests that a vector operator  $\nabla$  or nabla (called “del”) be defined in Cartesian coordinates by

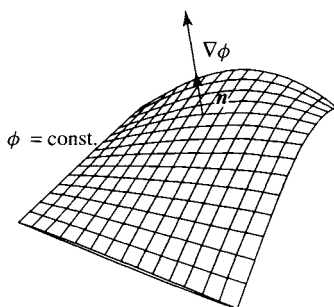
$$\nabla = \mathbf{i} \frac{\partial}{\partial x} + \mathbf{j} \frac{\partial}{\partial y} + \mathbf{k} \frac{\partial}{\partial z}. \quad (46)$$

This operator is not a vector in the geometrical sense, as it has no scalar magnitude. However, it transforms as a vector and thus can be treated formally as such.

## 4.9 THE GRADIENT

The operator del is defined in Cartesian coordinates by Eq. (46). The result of its operation on a scalar is called the gradient. Thus, Eq. (45) is an expression for the gradient of  $\phi$ , namely,  $\nabla\phi = \mathbf{grad} \phi$ , which is of course a vector quantity. The form of the differential operator del varies, however, depending on the choice of coordinates, as demonstrated in the following chapter.

To obtain a physical picture of the significance of the gradient, consider Fig. 9. The condition  $d\phi = 0$  produces a family of surfaces such as that shown. The change in  $\phi$  in passing from one surface to another will be the same regardless of the direction chosen. However, in the direction of  $\mathbf{n}$ , the normal



**Fig. 9** The normal  $\mathbf{n}$  to a surface and the gradient.

to the surface, the space rate of change of  $\phi$  will be maximum. It is the change in  $\phi$  in this direction that corresponds to the gradient.

#### 4.10 THE DIVERGENCE

The scalar product of the vector operator  $\nabla$  and a vector  $\mathbf{A}$  yields a scalar quantity, the divergence of  $\mathbf{A}$ . Thus,

$$\nabla \cdot \mathbf{A} = \text{div } \mathbf{A} = \left[ \mathbf{i} \frac{\partial}{\partial x} + \mathbf{j} \frac{\partial}{\partial y} + \mathbf{k} \frac{\partial}{\partial z} \right] \cdot [\mathbf{i} A_x + \mathbf{j} A_y + \mathbf{k} A_z] \quad (47)$$

$$= \frac{\partial A_x}{\partial x} + \frac{\partial A_y}{\partial y} + \frac{\partial A_z}{\partial z}. \quad (48)$$

If  $\mathbf{A}$  represents a vector field, the derivatives such as  $\partial A_x / \partial x$  transform normally under a change of coordinates.

As a simple example of the divergence, consider the quantity  $\nabla \cdot \mathbf{r}$ , where  $\mathbf{r} = x\mathbf{i} + y\mathbf{j} + z\mathbf{k}$ . Then,

$$\begin{aligned} \nabla \cdot \mathbf{r} &= \left( \mathbf{i} \frac{\partial}{\partial x} + \mathbf{j} \frac{\partial}{\partial y} + \mathbf{k} \frac{\partial}{\partial z} \right) \cdot (x\mathbf{i} + y\mathbf{j} + z\mathbf{k}) \\ &= \frac{\partial x}{\partial x} + \frac{\partial y}{\partial y} + \frac{\partial z}{\partial z} = 3. \end{aligned} \quad (49)$$

#### 4.11 THE CURL OR ROTATION

The vector product of  $\nabla$  and the vector  $\mathbf{A}$  is known as the curl or rotation of  $\mathbf{A}$ . Thus in Cartesian coordinates,

$$\begin{aligned} \text{curl } \mathbf{A} = \nabla \times \mathbf{A} &= \mathbf{i} \left[ \frac{\partial A_z}{\partial y} - \frac{\partial A_y}{\partial z} \right] + \mathbf{j} \left[ \frac{\partial A_x}{\partial z} - \frac{\partial A_z}{\partial x} \right] \\ &\quad + \mathbf{k} \left[ \frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y} \right] \end{aligned} \quad (50)$$

$$= \begin{vmatrix} \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ A_x & A_y & A_z \\ \mathbf{i} & \mathbf{j} & \mathbf{k} \end{vmatrix}. \quad (51)$$

In the development of the determinant in Eq. (51), care must be taken to preserve the correct order of the elements.

