

RESEARCH ARTICLE

Wigner active and passive rotation matrices applied to NMR tensor

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Abstract

NMR Hamiltonians are double contraction of two spherical rank-2 tensors, their space parts are represented by a spherical tensor and their spin parts are composed of spherical tensor operators. The comprehension of modern NMR experiments is very often based on the rotation of these tensors. We present the active and passive rotations in a progressive way from position vector to spherical tensor operator via space function, spherical harmonic, and vector operator. The passive rotation of a physical quantity is described by the rotation of coordinate system. Both the left- and right-handed rotation conventions are applied whereas the right-handed rotation convention is mainly used in the literature. Throughout the article, we explore the equivalence between the active rotation of a physical quantity in one direction and the rotation of the coordinate system in the opposite direction. The article presents redundant mathematical demonstrations between active and passive rotations, but they clarify the meanings of some important expressions not well developed in the literature.

KEYWORDS

active rotation, canonical transformation, Euler angles, passive rotation, Wigner rotation matrix

1 | INTRODUCTION

NMR Hamiltonians may be defined with Cartesian or spherical tensors.¹ In the latter case, they are double contractions of two spherical rank-2 tensors, one representing the space part and the other the spin part. Very often, the space part has to be expressed in several coordinate systems (principal-axis system, MAS rotor system, laboratory-axis system), whereas the spin part is mainly described in the laboratory-axis system in simple pulse experiments. For example, the electric-field gradient tensor of quadrupole spins in powder is well studied in static, MAS, DOR, DAS, and MQMAS experiments. Multi-pulse experiments on spin- $\frac{1}{2}$ systems reduce the homonuclear dipole-dipole Hamiltonian. These methods aim to narrow the line widths using rotations. Descriptions of rotation in classical and quantum mechanics are numerous in literature. We explore the active and passive points of view, which are sources of confusion.

In this article, we present the active and passive rotations in a progressive way from position vector to spherical tensor operator via space function, spherical harmonic, and vector operator. The passive rotation of a physical quantity is described by the rotation of coordinate system.

Section 2 describes two equivalent points of view for the rotation of axes by an angle θ in a plane of 3-D Euclidean space using left- and right-handed conventions. Throughout the article, right-handed coordinate systems are used for left- and right-handed rotations.

Active, passive, and canonical transformations are extensively discussed in the literature. As we mainly deal with spin operators and the density matrix operator in NMR, we define not only the active and passive rotations of operators but also the canonical transformation of operators in Section 3.

Section 4 details the active and passive rotations of space function $\Psi(\mathbf{r})$ about a single axis using active $R_A(\alpha, z)$ and passive $R_P(\alpha, z)$ rotation operators. We also use

Dirac notations,² which have the advantages to represent not only the space function by ket state $|\Psi\rangle$ but also the coordinate system by bra position basis $\langle\mathbf{r}|$. This is not the case in standard notation about the rotation of space function such as $R_A(\alpha, z) \Psi(\mathbf{r})$. We show that right- and left-handed rotations of coordinate system about z -axis by angle α are expressed mathematically by the application of the operators $R_P(\alpha, z)$ and $R_A(\alpha, z)$ to bra position basis, respectively. In contrast, right- and left-handed active rotations of space function about z -axis by angle α are expressed by the application of $R_A(\alpha, z)$ and $R_P(\alpha, z)$ to ket state, respectively.

In Section 5, active and passive rotation operators for space function are expressed in terms of Euler angles about fixed or rotated axes. These rotation operators are extensively discussed in the literature. Some examples are provided for clarifying the notations used in these rotation operators.

We recall in Section 6 the reasons for which rotations of spin components or those of spherical tensor operator components should be performed about fixed axes. As a result, we only present active and passive rotations about fixed axes in the remaining of the article.

Section 7 presents the Wigner active and passive rotation matrices because they are involved in the active and passive rotations of spherical harmonics, spherical tensors, and spherical tensor operators.

