

Correlations between two sets of angular relation equations

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Abstract It is shown here that the angular relation equations between direct and reciprocal vectors are very similar to the angular relation equations in Euler's theorem. These two sets of equations are usually treated separately as unrelated equations in different fields. In this careful study, the connection between the two sets of angular equations is revealed by considering the cosine rule for the spherical triangle. It is found that understanding of the correlation is hindered by the facts that the same variables are defined differently and different symbols are used to represent them in the two fields. Understanding the connection between different concepts is not only stimulating and beneficial, but also a fundamental tool in innovation and research, and has historical significance. The background of the work presented here contains elements of many scientific disciplines. This work illustrates the common ground of two theories usually considered separately and is therefore of benefit not only for its own sake but also to illustrate a general principle that a theory relevant to one discipline can often be used in another. The paper works with chemistry related concepts using mathematical methodologies unfamiliar to the usual audience of mainstream experimental and theoretical chemists.

Keywords Solid state chemistry · Crystallography · Euler's theorem · Reciprocal vectors · Spherical trigonometry · Analogies · Interdiscipline

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1 Introduction

Two well-established scientific concepts are the reciprocal lattice, fundamental to X-ray crystallography, and Euler's theorem important in computer graphics [1–3], symmetry operations, and quantum chemistry [4–6]. These two concepts, both involving angular relation equations, are usually treated separately, particularly as they are involved in different scientific disciplines. The angular relationships in X-ray Crystallography between direct and reciprocal vectors are given in Eqs. 4–6 in Sect. 2.2 and those in Euler's theorem are given in Eqs. 14–16 in Sect. 3.2. These two sets of equations are very similar though they may appear at first sight to be different. Unrelated derivations and different names used for the equivalent variables mask the similarities between them. In Sects. 5.1 and 5.3 we show that the two sets of equations are in fact different sides of the same coin, though they are commonly derived by different mathematical techniques in the literature. The basic principle involved in the correlation is the cosine rule for the spherical triangle shown in Eqs. 17–19 in Sect. 4 or 17'–19' in Sect. 5.1 and their proofs are given in Appendix 1. The keys for the correlation are Eqs. 22 and 23 in Sect. 5.1. The similarity between the two sets of equations is illustrated in Sect. 5 and seems obvious in retrospect but lateral thinking is required to make the connection. The problem involves quite a diversity of different disciplines and the correlation is therefore difficult to establish. The paper works with chemistry related concepts with mathematical methodologies unfamiliar to the usual audience of mainstream experimental and theoretical chemists. The usual unrelated derivations and related background concerning these two sets of equations show the important connection between mathematics and chemistry. Working out the connection between different concepts deserves a place in research and teaching because it is not only stimulating and beneficial, but also an important way of original thinking and important in the learning process. We advocate looking at a concept from different angles. So, besides the correlation, each angular relation is derived with different methods to correlate with different concepts.

2 Angular relations between direct vectors and reciprocal vectors

2.1 Definition of reciprocal vectors

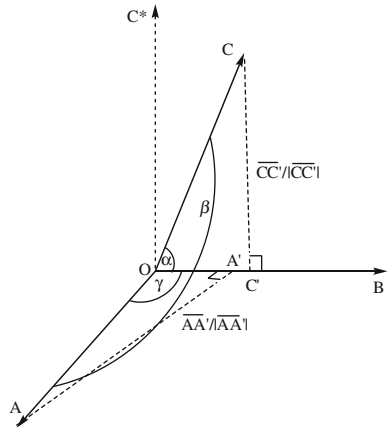
The reciprocal vectors are defined by Eqs. 1–3 from direct vectors as illustrated in Fig. 1

$$\overline{OA}^* = \frac{\overline{OB} \times \overline{OC}}{\overline{OA} \cdot (\overline{OB} \times \overline{OC})}; \quad |\overline{OA}^*| = \frac{|\overline{OB}| \cdot |\overline{OC}| \sin \alpha}{V} \quad (1)$$

$$\overline{OB}^* = \frac{\overline{OC} \times \overline{OA}}{\overline{OB} \cdot (\overline{OC} \times \overline{OA})}; \quad |\overline{OB}^*| = \frac{|\overline{OC}| \cdot |\overline{OA}| \sin \beta}{V} \quad (2)$$

$$\overline{OC}^* = \frac{\overline{OA} \times \overline{OB}}{\overline{OC} \cdot (\overline{OA} \times \overline{OB})}; \quad |\overline{OC}^*| = \frac{|\overline{OA}| \cdot |\overline{OB}| \sin \gamma}{V} \quad (3)$$

Fig. 1 3-dimensional basis vectors for direct lattice. The reciprocal vectors are defined as $\overline{OX} \cdot \overline{OY}^* = \delta_{XY^*}$ where $X = A, B, C; Y^* = A^*, B^*, C^*$; $\delta_{XY^*} = 1$ when $X = Y$. A^* and B^* are not shown here for simplicity. Unit vectors along $\overline{AA'}$ and $\overline{CC'}$ are indicated by $\frac{\overline{AA'}}{|\overline{AA'}|}$ and $\frac{\overline{CC'}}{|\overline{CC'}|}$, respectively



V and V^* represent the volumes of the lattice cell and its reciprocal lattice cell, respectively. α, β, γ are the angles between \overline{OB} and \overline{OC} , \overline{OC} and \overline{OA} , and \overline{OA} and \overline{OB} , respectively; $\alpha^*, \beta^*, \gamma^*$ are the angles between \overline{OB}^* and \overline{OC}^* , \overline{OC}^* and \overline{OA}^* , and \overline{OB}^* and \overline{OA}^* , respectively. $\{\overline{OA} \ \overline{OB} \ \overline{OC}\}$ and $\{\overline{OA}^* \ \overline{OB}^* \ \overline{OC}^*\}$ are the 3-dimensional direct vectors (Fig. 1) and reciprocal vectors, respectively.