The following important relations involving the curl can be verified by expanding the vectors in terms of their components  $i$ ,  $j$  and  $k$  in Cartesian coordinates:

$$\nabla \times (\mathbf{A} + \mathbf{B}) = \nabla \times \mathbf{A} + \nabla \times \mathbf{B}, \quad (52)$$

$$\nabla \times (\phi \mathbf{A}) = \nabla \phi \times \mathbf{A} + \phi \nabla \times \mathbf{A}, \quad (53)$$

$$\begin{aligned} \nabla(\mathbf{A} \cdot \mathbf{B}) &= (\mathbf{B} \cdot \nabla)\mathbf{A} + (\mathbf{A} \cdot \nabla)\mathbf{B} \\ &\quad + \mathbf{B} \times (\nabla \times \mathbf{A}) + \mathbf{A} \times (\nabla \times \mathbf{B}), \end{aligned} \quad (54)$$

$$\nabla \cdot (\mathbf{A} \times \mathbf{B}) = \mathbf{B} \cdot \nabla \times \mathbf{A} - \mathbf{A} \cdot \nabla \times \mathbf{B} \quad (55)$$

and

$$\nabla \times (\mathbf{A} \times \mathbf{B}) = (\mathbf{B} \cdot \nabla)\mathbf{A} - \mathbf{B}(\nabla \cdot \mathbf{A}) - (\mathbf{A} \cdot \nabla)\mathbf{B} + \mathbf{A}(\nabla \cdot \mathbf{B}) \quad (56)$$

(problem 10).

## 4.12 THE LAPLACIAN\*

In addition to the above vector relations involving del, there are six combinations in which del appears twice. The most important one, which involves a scalar, is

$$\nabla \cdot \nabla \phi = \nabla^2 \phi = \mathit{div grad} \phi. \quad (57)$$

The operator  $\nabla^2$ , which is known as the Laplacian, takes on a particularly simple form in Cartesian coordinates, namely,

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}. \quad (58)$$

However, as shown in Section 5.15 it can become more complicated in other coordinate systems. When applied to a vector, it yields a vector, which is given in Cartesian coordinates by

$$\nabla^2 \mathbf{A} = \frac{\partial^2 \mathbf{A}}{\partial x^2} + \frac{\partial^2 \mathbf{A}}{\partial y^2} + \frac{\partial^2 \mathbf{A}}{\partial z^2}. \quad (59)$$

\*Pierre Simon de Laplace, French astronomer and mathematician (1749–1827).

A third combination which involves del operating twice on a vector is

$$\begin{aligned} \nabla(\nabla \cdot \mathbf{A}) = \mathbf{grad\,div\,A} = & \mathbf{i} \frac{\partial^2 A_x}{\partial x^2} + \mathbf{j} \frac{\partial^2 A_y}{\partial y^2} + \mathbf{k} \frac{\partial^2 A_z}{\partial z^2} \\ & + \mathbf{i} \left[ \frac{\partial^2 A_y}{\partial x \partial y} + \frac{\partial^2 A_z}{\partial x \partial z} \right] + \mathbf{j} \left[ \frac{\partial^2 A_x}{\partial x \partial y} + \frac{\partial^2 A_z}{\partial y \partial z} \right] + \mathbf{k} \left[ \frac{\partial^2 A_x}{\partial x \partial z} + \frac{\partial^2 A_y}{\partial y \partial z} \right]. \end{aligned} \quad (60)$$

The cross product of two del's operating on a scalar function  $\phi$  yields

$$\begin{aligned} \nabla \times \nabla \phi = \mathbf{curl\,grad\,\phi} \\ = \begin{vmatrix} \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ \frac{\partial \phi}{\partial x} & \frac{\partial \phi}{\partial y} & \frac{\partial \phi}{\partial z} \\ \mathbf{i} & \mathbf{j} & \mathbf{k} \end{vmatrix} = 0. \end{aligned} \quad (61)$$

If  $\nabla \times \mathbf{A} = 0$  for any vector  $\mathbf{A}$ , then  $\mathbf{A} = \nabla \phi$ . In this case  $\mathbf{A}$  is irrotational. Similarly,

$$\nabla \cdot \nabla \times \mathbf{A} = \mathbf{div\,curl\,A} = 0. \quad (62)$$

Finally, a useful expansion is given by the relation

$$\nabla \times (\nabla \times \mathbf{A}) = \mathbf{curl\,curl\,A} = \nabla(\nabla \cdot \mathbf{A}) - \nabla^2 \mathbf{A}. \quad (63)$$