Section 8 presents the spherical harmonics, which are space functions. Properties of spherical tensors are deduced from those of spherical harmonics. Furthermore, spherical harmonics are related to Wigner rotation matrices via simple relations. These relations allow us to determine the type (active or passive) of Wigner rotation matrix.

Section 9 details the active rotations of spherical harmonics about fixed axes and the rotations of coordinate system about fixed axes, which allows us to define the rotations of spherical tensors. For simplicity, we replace the passive rotations of spherical harmonics by rotations of coordinate system. We explore the two points of view (active and passive) of the two rotation operators $R_A^{\text{fixed}}(\alpha, \beta, \gamma)$ and $R_P^{\text{fixed}}(\gamma, \beta, \alpha)$ in Dirac notations. In each case we provide a simple example.

Section 10 details the rotations of vector operator and those of coordinate system. A vector operator is the simplest spherical tensor operator, whose rank is 1. In NMR, the spin $\mathbf{I}$ is a vector operator. The study of rotation of vector operator is more complex than that of space function because vector operator is sandwiched by the rotation operator and its adjoint operator. In contrast, the rotation operator is sandwiched by a bra position basis and a ket state in the case of space function. We discuss the rotations of vector operator with Cartesian components and

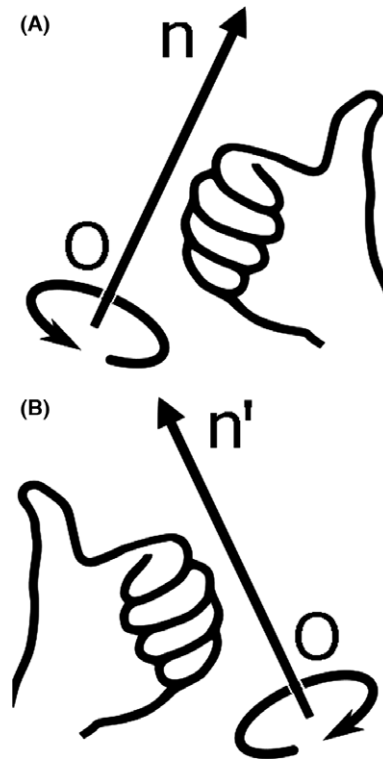


FIGURE 1 (A) Right-handed counter-clockwise rotations about the axis n ; (B) left-handed clockwise rotations about the axis n'

with spherical components. In each case we provide a simple example.

Section 11 provides the definitions of spherical tensor operator and an application example about the excitation of a spin by an off-resonance RF pulse using Wigner rotation matrices.

2 | ROTATION IN 3-D EUCLIDEAN SPACE

A right-handed rotation in 3-D Euclidean space is defined by an axis of rotation (n) through the origin (O) and an angle (θ) about that axis (Figure 1A). This rotation is denoted as $R(n, \theta)$. The positive sense of rotation³ is counter-clockwise when looking down the axis n toward the origin O . This description of rotation only involves the right hand. A second description of rotation involves the two hands: right-handed rotation (Figure 1A) and left-handed rotation (Figure 1B). In left-handed rotation, the positive sense of rotation is clockwise when looking down the axis n' toward the origin O .

Figure 2 adopted from Jackson⁴ shows a right-handed orthonormal Cartesian coordinate system (O, x, y, z). The point B in the $\{x, y\}$ plane is specified by the position vector $\mathbf{V}$ with components $(x_1, y_1, 0)$ along the axes as shown in Figure 2A. The latter shows that a left-handed rotation