2.2 The angular relationships

The angular relationships [7] between the direct and reciprocal vectors are given by Eqs. 4–6 and can be derived simply by manipulating the vector products or metric matrices

$$\cos \alpha^* = \frac{\cos \beta \cos \gamma - \cos \alpha}{\sin \beta \sin \gamma} \tag{4}$$

$$\cos \beta^* = \frac{\cos \gamma \cos \alpha - \cos \beta}{\sin \gamma \sin \alpha} \tag{5}$$

$$\cos \gamma^* = \frac{\cos \alpha \cos \beta - \cos \gamma}{\sin \alpha \sin \beta} \tag{6}$$

2.3 Derivation of Eqs. 4–6 from vector products

Equations 1 and 2 can be combined to obtain Eq. 7

$$\overline{OA}^* \cdot \overline{OB}^* = \frac{\overline{OB} \times \overline{OC}}{\overline{OA} \cdot (\overline{OB} \times \overline{OC})} \cdot \frac{\overline{OC} \times \overline{OA}}{\overline{OB} \cdot (\overline{OC} \times \overline{OA})} \tag{7}$$

By Lagrange’s identity [8,9] we have

$$(\overline{OB} \times \overline{OC}) \cdot (\overline{OC} \times \overline{OA}) = (\overline{OB} \cdot \overline{OC}) \cdot (\overline{OC} \cdot \overline{OA}) - (\overline{OB} \cdot \overline{OA}) \cdot (\overline{OC} \cdot \overline{OC}) \tag{8}$$

Since our only concern here is for angular relationships, unit vectors \overline{OA} , \overline{OB} , and \overline{OC} are used for simplicity and the generality has not been lost. Inserting Eqs. 1, 2, and 8 into Eq. 7, we can obtain Eq. 6 in the form

$$\sin \alpha \sin \beta \cos \gamma^* = \cos \alpha \cos \beta - \cos \gamma.$$

Equations 4 and 5 can be obtained similarly.

2.4 Derivation of Eqs. 4–6 from metric matrix

The metric matrices G and G^* are defined as

$$G = \begin{pmatrix} \overline{OA} \\ \overline{OB} \\ \overline{OC} \end{pmatrix} (\overline{OA} \ \overline{OB} \ \overline{OC}) = \begin{pmatrix} 1 & \cos \gamma & \cos \beta \\ \cos \gamma & 1 & \cos \alpha \\ \cos \beta & \cos \alpha & 1 \end{pmatrix}; |G| = V^2 \tag{9}$$

$$\begin{aligned} G^* &= \begin{pmatrix} \overline{OA}^* \\ \overline{OB}^* \\ \overline{OC}^* \end{pmatrix} (\overline{OA}^* \ \overline{OB}^* \ \overline{OC}^*) \\ &= \begin{pmatrix} |\overline{OA}^*| |\overline{OA}^*| & |\overline{OA}^*| |\overline{OB}^*| \cos \gamma^* & |\overline{OA}^*| |\overline{OC}^*| \cos \beta^* \\ |\overline{OB}^*| |\overline{OA}^*| \cos \gamma^* & |\overline{OB}^*| |\overline{OB}^*| & |\overline{OB}^*| |\overline{OC}^*| \cos \alpha^* \\ |\overline{OC}^*| |\overline{OA}^*| \cos \beta^* & |\overline{OC}^*| |\overline{OB}^*| \cos \alpha^* & |\overline{OC}^*| |\overline{OC}^*| \end{pmatrix} \\ |G^*| &= (V^*)^2 \end{aligned} \tag{10}$$

where

$$\begin{aligned} V^2 &= [\overline{OA} \cdot (\overline{OB} \times \overline{OC})] [\overline{OA} \cdot (\overline{OB} \times \overline{OC})] \\ &= \left| \begin{pmatrix} \overline{OA}_x & \overline{OA}_y & \overline{OA}_z \\ \overline{OB}_x & \overline{OB}_y & \overline{OB}_z \\ \overline{OC}_x & \overline{OC}_y & \overline{OC}_z \end{pmatrix} \right| \left| \begin{pmatrix} \overline{OA}_x & \overline{OB}_x & \overline{OC}_x \\ \overline{OA}_y & \overline{OB}_y & \overline{OC}_y \\ \overline{OA}_z & \overline{OB}_z & \overline{OC}_z \end{pmatrix} \right| \\ &= \left| \begin{pmatrix} \overline{OA}_x & \overline{OA}_y & \overline{OA}_z \\ \overline{OB}_x & \overline{OB}_y & \overline{OB}_z \\ \overline{OC}_x & \overline{OC}_y & \overline{OC}_z \end{pmatrix} \begin{pmatrix} \overline{OA}_x & \overline{OB}_x & \overline{OC}_x \\ \overline{OA}_y & \overline{OB}_y & \overline{OC}_y \\ \overline{OA}_z & \overline{OB}_z & \overline{OC}_z \end{pmatrix} \right| = \left| \begin{pmatrix} \overline{OA} \\ \overline{OB} \\ \overline{OC} \end{pmatrix} (\overline{OA} \ \overline{OB} \ \overline{OC}) \right| = |G| \\ &= \left| \begin{pmatrix} \overline{OA} \cdot \overline{OA} & \overline{OA} \cdot \overline{OB} & \overline{OA} \cdot \overline{OC} \\ \overline{OB} \cdot \overline{OA} & \overline{OB} \cdot \overline{OB} & \overline{OB} \cdot \overline{OC} \\ \overline{OC} \cdot \overline{OA} & \overline{OC} \cdot \overline{OB} & \overline{OC} \cdot \overline{OC} \end{pmatrix} \right| \end{aligned} \tag{11}$$

Still using unit vectors for \overline{OA} , \overline{OB} , and \overline{OC} , G^{-1} can be obtained from G via Eq. 9 to give Eq. 12

$$G^{-1} = \frac{1}{V^2} \begin{pmatrix} \sin^2 \alpha & \cos \alpha \cos \beta - \cos \gamma & \cos \alpha \cos \gamma - \cos \beta \\ \cos \alpha \cos \beta - \cos \gamma & \sin^2 \beta & \cos \beta \cos \gamma - \cos \alpha \\ \cos \alpha \cos \gamma - \cos \beta & \cos \beta \cos \gamma - \cos \alpha & \sin^2 \gamma \end{pmatrix} \tag{12}$$

Since

$$\begin{aligned} G^{-1}G &= G^{-1} \begin{pmatrix} \overline{OA} \\ \overline{OB} \\ \overline{OC} \end{pmatrix} (\overline{OA} \ \overline{OB} \ \overline{OC}) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \\ G^*G &= \begin{pmatrix} \overline{OA^*} \\ \overline{OB^*} \\ \overline{OC^*} \end{pmatrix} \left\{ (\overline{OA^*} \ \overline{OB^*} \ \overline{OC^*}) \begin{pmatrix} \overline{OA} \\ \overline{OB} \\ \overline{OC} \end{pmatrix} \right\} (\overline{OA} \ \overline{OB} \ \overline{OC}) \\ &= \begin{pmatrix} \overline{OA^*} \\ \overline{OB^*} \\ \overline{OC^*} \end{pmatrix} \left\{ \begin{pmatrix} \overline{OA^*}_x & \overline{OB^*}_x & \overline{OC^*}_x \\ \overline{OA^*}_y & \overline{OB^*}_y & \overline{OC^*}_y \\ \overline{OA^*}_z & \overline{OB^*}_z & \overline{OC^*}_z \end{pmatrix} \begin{pmatrix} \overline{OA}_x & \overline{OA}_y & \overline{OA}_z \\ \overline{OB}_x & \overline{OB}_y & \overline{OB}_z \\ \overline{OC}_x & \overline{OC}_y & \overline{OC}_z \end{pmatrix} \right\} (\overline{OA} \ \overline{OB} \ \overline{OC}) \\ &= \begin{pmatrix} \overline{OA^*} \\ \overline{OB^*} \\ \overline{OC^*} \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} (\overline{OA} \ \overline{OB} \ \overline{OC}) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \\ G^{-1} \cdot G &= G^*G; |G^*| |G| = (V^*)^2 \frac{1}{V^2} = 1 \end{aligned} \tag{13}$$