### 4.13 MAXWELL'S EQUATIONS

To illustrate the use of the vector operators described in the previous section, consider the equations of Maxwell. In a vacuum they provide the basic description of an electromagnetic field in terms of the vector quantities  $\mathcal{E}$  the electric field and  $\mathcal{H}$  the magnetic field. The definition of the field in a dielectric medium requires the introduction of two additional quantities, the electric displacement  $\mathcal{D}$  and the magnetic induction  $\mathcal{B}$ . The macroscopic electromagnetic properties of the medium are then determined by Maxwell's equations, *viz.*

$$\nabla \cdot \mathcal{D} = \rho, \quad (64)$$

$$\nabla \cdot \mathcal{B} = 0, \quad (65)$$

$$\nabla \times \mathcal{H} = \mathbf{J} + \dot{\mathcal{D}} \quad (66)$$

and

$$\nabla \times \mathcal{B} = -\dot{\mathcal{A}}. \quad (67)$$

In these expressions  $\rho$  is the charge density in the medium and  $\mathbf{J}$  is the current density.

In isotropic media  $\mathcal{D}$  and  $\mathcal{B}$  are related by  $\mathcal{D} = \varepsilon\mathcal{B}$ , where the scalar parameter  $\varepsilon$  is now referred to as the permittivity.\* In the international (SI) system it is given by  $\varepsilon = \varepsilon_r\varepsilon_0$ , where  $\varepsilon_0$  is the permittivity of vacuum (see Appendix II) and  $\varepsilon_r$  is a dimensionless permittivity that characterizes the medium. Furthermore, according to Ohm's law<sup>†</sup> the current is given by  $\mathbf{J} = \sigma\mathcal{B}$ , where  $\sigma$  is the electrical conductivity. The relation  $\nabla \cdot \mathcal{B} = 0$  is a mathematical statement of the observation that isolated magnetic poles do not exist.

A very general relation, that is known as the equation of continuity, has applications in many branches of physics and chemistry. It can be derived by taking the divergence of Eq. (66). Then, from Eq. (62) the relation

$$\nabla \cdot \nabla \times \mathcal{H} = \nabla \cdot (\mathbf{J} + \dot{\mathcal{D}}) = \nabla \cdot \mathbf{J} + \dot{\rho} = 0, \quad (68)$$

and hence

$$\nabla \cdot \mathbf{J} = -\frac{\partial \rho}{\partial t}, \quad (69)$$

is easily obtained. This result can be interpreted in electromagnetic theory as follows. The divergence of the current density (flux) from a system must be compensated by the rate of decrease in charge density within the system. This statement is a special case of the general divergence theorem, which is derived in Appendix VI.

In atomic and molecular spectroscopy it is the electric field created by the light excitation that is the origin of the interaction with a sample. The effect of the magnetic field is several orders of magnitude weaker. In this application, then, unit relative permeability<sup>‡</sup> will be assumed and  $\mathcal{B}$  will be replaced by  $\mu_0\mathcal{H}$  in Eqs. (65) and (67). Equations (64) to (67) become

$$\nabla \cdot \mathcal{D} = \rho, \quad (70)$$

$$\nabla \cdot \mathcal{H} = 0, \quad (71)$$

$$\nabla \times \mathcal{H} = \sigma\mathcal{B} + \varepsilon\dot{\mathcal{B}} \quad (72)$$

and

$$\nabla \times \mathcal{B} = -\mu_0\dot{\mathcal{H}}, \quad (73)$$

\*This quantity was previously called the dielectric constant. It is in general a function of frequency and therefore not a constant.

<sup>†</sup>Georg Simon Ohm, German Physicist (1789–1854).

<sup>‡</sup>In the SI system  $\mathcal{B} = \mu\mathcal{H} = \mu_r\mu_0\mathcal{H}$ , where  $\mu$  is the permeability of the medium. Here again it is written as the product of the permeability of vacuum and a relative quantity  $\mu_r$ , by analogy with the permittivity (see Appendix II).



respectively. The curl of Eq. (73) yields the relation

$$\nabla \times (\nabla \times \mathcal{E}) = -\mu_0 \nabla \times \dot{\mathcal{H}}, \quad (74)$$

$$= -\mu_0 \sigma \dot{\mathcal{E}} - \mu_0 \varepsilon \ddot{\mathcal{E}}, \quad (75)$$

where the time derivative of Eq. (72) has been substituted. With the use of the vector relation given by Eq. (63) the differential equation for the electric field can be written as

$$\nabla^2 \mathcal{E} - \nabla(\nabla \cdot \mathcal{E}) = \mu_0 \varepsilon \ddot{\mathcal{E}} + \mu_0 \sigma \dot{\mathcal{E}}. \quad (76)$$

It can be easily demonstrated that plane-wave solutions to Eq. (76) are of the form

$$\mathcal{E} = \mathcal{E}^0 e^{-2\pi i(\mathbf{k} \cdot \mathbf{r} + \nu t)} \quad (77)$$

for monochromatic waves of frequency  $\nu$  propagating in the direction of  $\mathbf{r}$  (see problem 14). Here,  $\mathbf{k}$  is the propagation vector in reciprocal space.