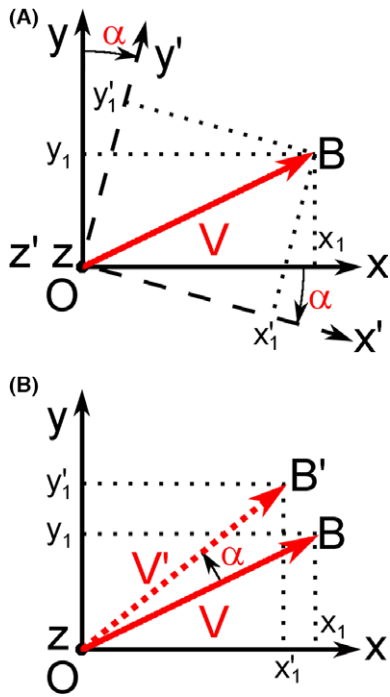


FIGURE 2 Two equivalent points of view for a rotation of axes by an angle α in a plane: (A) the vector $\mathbf{V}$ is fixed in the plane, whereas the axes are left-hand rotated about z -axis by a positive angle α in passive point of view; (B) the axes are fixed while the vector $\mathbf{V}$ is right-hand rotated to a new position $\mathbf{V}'$ about z -axis by a positive angle α in active point of view

about the z -axis by angle α applied to the coordinate system transforms (O, x, y, z) into (O, x', y', z') , keeping the point B fixed. Figure 2B shows that a right-handed rotation about the z -axis by angle α applied to the position vector transforms $\mathbf{V}$ into $\mathbf{V}'$, keeping the coordinate system (O, x, y, z) fixed. In either case, the primed coordinates $(x_1', y_1', 0)$ are given by

$$\begin{pmatrix} x_1' \\ y_1' \\ 0 \end{pmatrix} = \begin{pmatrix} \cos \theta & -\sin \theta & 0 \\ \sin \theta & \cos \theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ y_1 \\ 0 \end{pmatrix}. \quad (1)$$

We replace θ in Eq. (1) with the positive angle α used in Figure 2. This means that left-handed rotation of the coordinate system (O, x, y, z) keeping the position vector $\mathbf{V}$ fixed is equivalent to right-handed rotation of the position vector $\mathbf{V}$ keeping the coordinate system (O, x, y, z) fixed.

A single transformation matrix (Eq. (1)) can represent either left-handed rotation of coordinate system or right-handed rotation of position vector. An important point to note is that we use the same symbol α for two opposite senses of rotation.^{5–9} These opposite senses are shown by arrows. This point is not emphasized enough in the literature.

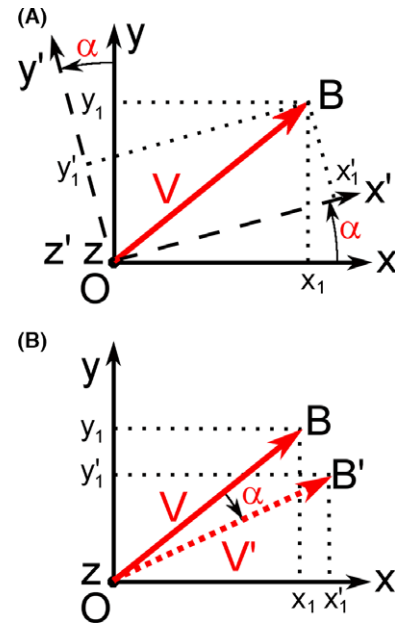


FIGURE 3 Two equivalent points of view for a rotation of axes by an angle α in a plane: (A) the vector $\mathbf{V}$ is fixed in the plane while the axes are right-hand rotated about z -axis by a positive angle α in passive point of view; (B) the axes are fixed while the vector $\mathbf{V}$ is left-hand rotated to a new position $\mathbf{V}'$ about z -axis by a positive angle α in active point of view

Heine¹⁰ presents a similar example (Figure 3). Figure 3A shows that a right-handed rotation about z -axis by angle α applied to the coordinate system transforms (O, x, y, z) into (O, x', y', z') , keeping the point B fixed. Figure 3B shows that a left-handed rotation about z -axis by angle α applied to the position vector transforms $\mathbf{V}$ into $\mathbf{V}'$, keeping the coordinate system (O, x, y, z) fixed. In either case, the primed coordinates $(x_1', y_1', 0)$ are given by

$$\begin{pmatrix} x_1' \\ y_1' \\ 0 \end{pmatrix} = \begin{pmatrix} \cos \theta & \sin \theta & 0 \\ -\sin \theta & \cos \theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ y_1 \\ 0 \end{pmatrix}. \quad (2)$$

Equation (2) is deduced from Eq. (1) by changing the sign of θ as the senses of rotation described by angles α in Figure 3 are the opposite of those in Figure 2. This means that right-handed rotation of the coordinate system (O, x, y, z) keeping the position vector $\mathbf{V}$ fixed is equivalent to left-handed rotation of the position vector $\mathbf{V}$ keeping the coordinate system (O, x, y, z) fixed.