Thus from Eq. 13, we prove that $G^{-1} = G^*$. By $(G^{-1})_{12} = (G^*)_{12}$, $(G^{-1})_{13} = (G^*)_{13}$, and $(G^{-1})_{23} = (G^*)_{23}$, where subscripts denote row and column respectively, and from Eqs. 1–3, together with Eqs. 10, 12, and 13, Eqs. 4–6 are obtained. e.g. By $(G^{-1})_{12} = (G^*)_{12}$ to give Eq. 6

$$\begin{aligned} \frac{\cos \alpha \cos \beta - \cos \gamma}{V^2} &= |\overline{OA^*}| |\overline{OB^*}| \cos \gamma^* \\ &= \frac{|\overline{OB}| \cdot |\overline{OC}| \sin \alpha}{V} \frac{|\overline{OC}| \cdot |\overline{OA}| \sin \beta}{V} \cos \gamma^* \\ &= \frac{\sin \alpha \sin \beta \cos \gamma^*}{V^2} \end{aligned}$$

Note that \overline{OA} , \overline{OB} , and \overline{OC} are supposed to be unit vectors, here.

3 Euler's theorem

3.1 The proof of Euler's theorem

Euler's Theorem states that any rotation (or sequence of rotations) about a point is equivalent to a single rotation about some axis through that point [10,11]. One of the derivations is given below.

As shown in Fig. 2, spherical triangles 1, 2, 3, and ABC are congruent with each other. Spherical triangle 1 matches spherical triangle 2 after rotating about \overrightarrow{OA} by an angle of $2^*\angle A$.^{1,2} Similarly spherical triangle 2 matches spherical triangle 3 after rotating about by an angle of $2^*\angle B$. The final result is equivalent to rotating spherical triangle 1 about by an angle of $2(\pi - \angle C)$ [or $-2\angle C$] to match spherical triangle 3. Note that it is sufficient to check three points to establish that two spherical triangles are in equivalent positions.

The value of $\angle C$ and the position of \overrightarrow{OC} are completely determined by the spherical triangle ABC. With the additional information provided in Sect. 5.3, the relevant angular relationships are provided by the cosine rule for spherical triangle as shown in method 1 of Appendix 1.

3.2 Angular relations in Euler's theorem

The theorem can be described by reference to Fig. 2 as follows. Rotate about a vector \overrightarrow{OA} by an arbitrary angle of $2^*\angle A$, then rotate about another vector \overrightarrow{OB} by an arbitrary angle of $2^*\angle B$, \overrightarrow{OA} will intersect \overrightarrow{OB} at point O by an angle defined as γ . The final result is equivalent to rotation about a definite vector \overrightarrow{OC} passing through the intersecting point O of \overrightarrow{OA} and \overrightarrow{OB} by a given angle of $2^*(\pi - \angle C)$ [or $-2^*\angle C$]. The position of \overrightarrow{OC} is fixed by angles α and β with respect to \overrightarrow{OB} and \overrightarrow{OA} , respectively. The three parameters, two concerning the position of \overrightarrow{OC} are fixed by α and β and the third dependent upon the value of $\angle C$, can be determined from Eqs. 14–16 by the angle between axes \overrightarrow{OA} and \overrightarrow{OB} , γ , and the rotation angles related to $\angle A$, $\angle B$.

¹ Positive angles are clockwise, negative angles, anticlockwise.

² When direct and reciprocal vectors are dealt with, α , β , and γ are usually used for the angles between \overrightarrow{OA} , \overrightarrow{OB} , and \overrightarrow{OC} . But when spherical triangle is dealt with, $\frac{a}{R}$, $\frac{b}{R}$, and $\frac{c}{R}$ are used for the angles between \overrightarrow{OA} , \overrightarrow{OB} , and \overrightarrow{OC} , where α , β , and γ are usually used for the dihedral angles defined by the spherical triangle. In Euler's theorem, the dihedral angles which are related with rotations are usually denoted by the more frequently used symbols u, v, and w or the less frequently used symbols $\angle A$, $\angle B$, and $\angle C$. Since there are symbol denoting conflicts, we use symbols $\angle A$, $\angle B$, and $\angle C$ for the dihedral angles because it is more convenient to remember that dihedral angle $\angle A$ is opposite to arc a, $\angle B$ to b, and $\angle C$ to c.

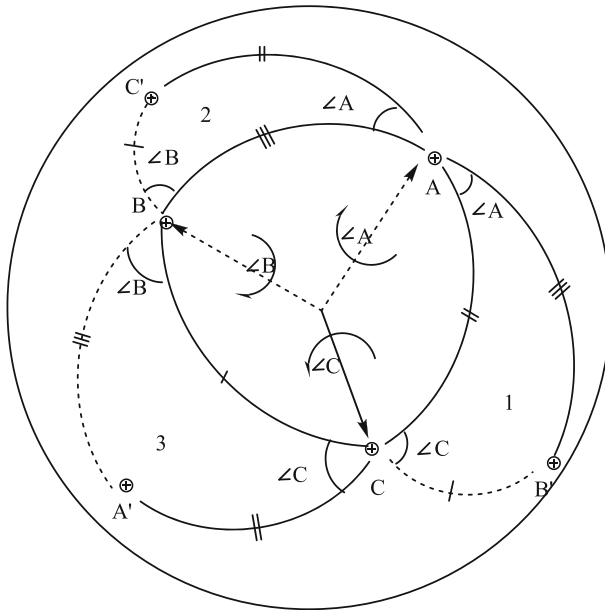


Fig. 2 The relationships between rotations as specified in Euler’s theorem. Points $A, B, C, A', B',$ and C' are all on the surface of a sphere. Spherical triangles $ACB', ABC',$ and BCA' are congruent with spherical triangle $ABC,$ and denoted as 1, 2 and 3, respectively

$$\cos \angle C = -\cos \angle A \cos \angle B + \sin \angle A \sin \angle B \cos \gamma \tag{14}$$

$$\cos \alpha = \frac{\cos \angle B \cos \angle C + \cos \angle A}{\sin \angle B \sin \angle C} \tag{15}$$

$$\cos \beta = \frac{\cos \angle C \cos \angle A + \cos \angle B}{\sin \angle C \sin \angle A} \tag{16}$$

In computer graphics and symmetry operations, Euler’s theorem is used to derive the matrix representation of a general rotation about an arbitrary axis from the matrix describing rotation about the z axis. In the matrix generation process, the z axis is first made coincident with the general rotation axis by two easily defined rotations. The two rotation angles plus the rotation angle about the general axis define three parameters which are equivalent to those involved in Eqs. 14–16. The final step of rotating the z axis back to its original position does not generate new parameters. The three rotation angles involved are called Euler angles that might be not easy to find.³ This is the essential feature of Euler’s theorem [11] and Eqs. 14–16 can be considered as another mathematical representation of Euler’s theorem.

