$$v^i\mathbf{a}_i = (v_k g^{ik})\mathbf{a}_i = v_k\mathbf{a}^k.$$

Hence

$$\mathbf{a}^k = g^{ik}\mathbf{a}_i \qquad (1.1.4.13)$$

and, similarly,

$$\mathbf{a}_k = g_{ik}\mathbf{a}^i. \qquad (1.1.4.14)$$

(iii) The tensors g_{ij} and g^{ij} are symmetric, by definition.

(iv) It follows from (1.1.4.11) and (1.1.4.12) or (1.1.4.13) and (1.1.4.14) that the matrices of the direct and reciprocal metric tensors are mutually inverse, *i.e.*

$$\begin{pmatrix} g_{11} & g_{12} & g_{13} \\ g_{21} & g_{22} & g_{23} \\ g_{31} & g_{32} & g_{33} \end{pmatrix}^{-1} = \begin{pmatrix} g^{11} & g^{12} & g^{13} \\ g^{21} & g^{22} & g^{23} \\ g^{31} & g^{32} & g^{33} \end{pmatrix}, \qquad (1.1.4.15)$$

and their determinants are mutually reciprocal.

1.1.4.4. *Examples*

There are numerous applications of tensor notation in crystallographic calculations, and many of them appear in the various chapters of this volume. We shall therefore present only a few examples.

(i) The (squared) magnitude of the diffraction vector $\mathbf{h} = h_i\mathbf{a}^i$ is given by

$$|h|^2 = \frac{4\sin^2\theta}{\lambda^2} = h_i h_j g^{ij}. \qquad (1.1.4.16)$$

This concise relationship is a starting point in a derivation of unit-cell parameters from experimental data.

(ii) The structure factor, including explicitly anisotropic displacement tensors, can be written in symbolic matrix notation as

$$F(\boldsymbol{h}) = \sum_{j=1}^{N} f_{(i)} \exp(-\boldsymbol{h}^T\boldsymbol{\beta}_{(j)}\boldsymbol{h}) \exp(2\pi i\boldsymbol{h}^T\boldsymbol{r}_{(j)}), \qquad (1.1.4.17)$$

where $\boldsymbol{\beta}_{(j)}$ is the matrix of the anisotropic displacement tensor of the jth atom. In tensor notation, with the quantities referred to their natural bases, the structure factor can be written as

$$F(h_1h_2h_3) = \sum_{j=1}^{N} f_{(j)} \exp(-h_ih_k\beta^{ik}_{(j)}) \exp(2\pi i h_i x^i_{(j)}), \qquad (1.1.4.18)$$

and similarly concise expressions can be written for the derivatives of the structure factor with respect to the positional and displacement parameters. The summation convention applies only to indices denoting components of vectors and tensors; the atom subscript j in (1.1.4.18) clearly does not qualify, and to indicate this it has been surrounded by parentheses.

(iii) Geometrical calculations, such as those described in the chapters of Part 3, may be carried out in any convenient basis but there are often some definite advantages to computations that are referred to the natural, non-Cartesian bases (see Chapter 3.1). Usually, the output positional parameters from structure refinement are available as contravariant components of the atomic position vectors. If we transform them by (1.1.4.11) to their covariant form, and store these covariant components of the atomic position vectors, the computation of scalar products using equations (1.1.4.9) or (1.1.4.10) is *almost as efficient as it would be if the coordinates were referred to a Cartesian system.* For example, the right-hand side of the vector identity (1.1.3.5), which is employed in the computation of dihedral angles, can be written as

$$(A_iC^i)(B_kD^k) - (A_iD^i)(B_kC^k).$$

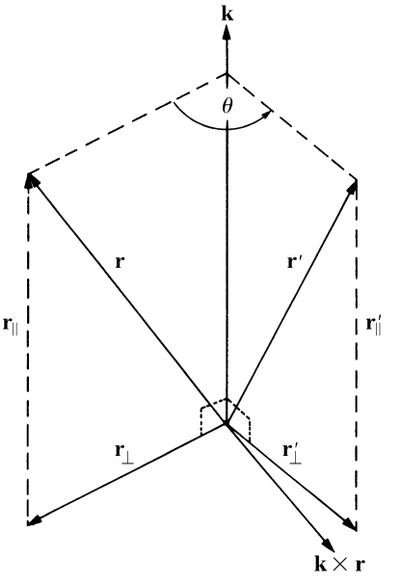

Fig. 1.1.4.1. Derivation of the general expression for the rotation operator. The figure illustrates schematically the decompositions and other simple geometrical considerations required for the derivation outlined in equations (1.1.4.22)–(1.1.4.28).

This is a typical application of reciprocal space to ordinary direct-space computations.

(iv) We wish to derive a tensor formulation of the vector product, along similar lines to those of Chapter 3.1. As with the scalar product, there are several such formulations and we choose that which has both vectors, say $\mathbf{u}$ and $\mathbf{v}$, and the resulting product, $\mathbf{u}\times\mathbf{v}$, referred to a covariant basis. We have

$$\begin{aligned}\mathbf{u}\times\mathbf{v} &= u^i\mathbf{a}_i \times v^j\mathbf{a}_j \\ &= u^iv^j(\mathbf{a}_i\times\mathbf{a}_j).\end{aligned} \qquad (1.1.4.19)$$

If we make use of the relationships (1.1.3.3) between the direct and reciprocal basis vectors, it can be verified that

$$\mathbf{a}_i\times\mathbf{a}_j = Ve_{kij}\mathbf{a}^k, \qquad (1.1.4.20)$$

where V is the volume of the unit cell and the antisymmetric tensor e_{kij} equals $+1$, -1, or 0 according as kij is an even permutation of 123, an odd permutation of 123 or any two of the indices kij have the same value, respectively. We thus have

$$\begin{aligned}\mathbf{u}\times\mathbf{v} &= Ve_{kij}u^iv^j\mathbf{a}^k \\ &= Vg^{lk}e_{kij}u^iv^j\mathbf{a}_l,\end{aligned} \qquad (1.1.4.21)$$

since by (1.1.4.13), $\mathbf{a}^k = g^{lk}\mathbf{a}_l$.

(v) *The rotation operator.* The general formulation of an expression for the rotation operator is of interest in crystal structure determination by Patterson techniques (see Chapter 2.3) and in molecular modelling (see Chapter 3.3), and another well known crystallographic application of this device is the derivation of the translation, libration and screw-motion tensors by the method of Schomaker & Trueblood (1968), discussed in Part 8 of Volume C (*IT* C, 1999) and in Chapter 1.2 of this volume. A digression on an elementary derivation of the above seems to be worthwhile.

Suppose we wish to rotate the vector $\mathbf{r}$, about an axis coinciding with the unit vector $\mathbf{k}$, through the angle θ and in the positive sense, *i.e.* an observer looking in the direction of $+\mathbf{k}$ will see $\mathbf{r}$ rotating in the clockwise sense. The vectors $\mathbf{r}$, $\mathbf{k}$ and the rotated (target) vector $\mathbf{r}'$ are referred to an origin on the axis of rotation (see Fig. 1.1.4.1). Our purpose is to express $\mathbf{r}'$ in terms of $\mathbf{r}$, $\mathbf{k}$ and θ by a general vector

 references