In practice, Figure 2 is suitable for the analysis of rotation of vector because Figure 2B describes the right-handed rotation of vector.^{9,11} In contrast, Figure 3 is suitable for the analysis of rotation of coordinate system because Figure 3A describes the right-handed rotation of coordinate system.^{12,13}

Figure 4 shows the typical rotation angle notations suitable for rotation of vector. In this case, all rotations are described

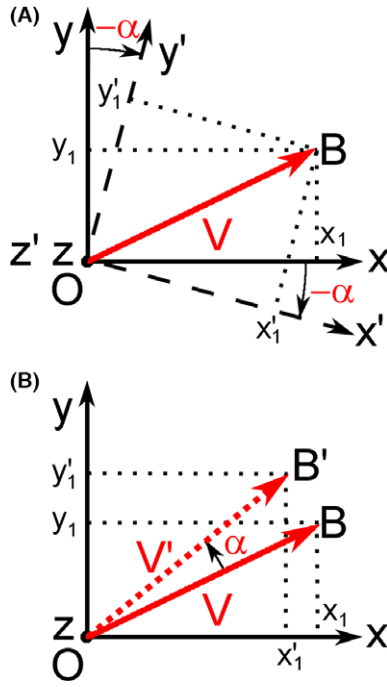


FIGURE 4 Two equivalent points of view for a rotation of axes by an angle α in a plane: (A) the vector $\mathbf{V}$ is fixed in the plane while the axes are right-hand rotated about z -axis by a negative angle $-\alpha$ in passive point of view; (B) the axes are fixed while the vector $\mathbf{V}$ is right-hand rotated to a new position $\mathbf{V}'$ about z -axis by a positive angle α in active point of view

by right-handed rotations^{1,3,11,14–16} in right-handed coordinate systems. The sense of rotation is either negative as shown in Figure 4A by angle $-\alpha$ or positive as shown in Figure 4B by angle α . As a result, two rotation matrices are involved. That corresponding to Figure 4A describes a right-handed rotation of coordinate system about z -axis by angle θ :³

$$\begin{pmatrix} x'_1 \\ y'_1 \\ 0 \end{pmatrix} = \begin{pmatrix} \cos \theta & \sin \theta & 0 \\ -\sin \theta & \cos \theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ y_1 \\ 0 \end{pmatrix}. \quad (3)$$

This angle θ is negative ($-\alpha$) in Figure 4A. That corresponding to Figure 4B describes a right-handed rotation of vector about z -axis by angle θ :³

$$\begin{pmatrix} x'_1 \\ y'_1 \\ 0 \end{pmatrix} = \begin{pmatrix} \cos \theta & -\sin \theta & 0 \\ \sin \theta & \cos \theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ y_1 \\ 0 \end{pmatrix}. \quad (4)$$

This angle θ is positive (α) in Figure 4B.

Replacing θ by $-\alpha$ in Eq. (3) and by α in Eq. (4) yield the same primed coordinates $(x'_1, y'_1, 0)$. Therefore, right-handed positive rotation of the position vector $\mathbf{V}$ keeping the coordinate system (O, x, y, z) fixed is equivalent to right-handed negative rotation of the coordinate system $(O,$

$x, y, z)$ keeping the position vector $\mathbf{V}$ fixed. Another way to express the same thing is the following. Right-handed counter-clockwise rotation of the position vector $\mathbf{V}$ keeping the coordinate system (O, x, y, z) fixed is equivalent to right-handed clockwise rotation of the coordinate system (O, x, y, z) keeping the position vector $\mathbf{V}$ fixed.