In classical mechanics, still another mathematical representation of Euler’s theorem is used to transform one system of Descartes coordinates into another, and only three parameters of Euler angles are involved. Furthermore, Euler’s theorem is stated

³ For example, rotating an object around the x axis by $\pi/2$ and then rotating it around the y axis by $\pi/2$ is equivalent to threefold rotation.

alternatively as: The general displacement of a rigid body with one point fixed (any number of rotations about a point) is a rotation about some axis. [5]

The derivations for Eqs. 14–16 are given in Sect. 5.1. The validity of Eqs. 14–16 can be checked by an example. For example, a rotation by $\pi/2$ around axis \vec{OA} followed by another rotation by $\pi/2$ about axis \vec{OB} perpendicular to \vec{OA} gives a 3-fold axis in a cubic cell. When these angles $\angle A = \angle B = \pi/4$ and $\gamma = \pi/2$ in the above case are substituted into Eq. 14, we have

$$\cos \angle C = -\cos 45^\circ \cos 45^\circ + \sin 45^\circ \sin 45^\circ \cos 90^\circ = -1/2, \text{ so } \angle C = 120^\circ$$

Accordingly $2^*(\pi - \angle C) = 2x(180^\circ - 120^\circ) = 120^\circ$, demonstrating that the resulting rotation is a 3-fold rotation. α and β define the position of the 3-fold axis. The actual values of α and β , both of which are 54.74° , can also be verified from equations 15–16.

It can now be seen that Eqs. 4–6 are very similar to Eqs. 14–16. When students come across the two sets of equations, they should think laterally and realize that there will be some mathematical relationship between the two sets of equations and find that working out the relationship is educationally stimulating and beneficial. In fact, we show in Sect. 5 that both Eqs. 4–6 and Eqs. 14–16 can be derived from the cosine rule for the spherical triangle.

4 The cosine rule for spherical triangle

Points A , B , and C in Fig. 1 can be positioned on the same sphere as in Figs. 3 and 4 in order to deduce the angular relationships. This approach can be justified because we are only concerned here with the correlations between angular Eqs. 4–6 and 14–16.

For three points A , B and C on a sphere (Figs. 3 and 4), the cosine rule for the spherical triangle [12] can be expressed by Eqs. 17–19

$$\cos \frac{a}{R} = \cos \frac{b}{R} \cos \frac{c}{R} + \sin \frac{b}{R} \sin \frac{c}{R} \cos \angle A \quad (17)$$

$$\cos \frac{b}{R} = \cos \frac{a}{R} \cos \frac{c}{R} + \sin \frac{a}{R} \sin \frac{c}{R} \cos \angle B \quad (18)$$

$$\cos \frac{c}{R} = \cos \frac{a}{R} \cos \frac{b}{R} + \sin \frac{a}{R} \sin \frac{b}{R} \cos \angle C \quad (19)$$

where R is the radius of the sphere. Here the angle $\angle A$ in the triangle is the dihedral angle between planes AOB and AOC (Fig. 1), $\angle B$ is the dihedral angle between planes AOB and BOC , and $\angle C$ the dihedral angle between planes AOC and COB . In fact, these three angles are just the angles related to rotation in Eqs. 14–16 as will be become clear in the following discussion. O is the center of the sphere. a is the length of \widehat{BC} , i.e.

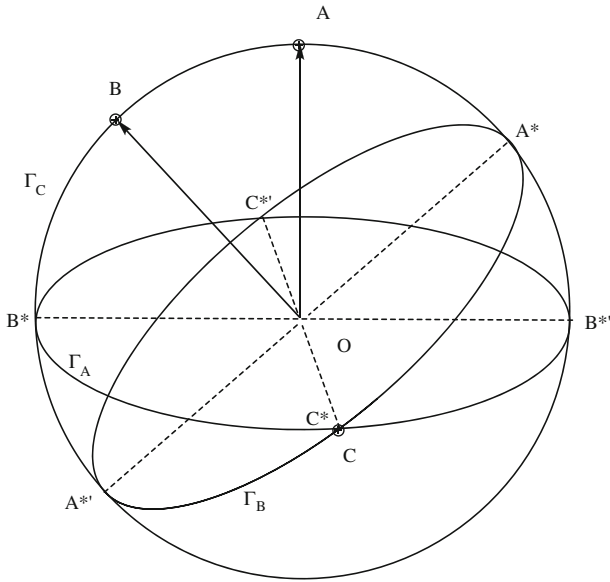
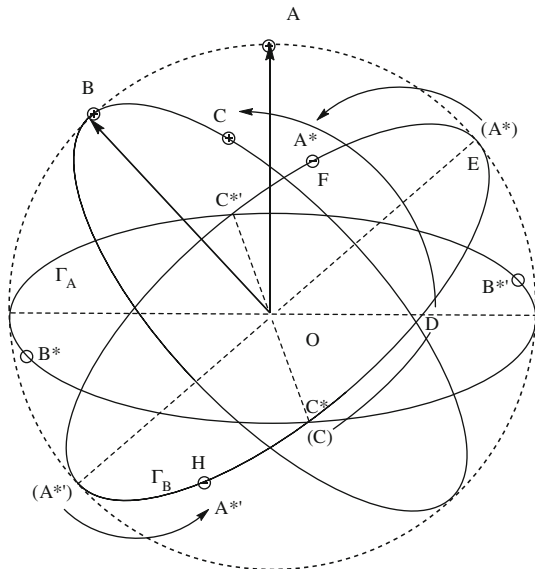