From Eq. (77) the relations

$$\dot{\mathcal{E}} = -2\pi i \nu \mathcal{E}, \quad (78)$$

$$\nabla \cdot \mathcal{E} = -2\pi i \mathbf{k} \cdot \mathcal{E} \quad (79)$$

and

$$\nabla \times \mathcal{E} = -2\pi i \mathbf{k} \times \mathcal{E} \quad (80)$$

can be easily obtained. Their substitution in Eq. (76) yields

$$-(\mathbf{k} \cdot \mathcal{E})\mathbf{k} + (\mathbf{k} \cdot \mathbf{k})\mathcal{E} = -\nu^2 \mu_0 \left( \varepsilon + \frac{\sigma i}{2\pi \nu} \right) \mathcal{E} = \left( \frac{\nu}{c_0} \right)^2 \hat{n}^2 \mathcal{E}, \quad (81)$$

where by definition  $\hat{n}^2 = \varepsilon_r + \sigma i / 2\pi \nu \varepsilon_0$  is the square of the complex refractive index of the medium. By taking the scalar product of  $\mathbf{k}$  with Eq. (81) it is found that

$$\hat{n}^2 \mathbf{k} \cdot \mathcal{E} = 0. \quad (82)$$

Thus, as  $\hat{n}$  is not in general equal to zero,  $\mathbf{k} \cdot \mathcal{E} = 0$ , which describes a transverse wave, with the electric field perpendicular to the direction of propagation. The complex refractive index is then given by

$$\hat{n} = \sqrt{\varepsilon_r + \frac{\sigma i}{2\pi \nu \varepsilon_0}} = n + i\kappa, \quad (83)$$

the fundamental relation between the electrical and optical properties of a material. Note that in a nonconducting medium ( $\sigma = 0$ ) the permittivity is equal to the square of the (real) refractive index.

In an anisotropic solid both  $\varepsilon$  and  $\sigma$  become tensor quantities, that is they are represented by  $3 \times 3$  matrices (see Section 7.3). In general, then, a solid may exhibit anisotropy with respect to both the real and imaginary parts of the refractive index.

#### 4.14 LINE INTEGRALS

Line integrals were introduced in Section 3.4.3. The principles presented there can be easily recast within the vector formalism of this chapter. Thus,

$$\int_c \mathbf{A} \cdot d\mathbf{s} \quad (84)$$

is one form of the line integral from  $a$  to  $b$  along curve 1, as shown in Fig. 10. Its evaluation, which results in a scalar quantity, can be carried out if  $\mathbf{A} \cdot d\mathbf{s}$  is known as a function of the coordinates, say,  $x, y, z$ . A special case arises in which the function to be integrated is an exact differential (see Section 2.13). Thus, if

$$\mathbf{A} = \nabla\phi, \quad (85)$$

where  $\phi$  is a scalar point function,

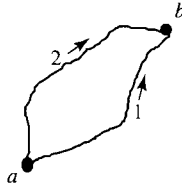
$$\begin{aligned} \int_a^b \mathbf{A} \cdot d\mathbf{s} &= \int_a^b \nabla\phi \cdot d\mathbf{s} = \int_a^b \left[ \frac{\partial\phi}{\partial x} dx + \frac{\partial\phi}{\partial y} dy + \frac{\partial\phi}{\partial z} dz \right] \\ &= \int_a^b d\phi = \phi_b - \phi_a. \end{aligned} \quad (86)$$

If the integration is taken around a closed curve, as shown in Fig. 10,\*

$$\int_a^a \nabla\phi \cdot d\mathbf{s} = \oint \nabla\phi \cdot d\mathbf{s} = 0. \quad (87)$$

Conversely, if  $\oint \nabla\phi \cdot d\mathbf{s} = 0$ , then Eq. (85) must hold and  $\mathbf{A}$  is the gradient of some scalar point function  $\phi$ . In conclusion, if  $\mathbf{A} = \nabla\phi$ , the line integral

\*The symbol  $\oint d\mathbf{s}$  represents a line integral around a closed path.