3 | ACTIVE, PASSIVE, AND CANONICAL TRANSFORMATIONS OF OPERATOR

Thaller¹⁷ suggests a test of the isotropy of space in performing an experiment with a physical system S in a fixed coordinate system C and then repeating the experiment in a rotated coordinate system C' . The response of S to an experiment should not depend on its orientation in space. This can be done in three ways.

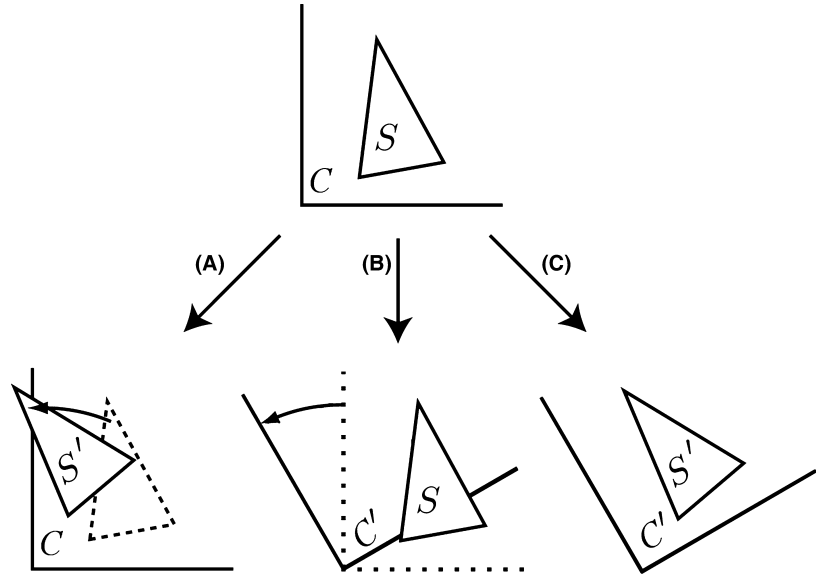
1. Rotate the system S but not the observer (Figure 5A). The experiment on the rotated physical system S' is described by an observer sitting in the fixed coordinate system C . The observer represents the measuring apparatus.¹⁸
2. Rotate the observer but not the system S (Figure 5B). The experiment on the system S in the fixed coordinate system C is described by an observer sitting in the rotating coordinate system C' .
3. Rotate the system S and the observer (Figure 5C). The procedure consists in rotating the whole experimental setup (the physical system and the observer). The experiment on the rotated system S' is performed and described in the rotated coordinate system C' . If the space is isotropic, the rotated system S' in the rotated coordinate system C' behaves exactly as the system S did in the fixed coordinate system C .

In classical mechanics, “rotate the system S but not the observer” is called an active transformation, whereas “rotate the observer but not the system S ” is called a passive transformation.¹⁷

In quantum mechanics, the physical system is represented by a state vector in Hilbert space of the physical system and observables are provided by measuring apparatus (or an observer in classical mechanics) sitting in a coordinate system. As a result, moving a measuring apparatus means moving the coordinate system.¹⁹ Observables (or more generally operators) T defined before moving the measuring apparatus becomes observables T' after moving the measuring apparatus. In other words, observables are defined for a coordinate system.

Shankar,²⁰ Rembold,²¹ and Auletta and Wang⁵ provide the definition of active and passive transformations. The state vectors in Hilbert space are affected in an active transformation and left alone in the passive case. The operators

FIGURE 5 Transformations of physical system: (A) In an active transformation, the physical system S is transformed with respect to a fixed coordinate system C . (B) In a passive transformation, the coordinate system C is transformed while the physical system S is left unchanged. (C) In a canonical transformation, both the physical system S and the coordinate system C are simultaneously transformed in the same way. C and C' are called body-attached coordinate system



or the measurement apparatus are left alone in an active transformation and are affected in the passive case. This presentation of active and passive transformations opposes transformed states against transformed operators. The coordinate system is implicitly related to measuring apparatus or operators.