Fig. 3 Spherical Triangle ABC and its polar triangle $A^*B^*C^*$. $R = 1 \cdot \Gamma_A, \Gamma_B$ and Γ_C are great circles as is defined in Sect. 5.1. A is the pole of circle Γ_A ; B is the pole of Γ_B ; and C is the pole of Γ_C (see Sect. 2). The three basis vectors shown in Fig. 1 are also presented. OA and OB are arbitrarily positioned. Here OC is chosen to be perpendicular to OA and OB . But for the general derivation shown in Fig. 4, point C is moved to a general position. A^* and $A^{*'}$ are the intersections of Γ_B and $\Gamma_C \cdot B^*$ and $B^{*'}$ are the intersections of Γ_A and $\Gamma_C \cdot C^*$ and $C^{*'}$ are the intersections of Γ_A and Γ_B

Fig. 4 A specified position of point C in Fig. 3 (indicated here in *parenthesis*) moves to a general position (*without parenthesis*) through point D . The great circle Γ_C moves from the dotted position to a new position as its pole C moves. See text for detail. Points A^* and F are identical as are $A^{*'}$ and H . As Γ_C moves, the points indicated in parentheses, (C) , (A^*) , and $(A^{*'})$, also move to new positions, indicated by C , F , and H , respectively



$$\begin{aligned}
 a &= \widehat{BC} & b &= \widehat{AC} & c &= \widehat{AB} \\
 a^* &= \widehat{B^*C^*} & b^* &= \widehat{A^*C^*} & c^* &= \widehat{A^*B^*}
 \end{aligned}
 \tag{20}$$

The radians of the sides, \widehat{BC} , \widehat{AC} and \widehat{AB} , of the spherical triangle are

$$\begin{aligned}
 \frac{a}{R} &= \angle COB = \alpha; & \frac{b}{R} &= \angle COA = \beta; & \frac{c}{R} &= \angle AOB = \gamma \\
 \frac{a^*}{R} &= \angle C^*OB^* = \alpha^*; & \frac{b^*}{R} &= \angle C^*OA^* = \beta^*; & \frac{c^*}{R} &= \angle A^*OB^* = \gamma^*
 \end{aligned}
 \tag{21}$$

The angle symbols, α , β , and γ , are not usually used in Eqs. 14–16 for the definitions of these angles. But they are indicated here because these symbols are used in Eqs. 4–6 and defined differently as the angles between pairs of axes \overrightarrow{OA} , \overrightarrow{OB} , and \overrightarrow{OC} . Similarly, α^* , β^* , and γ^* are the angles between pairs of axes $\overrightarrow{O^*A^*}$, $\overrightarrow{O^*B^*}$, and $\overrightarrow{O^*C^*}$ or the relevant radians of the sides in Eq. 21 (Figs. 1, 3 and 4). The derivations for Eqs. 17–19 are given in Appendix 1.

5 Relationship of the two sets of angular equations

5.1 Equations 14–16 and the cosine rule for the spherical triangle

In this section we will show how Eqs. 14–16 are derived from the cosine rule for the spherical triangle. The intersection of the surface of a sphere made by a plane is called a great circle Γ if the plane passes through the center of the sphere. The diameter of a sphere perpendicular to the plane of a circle of the sphere is called the axis of that circle. The points where the axes of a circle of a sphere intersect the surface of the sphere are called the poles of the circle. If the vertices of a spherical triangle are used as the poles and their great circles are drawn, another triangle is formed, called the polar triangle of the first. Thus in Figs. 3 and 4, A is the pole of a^* , B the pole of b^* , C the pole of c^* , and $A^*B^*C^*$ is the polar triangle of ABC .

The sides (in radians) and the angles of a spherical triangle are supplementary to the angles and the sides opposite in the polar triangle, and, conversely [13, 14]. The supplementary relationships are expressed as Eqs. 22 and 23

$$\angle A + \frac{a^*}{R} = \angle B + \frac{b^*}{R} = \angle C + \frac{c^*}{R} = \angle A^* + \frac{a}{R} = \angle B^* + \frac{b}{R} = \angle C^* + \frac{c}{R} = \pi
 \tag{22}$$

or

$$\angle A + \alpha^* = \angle B + \beta^* = \angle C + \gamma^* = \angle A^* + \alpha = \angle B^* + \beta = \angle C^* + \gamma = \pi
 \tag{23}$$

with the relevant symbols defined in Eqs. 20 and 21. The derivations for Eqs. 22 and 23 are given in Sect. 5.2 and “Appendix 2”.

Equations 14–16 for Euler’s theorem can be obtained from Eqs. 22 and 23 together with the cosine rule for the spherical triangle. The derivations of Eqs. 22 and 23 are given in Sect. 5.2 and “Appendix 2” for completeness but are not necessary for a complete understanding of the angular relationship correlation.

The first parts of Eq. 22 and the last parts of Eq. 23 are shown below

$$\begin{aligned} \angle A + \frac{a^*}{R} &= \angle B + \frac{b^*}{R} = \angle C + \frac{c^*}{R} = \pi \\ \angle A^* + \alpha &= \angle B^* + \beta = \angle C^* + \gamma = \pi \end{aligned}$$

These relationships can be inserted into the cosine rule for the polar triangle $A^*B^*C^*$ to give Eqs. 17’–19’, which can also be obtained by applying Eqs. 17–19 to the polar triangle of ABC

$$\cos \frac{a^*}{R} = \cos \frac{b^*}{R} \cos \frac{c^*}{R} + \sin \frac{b^*}{R} \sin \frac{c^*}{R} \cos \angle A^* \tag{17’}$$

$$\cos \frac{b^*}{R} = \cos \frac{a^*}{R} \cos \frac{c^*}{R} + \sin \frac{a^*}{R} \sin \frac{c^*}{R} \cos \angle B^* \tag{18’}$$

$$\cos \frac{c^*}{R} = \cos \frac{a^*}{R} \cos \frac{b^*}{R} + \sin \frac{a^*}{R} \sin \frac{b^*}{R} \cos \angle C^* \tag{19’}$$

It will be noted that Eq. 19’ can be written as

$$\cos(\pi - \angle C) = \cos(\pi - \angle A) \cos(\pi - \angle B) + \sin(\pi - \angle A) \sin(\pi - \angle B) \cos(\pi - \gamma)$$

which is just Eq. 14 in a different form. Similarly Eqs. 17’ and 18’ are equivalent to Eqs. 15 and 16.

The angular relationship of Euler’s theorem is just defined by the spherical triangle (Fig. 2). And the angular relationship of the spherical triangle is described by the cosine rule. Thus, the connection between the two angular relationships is natural. Their connections with the angular relationship of the direct and reciprocal vectors are shown in Sect. 5.3 and can also be shown by another more simple method equipped with the information provided in Sect. 5.3 as shown in method 1 of Appendix 1.