**Fig. 10** Evaluation of line integrals.

$\int_a^b \mathbf{A} \cdot d\mathbf{s}$  depends only on the initial and final values of  $\phi$  and is independent of the path.

The results obtained above are of fundamental importance in many physical problems. In mechanics, for example, a system is said to be conservative if the force on a given particle is given by

$$\mathbf{f} = -\nabla\phi, \quad (88)$$

where  $\phi$  is a scalar potential function. Thus, from Eq. (61),  $\nabla \times \mathbf{f} = 0$ , and the force is irrotational. Furthermore,  $\oint \nabla\phi \cdot d\mathbf{s} = 0$ , as shown.

In thermodynamics the state functions are independent of the path. That is, the reversible processes involved in passing from a given initial state to the final state are not involved in the resulting changes in such functions. The differentials of state functions are of course exact, as shown in Section 3.5.

#### 4.15 CURVILINEAR COORDINATES

In previous sections of this chapter, vectors have been described by their components in a Cartesian system. However, for most physical problems it is not the most convenient one. It is generally important to choose a system of coordinates that is compatible with the natural symmetry of the problem at hand. This natural symmetry is determined by the boundary conditions imposed on the solutions.

If the Cartesian coordinates  $x$ ,  $y$  and  $z$  are related to three new variables by

$$x = x(\xi_1, \xi_2, \xi_3), \quad (89)$$

$$y = y(\xi_1, \xi_2, \xi_3) \quad (90)$$

and

$$z = z(\xi_1, \xi_2, \xi_3). \quad (91)$$

The chain rule leads to expressions such as

$$dx = \frac{\partial x}{\partial \xi_1} d\xi_1 + \frac{\partial x}{\partial \xi_2} d\xi_2 + \frac{\partial x}{\partial \xi_3} d\xi_3, \quad (92)$$

with analogous relations for the other differentials. The most important case is that in which the new coordinates are orthogonal; that is, their surfaces  $\xi_i = \text{constant}$ , ( $i = 1,2,3$ ) intersect at right angles. Then, the square of the distance between two adjacent points is given by

$$(ds)^2 = (dx)^2 + (dy)^2 + (dz)^2 = h_1^2(d\xi_1)^2 + h_2^2(d\xi_2)^2 + h_3^2(d\xi_3)^2, \quad (93)$$

where the  $h_i$ 's are scale factors, with

$$h_i^2 = \left(\frac{\partial x}{\partial \xi_i}\right)^2 + \left(\frac{\partial y}{\partial \xi_i}\right)^2 + \left(\frac{\partial z}{\partial \xi_i}\right)^2. \quad i = 1,2,3 \quad (94)$$

The distance between two points on a coordinate line is the line element

$$ds_i = h_i d\xi_i. \quad i = 1,2,3 \quad (95)$$

Thus, the element of volume becomes equal to

$$ds_1 ds_2 ds_3 = h_1 h_2 h_3 d\xi_1 d\xi_2 d\xi_3. \quad (96)$$

As explained in Section 5.9, each component of  $d\phi/ds_i = (1/h_i)(\partial\phi/\partial\xi_i)$  is its directional derivative. In a curvilinear system its component perpendicular to the surface  $\xi_i = \text{constant}$  (that is, in the direction of  $s_i$ ) is

$$\frac{d\phi}{ds_i} = \frac{1}{h_i} \frac{\partial\phi}{\partial\xi_i}, \quad (97)$$

following Eq. (95). Then  $\nabla\phi$  can be written in the form

$$\nabla\phi = \frac{\mathbf{e}_1}{h_1} \frac{\partial\phi}{\partial\xi_1} + \frac{\mathbf{e}_2}{h_2} \frac{\partial\phi}{\partial\xi_2} + \frac{\mathbf{e}_3}{h_3} \frac{\partial\phi}{\partial\xi_3}, \quad (98)$$

where the  $\mathbf{e}_i$ 's are unit vectors along the curvilinear coordinate axes.