Thompson²² and Lipkin²³ also distinguish three types of transformations as does Thaller:¹⁷ active, passive, and canonical transformations. State vectors are represented by kets. Dynamical operators are denoted by T and transformation operators by R_i .

In NMR, we essentially manipulate spin operators and density matrix operators, scarcely the state vector of the spin system. Therefore, we have to define the active and passive rotations of an operator. We focus on operators and coordinate systems, whereas state vector is hidden. The active transformation may be involved in one or two coordinate systems.¹ Two coordinate systems are involved in passive transformation.

3.1 | Active transformation of operator

Three entities are involved in our approach: state vector, operator, and right-handed coordinate system. An active transformation operator R_A changes the physical system but leaves the coordinate system unchanged.²⁴ That is,²²

$$|\Psi\rangle \xrightarrow{R_A} R_A|\Psi\rangle = |R_A\Psi\rangle = |\Psi'\rangle, \quad (5)$$

$|\Psi'\rangle$ is the transformed state vector and

$$T \xrightarrow{R_A} T. \quad (6)$$

The operators T are unchanged by an active transformation, because operators are defined for a coordinate

system that remains fixed in an active transformation. But the matrix elements of operators are usually changed:²⁵

$$\langle\Psi_1|T|\Psi_2\rangle \xrightarrow{R_A} \langle R_A\Psi_1|T|R_A\Psi_2\rangle. \quad (7)$$

In calculating matrix elements, the transformation operator R_A can always be shifted from the state vectors to the operators T . Equation (7) becomes⁹

$$\langle\Psi_1|T|\Psi_2\rangle \xrightarrow{R_A} \langle\Psi_1|(R_A)^\dagger T R_A|\Psi_2\rangle. \quad (8)$$

Sakurai and Napolitano²⁶ and Brink and Satchler⁹ also distinguish two approaches to describing R_A .

Approach 1: $|\Psi\rangle \xrightarrow{R_A} |R_A\Psi\rangle$ is a transformation of state vector with operators T unchanged (Eq. (7)).

Approach 2: $T \xrightarrow{R_A} (R_A)^\dagger T R_A$ is a transformation of operators T with state vectors unchanged (Eq. (8)).

In other words, we can either apply the active rotation operator to state vector ($|\Psi\rangle \xrightarrow{R_A} |R_A\Psi\rangle$) and leave operators unchanged, or we can leave state vectors unchanged and rotate operators $[T \xrightarrow{R_A} (R_A)^\dagger T R_A]$. Both yield the same matrix elements:

$$\langle\Psi_1|T|\Psi_2\rangle \xrightarrow{R_A} \langle R_A\Psi_1|T|R_A\Psi_2\rangle = \langle\Psi_1|(R_A)^\dagger T R_A|\Psi_2\rangle, \quad (9)$$

so the same physics.

If R_A is a right-handed counter-clockwise (Figure 1A) active rotation operator, the transformation defined in Eq. (7) describes a right-handed counter-clockwise rotation of the physical system, keeping the operators T fixed. It is equivalent to saying that the transformation defined in Eq. (8) describes a right-handed clockwise rotation of the operators T , keeping the physical system fixed. The same matrix element describes either the

right-handed counter-clockwise rotation of the state vectors or the right-handed clockwise rotation of the operators.

To distinguish these two ways to describe a matrix element, we call the first way ($|\Psi\rangle \xrightarrow{R_A} |R_A\Psi\rangle$) a right-handed (Figure 1A) active rotation of state vector and the second way $[T \xrightarrow{R_A} (R_A)^\dagger T R_A]$ a left-handed (Figure 1B) active rotation of operators T . In both ways, the coordinate system remains fixed.