5.2 Derivation of Eqs. 22 and 23

This section can be skipped without affecting the general understanding of our method but is included for completeness.

\overrightarrow{OA} , \overrightarrow{OB} and \overrightarrow{OC} in Fig. 1 could have the same length R since only angles are relevant to Eqs. 14–16. The angular relations thus obtained apply to any cell even if the lengths for the three axes are not equal.

The validity of Eqs. 22 and 23 can be proved by placing point C in Fig. 3 in a more general position as indicated in Fig. 4. Notice that the great circle Γ_C moves with its pole C . As the previous pole C [now indicated as (C) in Fig. 4], goes to point D [after rotation around OB], the great circle Γ_C (dotted) moves along Γ_B until the intersection points of Γ_C and Γ_B reach arbitrary points F and H . [Rotation around the new line A^*A^* or FH in Fig. 4 can move the pole of Γ_C away from D to a more general position but this operation will have no effect on C^*A^* and thus does not affect the following discussion.] The previous C^*A^* in Fig. 3 [indicated here in Fig. 4 as $C^*(A^*)$] becomes the small arc C^*F [indicated also as a new C^*A^* here in Fig. 4].

From the above operations, it is clear that $C^*D = EF$, so

$$\angle DOE + \angle C^*OD = \pi/2 \tag{24}$$

$$\angle DOE + \angle EOF = \pi/2 \tag{25}$$

Adding Eqs. 24 and 25 together we obtain Eq. 26

$$\begin{aligned} \pi/2 + \pi/2 &= (\angle DOE + \angle C^*OD) + (\angle DOE + \angle EOF) \\ &= \angle DOE + (\angle C^*OD + \angle DOE + \angle EOF) \end{aligned} \tag{26}$$

Since $\angle B = \angle DOE$, $\beta^* = b^*/R = C^*A^* = C^*F = \angle C^*OD + \angle DOE + \angle EOF$ where $R = 1$, so that

$$\angle B + (b^*/R) = \angle B + \beta^* = \pi \tag{27}$$

which is part of Eq. 23. The other parts of Eqs. 22 and 23 are obtained similarly.

With the additional information introduced in Sect. 5.3, a more simple proof is available and this is provided in “Appendix 2”.

5.3 Eqs. 4–6 and the cosine rule for the spherical triangle

In this section, we establish the connection between Eqs. 4–6 and the cosine rule for spherical triangle

For two-dimensional lattices, the angle between the reciprocal vectors, $\overrightarrow{OA^*}$ and $\overrightarrow{OB^*}$, is $\pi - \gamma = \gamma^*$ [15], similar to Eq. 23, where γ is the angle between the direct vectors, \overrightarrow{OA} and \overrightarrow{OB} . Equivalent equations for three-dimensional lattices are shown

by Eq. 23. In fact the relationships between the vectors $\vec{OA}, \vec{OB}, \vec{OC}$ for the spherical triangle ABC and the vectors $\vec{OA}^*, \vec{OB}^*, \vec{OC}^*$, for the polar triangle A*B*C* are the same as the relationships between the direct and the reciprocal vectors [16] as given by Eqs. 28–30 where k is a constant. This equivalence can also be observed by considering Figs. 3 and 4.

$$\vec{OA} \times \vec{OB} = k \cdot \vec{OC}^* \tag{28}$$

$$\vec{OB} \times \vec{OC} = k \cdot \vec{OA}^* \tag{29}$$

$$\vec{OC} \times \vec{OA} = k \cdot \vec{OB}^* \tag{30}$$

Equations 28–30 satisfy the definition of the direct and reciprocal vector relations as shown by Eqs. 1–3 when only angular relations are concerned. The length of R is immaterial because we are only concerned with angles here. In fact, Eqs. 28–30 shows that Eqs. 22 and 23 also represent the angular relationship between the direct and reciprocal vectors. By Eqs. 21, 22 and 23, and Eqs. 17–19, we can obtain Eqs. 4–6. e.g. From Eq. 17, together with Eqs. 21 and 23, we obtain

$$\cos \alpha = \cos \beta \cos \gamma + \sin \beta \sin \gamma \cos (\pi - \alpha^*)$$

which is Eq. 4. Eqs. 5 and 6 can be obtained similarly.

Thus taking into account the cosine rule for the spherical triangle, the correlations between Eqs. 4–6 and Eqs. 14–16 are revealed via Eqs. 22 and 23 in a manner that is straightforward and beautifully simple.

6 Conclusions

The angular relationships in two different concepts in different fields, namely Euler’s theorem and the direct and reciprocal vectors in crystallography, are shown to be equivalent and are derived from the same basic theory. This is despite the fact that their similarity has remained unrecognized in many text books because not only are they used in different scientific disciplines but also, on a more trivial level, use different names for equivalent parameters. For example, in the two fields different symbols are used for $\alpha, \beta,$ and γ as shown in Eq. 21, and the angles are defined differently. As is shown in the text, the angular relationships for the spherical triangle ABC and its polar triangle A*B*C*[16], illustrated in Eqs. 22 and 23, are the same as those for direct and reciprocal vectors since the concepts of reciprocal vectors and the polar triangle are essentially identical. But in discussions of direct and reciprocal vectors, Eqs. 22 and 23 are not usually emphasized. Facts such as these make understanding the correlations between angular relationships very difficult.

In this paper we point out the similarity of the two angular relationship and then show that they are in fact connected to each other by the cosine rule for the spherical triangle. In fact, Eqs. 17–19 (or 17’–19’) of the cosine rule for spherical triangles can

be derived by Method 1 in Appendix 1 from Eqs. 22 and 23 which shows that the two equations are related to the concept of direct and reciprocal vectors [16].

Thus the key to the connection between the two angular relationships is to be found in Eqs. 22 and 23 which together with the cosine rule for the spherical triangle allow the correlations between Equations 4–6 and 14–16 to follow naturally. In fact the cosine rule for spherical triangles is often derived by other geometrical means described as methods 2 to 4 in “Appendix 1” independent of the direct and reciprocal concept [14]. If Eqs. 4–6 and 14–16 are derived independently of each other as is usually done in the literature, then the correlation between them revealed by this work is a major step forward and will be of considerable interest to student in either discipline.

Research and innovation in well-developed traditional fields [17–19] is also very important. The achievements of the research are usually significant historically. Through the above work we show that research and innovation in well-developed traditional fields are interesting and rewarding intellectually.