It is now necessary to derive analogous relations for the divergence of a vector, *viz.*  $\nabla \cdot \mathbf{A}$ . The calculation can be carried out in at least two ways. The direct analytic approach is long, but does not involve any methods other than those of vector algebra. Otherwise, it is necessary to develop the divergence (Gauss's) theorem, after which the desired result is easily obtained (see Appendix VI). In either case it is given by

$$\nabla \cdot \mathbf{A} = \frac{1}{h_1 h_2 h_3} \left[ \frac{\partial}{\partial \xi_1} (A_1 h_2 h_3) + \frac{\partial}{\partial \xi_2} (A_2 h_1 h_3) + \frac{\partial}{\partial \xi_3} (A_3 h_1 h_2) \right]. \quad (99)$$

If  $A = \nabla\phi$ ,

$$\begin{aligned} \nabla \cdot \nabla\phi = \nabla^2\phi = \frac{1}{h_1 h_2 h_3} & \left[ \frac{\partial}{\partial \xi_1} \left( \frac{h_2 h_3}{h_1} \frac{\partial \phi}{\partial \xi_1} \right) + \frac{\partial}{\partial \xi_2} \left( \frac{h_1 h_3}{h_2} \frac{\partial \phi}{\partial \xi_2} \right) \right. \\ & \left. + \frac{\partial}{\partial \xi_3} \left( \frac{h_1 h_2}{h_3} \frac{\partial \phi}{\partial \xi_3} \right) \right] \end{aligned} \tag{100}$$

as the components of  $\nabla\phi$  are  $A_i = 1/h_i(\partial\phi/\partial\xi_i)$  [see Eq. (98)]. Analogous expressions for  $\nabla^2 A$  can be obtained with use of the expansion

$$\nabla^2 A = \nabla(\nabla \cdot A) - \nabla \times \nabla \times A. \tag{101}$$

The general expressions developed in this section can be applied to a given problem by calculating the  $h_i$ 's from Eq. (94), providing of course that the coordinate transformations given by Eqs. (89) to (91) are known. Some well-known examples will be treated in the following chapter.

### PROBLEMS

1. Show that Eqs. (16) and (17) are verified by the substitutions of Eqs. (18–20).
2. Given two vectors  $A = 4i + j + 3k$  and  $B = i - 3j - k$ , calculate:  $A + B$ ,  $A \cdot B$  and  $A \times B$ .  
 Ans.  $5i - 2j + 2k, -2, 8i + 7j - 13k$
3. If  $A = 2i + 4j + k$  and  $B = -2i + j + 2k$ , find  $A \cdot B$ ,  $A \times B$ , and  $\cos \theta$ .  
 Ans.  $\sqrt{21}, 3, 2, 0.1455$
4. Verify Eqs. (27) and (28).
5. Demonstrate the inequality of Eq. (29).
6. With the use of Eq. (24), calculate the volume of the parallelepiped defined by the vectors  $A = i + 2j + k$ ,  $B = j + k$  and  $C = i - j$ .  
 Ans. 4
7. Show that  $(A \times B) \cdot (C \times D) = (A \cdot C)(B \cdot D) - (A \cdot D)(B \cdot C)$ .
8. Calculate the angles between two diagonals of a cube.                      Ans.  $\cos^{-1} \frac{1}{3}$
9. Find the angle between the diagonal of a cube and a diagonal of a face.  
 Ans.  $\cos^{-1} \sqrt{2/3}$
10. Demonstrate Eqs. (52–56) by expansion in Cartesian coordinates.
11. Show that if a vector  $A$  is irrotational,  $A = \nabla\phi$ , where  $\phi$  is a scalar.
12. Prove Eqs. (62) and (63).

13. Given a force  $\mathbf{f} = i - zj - yk$ , show that it is conservative, *i.e.* that  $\nabla \times \mathbf{f} = 0$ . Find a scalar potential  $\phi$  such that  $\mathbf{f} = -\nabla\phi$ .      Ans.  $\phi = -x + yz$ .
14. Show that Eq. (77) represents a solution to Eq. (76).
15. From Eq. (3) derive the relations for the real and imaginary parts of the refractive index as functions of the permittivity and the electrical conductivity of a given medium. Note that both  $n$  and  $\kappa$  are defined as real quantities.

$$\text{Ans. } \kappa^2 = \frac{1}{2} \left[ -\varepsilon_r + \sqrt{\varepsilon_r^2 + \frac{\sigma^2}{4\pi^2\nu^2\varepsilon_0^2}} \right]$$

$$\text{and } n^2 = \frac{1}{2} \left[ \varepsilon_r + \sqrt{\varepsilon_r^2 + \frac{\sigma^2}{4\pi^2\nu^2\varepsilon_0^2}} \right],$$

where the positive square roots are to be taken.

15. Show that in the case of a relatively poor conductor,  $\kappa \approx (\sigma/4\pi\nu\varepsilon_0)$  and  $n \approx \sqrt{\varepsilon_r}$ .