3.2 | Passive transformation of operator

A passive transformation operator R_P leaves the physical system unchanged, but changes the coordinate system. The change in coordinate system is also called the change in description.²⁷ This means two coordinate systems are involved in passive transformation. We have²²

$$|\Psi\rangle \xrightarrow{R_P} |\Psi\rangle \quad (10)$$

and

$$T \xrightarrow{R_P} T', \quad (11)$$

T and T' being the same operators expressed in terms of the old and new coordinate systems, respectively. Matrix elements are usually changed under a passive transformation:

$$\begin{aligned} \langle \Psi_1 | T | \Psi_2 \rangle &\xrightarrow{R_P} \langle R_P \Psi_1 | T | R_P \Psi_2 \rangle = \langle \Psi_1 | (R_P)^\dagger T R_P | \Psi_2 \rangle \\ &= \langle \Psi_1 | T' | \Psi_2 \rangle. \end{aligned} \quad (12)$$

As it is well-known (see Section 4) that

$$(R_A)^\dagger = R_P, \quad (13)$$

the operators T' in Eqs. (11) and (12) are defined by^{19,23}

$$T \xrightarrow{R_P} T' = (R_P)^\dagger T R_P = R_A T (R_A)^\dagger. \quad (14)$$

Therefore, Eq. (12) becomes

$$\begin{aligned} \langle \Psi_1 | T | \Psi_2 \rangle &\xrightarrow{R_P} \langle \Psi_1 | T' | \Psi_2 \rangle = \langle \Psi_1 | (R_P)^\dagger T R_P | \Psi_2 \rangle \\ &= \langle \Psi_1 | R_A T (R_A)^\dagger | \Psi_2 \rangle. \end{aligned} \quad (15)$$

If R_A is a right-handed counter-clockwise active rotation operator, it follows that R_P is also a right-handed counter-clockwise, but passive rotation operator. We have just proposed that the transformation $T \xrightarrow{R_A} (R_A)^\dagger T R_A$ deduced from Eq. (8) describes a left-handed active rotation of operators T , keeping the coordinate system fixed. We deduce that the transformation $T \xrightarrow{R_P} T' = R_A T (R_A)^\dagger$ in Eq. (14) describes a right-handed active rotation of operators T , keeping the coordinate system fixed. Thanks to Eq. (14), it is equivalent to describing the transformation

$T \xrightarrow{R_P} T' = (R_P)^\dagger T R_P$ as a left-handed rotation of the coordinate system, keeping the operators T fixed. It is also called left-handed passive rotation of operators T .

3.3 | Canonical transformation of operator

A canonical transformation by the operator R_A changes both the physical system and the coordinate system. We have,²²

$$|\Psi\rangle \xrightarrow{R_A} R_A |\Psi\rangle = |R_A \Psi\rangle = |\Psi'\rangle, \quad (16)$$

and

$$T \xrightarrow{R_A} T'. \quad (17)$$

Recall in quantum mechanics, observables are provided by a measuring apparatus. Moving a measuring apparatus means moving the coordinate system.

The transformation defined by Eqs. (16) and (17) is called canonical because it transforms state vector and operators but leaves the matrix elements invariant:²⁸

$$\langle \Psi_1 | T | \Psi_2 \rangle \xrightarrow{R_A} \langle \Psi'_1 | T' | \Psi'_2 \rangle = \langle \Psi_1 | T | \Psi_2 \rangle. \quad (18)$$

The important point is that matrix elements do not change by a unitary transformation of state vector and a unitary transformation of observables. An important class of canonical transformations are those which correspond to symmetries of the physical system.²³ They are translations, rotations, space inversion, and time-reversal.

Equation (16) allows us to rewrite the matrix element in Eq. (18) as

$$\begin{aligned} \langle \Psi'_1 | T' | \Psi'_2 \rangle &= \langle R_A \Psi_1 | T' | R_A \Psi_2 \rangle = \langle \Psi_1 | (R_A)^\dagger T' R_A | \Psi_2 \rangle \\ &= \langle \Psi_1 | T | \Psi_2 \rangle. \end{aligned} \quad (19)$$

As a result, Eq. (17) becomes

$$T \xrightarrow{R_A} T' = R_A T (R_A)^\dagger. \quad (20)$$

The transformation in Eq. (20) differs with $T \xrightarrow{R_A} (R_A)^\dagger T R_A$ discussed in active transformation of operator. As the latter is a left-handed active rotation of operators T in a fixed coordinate system, the transformation in Eq. (20) is a right-handed active rotation of operators T in a fixed coordinate system.