Appendices

Appendix 1 Derivations of the cosine rule for the spherical triangle

Method 1 Derivation by vector products

As stated in Sect. 5.3, the relationships between the vectors $\vec{OA}, \vec{OB}, \vec{OC}$ for the spherical triangle ABC and the vectors OA^*, OB^*, OC^* for the polar triangle A*B*C* are the same as the relationships between the direct and the reciprocal vectors. Thus the cosine rule for the spherical triangle can be derived in similar ways as that via Eqs. 7 and 8. Eqs. 31–33 can be obtained by using Eqs. 1–3 and Lagrange’s identity.

$$\begin{aligned} & \overline{OA} \cdot \overline{OB} \\ &= \frac{\overline{OB^*} \times \overline{OC^*}}{OA^* \cdot (\overline{OB^*} \times \overline{OC^*})} \cdot \frac{\overline{OC^*} \times \overline{OA^*}}{OB^* \cdot (\overline{OC^*} \times \overline{OA^*})} \\ &= \frac{(\overline{OB^*} \cdot \overline{OC^*}) \cdot (\overline{OC^*} \cdot \overline{OA^*}) - (\overline{OB^*} \cdot \overline{OA^*}) \cdot (\overline{OC^*} \cdot \overline{OC^*})}{[OA^* \cdot (\overline{OB^*} \times \overline{OC^*})][OB^* \cdot (\overline{OC^*} \times \overline{OA^*})]} \end{aligned} \tag{31}$$

$$\begin{aligned} & \frac{|\overline{OB^*}| |\overline{OC^*}| \sin \alpha^*}{V^*} \cdot \frac{|\overline{OC^*}| |\overline{OA^*}| \sin \beta^*}{V^*} \cos \gamma \\ &= \frac{(|\overline{OB^*}| |\overline{OC^*}| \cos \alpha^*) \cdot (|\overline{OC^*}| |\overline{OA^*}| \cos \beta^*) - (|\overline{OB^*}| |\overline{OA^*}| \cos \gamma^*) \cdot (|\overline{OC^*}| |\overline{OC^*}|)}{V^{*2}} \end{aligned} \tag{32}$$

or

$$\sin \alpha^* \sin \beta^* \cos \gamma = \cos \alpha^* \cos \beta^* - \cos \gamma^* \tag{33}$$

By applying Eqs. 21–23 it can be easily seen that Eq. 33 is just Eq. 19’.

Thus with the information provided in Sect. 5.3, the angular relationship for the direct and reciprocal vectors in Sect. 2.2 and the angular relationship for Euler’s theorem in Sect. 3.1 are just the angular relationship for spherical triangle as described by the cosine rule for the spherical triangle.

Method 2 Derivation by orthogonal vectors

\overline{OA} and \overline{OC} in Fig. 1 can be decomposed into orthogonal vectors as Eqs. 34 and 35

$$\overline{OA} = (|\overline{OA}| \cos \gamma) \frac{\overline{OB}}{|\overline{OB}|} + (|\overline{OA}| \sin \gamma) \frac{\overline{AA'}}{|\overline{AA}|} \tag{34}$$

$$\overline{OC} = (|\overline{OC}| \cos \alpha) \frac{\overline{OB}}{|\overline{OB}|} + (|\overline{OC}| \sin \alpha) \frac{\overline{CC'}}{|\overline{CC}|} \tag{35}$$

For simplicity we use unit vectors for \overline{OA} , \overline{OB} , \overline{OC} , thus Eqs. 34 and 35 are simplified as Eqs. 36 and 37

$$\overline{OA} = \overline{OB} \cos \gamma + \frac{\overline{AA'}}{|\overline{AA}|} \sin \gamma \tag{36}$$

$$\overline{OC} = \overline{OB} \cos \alpha + \frac{\overline{CC'}}{|\overline{CC}|} \sin \alpha \tag{37}$$

From Eq. 38 we obtain Eq. 18

$$\begin{aligned} \overline{OC} \cdot \overline{OA} &= \cos \beta \\ \cos \beta &= \overline{OC} \cdot \overline{OA} = \left(\overline{OB} \cos \alpha + \frac{\overline{CC'}}{|\overline{CC}|} \sin \alpha \right) \cdot \left(\overline{OB} \cos \gamma + \frac{\overline{AA'}}{|\overline{AA}|} \sin \gamma \right) \\ &= \cos \alpha \cos \gamma + \sin \alpha \sin \gamma \cos \angle B \end{aligned} \tag{38}$$

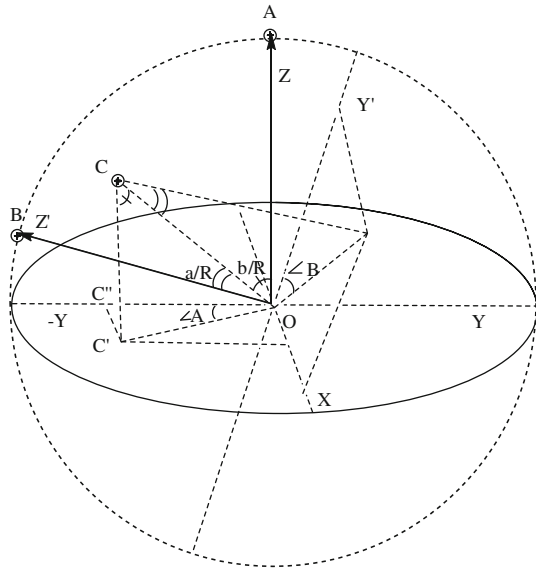
or

$$\cos \frac{b}{R} = \cos \frac{a}{R} \cos \frac{c}{R} + \sin \frac{a}{R} \sin \frac{c}{R} \cos \angle B \tag{18}$$

where

$$\overline{OB} \cdot \overline{OB} = 1; \overline{OB} \cdot \frac{\overline{CC'}}{|\overline{CC}|} = 0; \overline{OB} \cdot \frac{\overline{AA'}}{|\overline{AA}|} = 0; \frac{\overline{CC'}}{|\overline{CC}|} \cdot \frac{\overline{AA'}}{|\overline{AA}|} = \cos \angle B$$

Fig. 5 A spherical triangle ABC . Two coordinate systems, $OXYZ$ and $OXY'Z'$, are related by a rotation of $\frac{c}{R}$ around OX



Method 3 Derivation by coordinate system rotation

ABC (Fig. 5) is a spherical triangle from the surface of a sphere. CC' is perpendicular to XOY plane and C' is in XOY plane. Since the four points A, C, C' , and O are in a plane

$$\angle OCC' = \frac{\widehat{AC}}{R} = \frac{b}{R} \tag{39}$$

and \widehat{AB} and $\overline{OC''}$ are in a plane, and \widehat{AC} and $\overline{OC'}$ are in a plane

$$\angle C'OC'' = \angle A \tag{40}$$

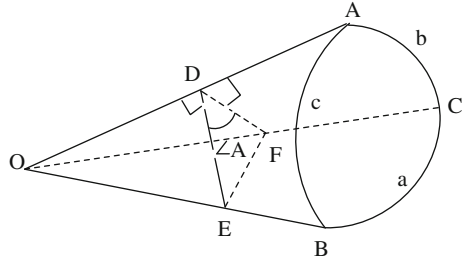
Thus the coordinates of C in the $OXYZ$ coordinate system are

$$C(x, y, z) = C \left(R \sin \frac{b}{R} \sin \angle A, -R \sin \frac{b}{R} \cos \angle A, R \cos \frac{b}{R} \right) \tag{41}$$

When the $OXYZ$ coordinate system is rotated by $\frac{\widehat{AB}}{R} = \frac{c}{R}$ around OX , OB becomes the new Z' . The new coordinates of C in the $OXY'Z'$ coordinate system are

$$C(x, y', z') = C \left(R \sin \frac{a}{R} \sin \angle B, R \sin \frac{a}{R} \cos \angle B, R \cos \frac{a}{R} \right) \tag{42}$$

Fig. 6 Spherical triangle ABC .
 $OA = OB = OC = R$



The old z coordinate of C in the old coordinate system $OXYZ$ is connected to the new z' in the new $OXY'Z'$ by rotation angle $\frac{c}{R}$.

$$z' = z \cos \frac{c}{R} - y \sin \frac{c}{R} \tag{43}$$

Inserting z' and the old y and z into the above coordinate system rotation formula, Eq. 43, we obtain Eq. 17

$$R \cos \frac{a}{R} = R \cos \frac{b}{R} \cos \frac{c}{R} + R \sin \frac{b}{R} \cos \angle A \sin \frac{c}{R} \tag{17}$$

Method 4 Derivation by trigonometry [14]

ABC (Fig. 6) is a spherical triangle from the surface of a sphere; O is the center; the length of radius OA is R . At an arbitrary point D in OA , draw a plane DEF perpendicular to the edge OA . Then

$$\angle EDF = \angle A \tag{44}$$

In the triangle DEF

$$\overline{EF}^2 = \overline{DE}^2 + \overline{DF}^2 - 2\overline{ED} \cdot \overline{DF} \cos \angle A \tag{45}$$

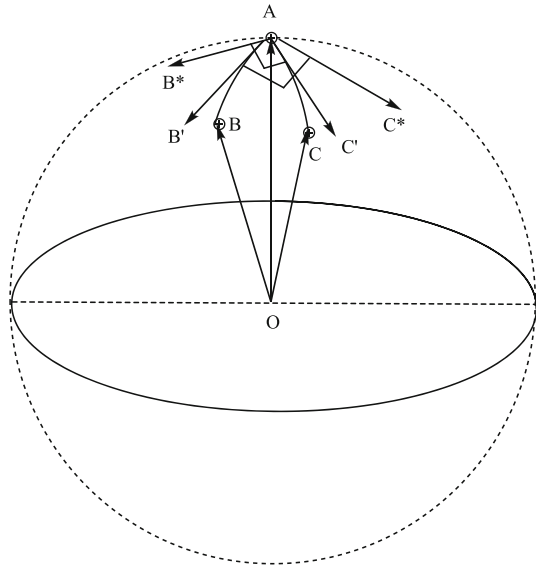
In the triangle OEF

$$\overline{EF}^2 = \overline{OE}^2 + \overline{OF}^2 - 2\overline{OE} \cdot \overline{OF} \cos \frac{a}{R} \tag{46}$$

Equating these values of \overline{EF}^2 with rearrangement

$$\begin{aligned} 2\overline{OE} \cdot \overline{OF} \cos \frac{a}{R} &= (\overline{OE}^2 - \overline{DE}^2) + (\overline{OF}^2 - \overline{DF}^2) + 2\overline{ED} \cdot \overline{DF} \cos \angle A \\ &= 2\overline{OD}^2 + 2\overline{ED} \cdot \overline{DF} \cos \angle A \end{aligned} \tag{47}$$

Fig. 7 A spherical triangle ABC and reciprocal vectors related polar vectors



Dividing Eq. 47 by $2\overline{OE} \cdot \overline{OF}$ and then arranging the factors results in Eq. 17

$$\begin{aligned} \cos \frac{a}{R} &= \frac{\overline{OD}}{\overline{OE}} \cdot \frac{\overline{OD}}{\overline{OF}} + \frac{\overline{ED}}{\overline{OE}} \cdot \frac{\overline{DF}}{\overline{OF}} \cos \angle A \\ &= \cos \frac{c}{R} \cos \frac{b}{R} + \sin \frac{c}{R} \sin \frac{b}{R} \cos \angle A \end{aligned} \tag{48}$$

Equations 18 and 19 can be obtained similarly. There is some kind of similarity between method 4 and method 2.

Appendix 2 Another derivation of Eqs. 22 and 23

ABC (Fig. 7) is a spherical triangle from the surface of a sphere. $\overline{AB'}$ and \widehat{AB} are in the same plane. $\overline{AC'}$ and \widehat{AC} are in the same plane. $\overline{AB'} \perp \overline{OA}$ and $\overline{AC'} \perp \overline{OA}$. Thus

$$\angle A = \angle B'AC' \tag{49}$$

$\overline{OA} \times \overline{OB}$ gives $\overline{AC^*}$. $\overline{OC} \times \overline{OA}$ gives $\overline{AB^*}$

$$\angle B^*AC' = \frac{\pi}{2} \tag{50}$$

$$\angle B'AC^* = \frac{\pi}{2} \tag{51}$$

Add the two Eqs.

$$\angle B^*AC' + \angle B'AC^* = \pi \quad (52)$$

or

$$\begin{aligned} \angle B^*AC' + \angle B'AC^* &= (\angle B^*AB' + \angle B'AC') + (\angle B'AC' + \angle C'AC^*) \\ &= (\angle B^*AB' + \angle B'AC' + \angle C'AC^*) + \angle B'AC' \\ &= \angle B^*AC^* + \angle A = \pi \end{aligned} \quad (53)$$

with the information provided in Sect. 5.3, we know that $\overline{AB^*}$ is parallel to $\overline{OB^*}$ as in Fig. 3 or 4 and that $\overline{AC^*}$ is parallel to $\overline{OC^*}$. When the plane containing $\overline{AB^*}$, $\overline{AC^*}$, $\overline{AB'}$, and $\overline{AC'}$ is moved down along \overline{OA} from A to O , it can easy to see that

$$\angle B^*AC^* = \angle B^*OC^* = \frac{a^*}{R} = \alpha^* \quad (54)$$

Thus Eq. 22 or 23 can be readily obtained from Eq. 53.

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