In quantum mechanics textbooks on symmetry operations (Chapter 3 in Ballentine,²⁹ Section 14 of Chapter 3 in Biedenharn and Louck,³⁰ Complement B_{VI} in Cohen-Tannoudji et al.,³¹ Pages 99-101 in Davydov,³² Chapter 1 in Haywood,²⁷ Chapter 29 in Hecht,²⁸ Section 7.4 in Konishi and Paffuti,³³ Chapter 2 and Section 6.3 in Mathur and Singh,¹⁴ Chapter 13 in Messiah,³⁴ Section 4.10 in Miller,³⁵

Section 2 in Rose,³⁶ Page 3 in Tung,³⁷ Chapter 3 in Zare,³⁸ Pages 102 and 116 in Zettili³⁹), the active transformation is defined as the following: In conjunction with the transformation of the state vectors induced by a symmetry operation (unitary transformation) given by Eq. (16), each operator T undergoes the transformation defined in Eq. (20).

In the canonical transformation by the operator R_A , both operators and coordinate system rotate together. The right-handed active rotation of operators T in a fixed coordinate system is followed by a right-handed rotation of the fixed coordinate system. The rotated coordinate system is called body-attached coordinate system.

In fact, the active transformation corresponds to our active rotation in one coordinate system, the fixed coordinate system associated with the unprimed operator. The canonical transformation corresponds to our active rotation in two coordinate systems:¹ the fixed coordinate system is associated with the unprimed operator and the body-attached coordinate system is attached to the operator and rotates with it. Equation (18) means that the primed operator in the body-attached coordinate system has the same matrix elements as those of the unprimed operator in the fixed coordinate system before the active rotation.

4 | ROTATION OF SPACE FUNCTION ABOUT A SINGLE AXIS

The study of active rotation of space function about a single axis involves one or two coordinate systems. When one coordinate system is used,⁴⁰ it corresponds to a space-fixed coordinate system (O, x, y, z).³⁸ When two coordinate systems are used,³⁶ one corresponds to the space-fixed coordinate system (O, x, y, z) and the other is attached to the space function, rotates with it, and is called body-attached coordinate system (O, x', y', z') or molecule-fixed frame.^{38,41} Viewed in its body-attached coordinate system, the space function remains motionless. We previously shown¹ that Rose³⁶ used this approach for deducing the active rotation operator involving Euler angles. As Rose did not use figures to support his presentation, Wolf⁴⁰ and Bouten⁴² understood that Rose dealt with passive rotation of space function.

In this section, we formulate the rotation of a space function in one direction and the equivalent rotation of coordinate system in the opposite direction using right and left hands. Two approaches are used: the standard one involving rotation operator and space function [$R_A(\alpha, z)\Psi(\mathbf{r})$] and that involving Dirac notations [$\langle \mathbf{r} | R_A(\alpha, z) | \Psi \rangle$]. The second approach has the advantage to exhibit both the coordinate system represented by bra position basis and the space function represented by ket space function. In the standard approach [$R_A(\alpha, z)\Psi(\mathbf{r})$], the coordinate system is not explicitly defined.

We first provide the definitions of terms such as Hilbert space, scalar product, position representation, and wave function used in quantum mechanics that are important for the comprehension of some common notations. Especially, scalar product and wave function have two possible interpretations.

4.1 | Hilbert space

A Hilbert space is an abstract vector space with a scalar product and a positive definite norm.^{28,39,43} In quantum mechanics, physical properties of a system are represented by linear operators $R, L, \dots$ and a state vector Φ or state for short by ket state $|\Phi\rangle$ or wave function $\Phi(\mathbf{r})$, and by bra state $\langle \Phi |$ or complex conjugate $\Phi^*(\mathbf{r})$ of wave function. While ket state belongs to a Hilbert space, its bra state belongs to the corresponding dual Hilbert space. Wave functions, complex-valued functions of space, are square-integrable functions. Their space possesses the properties of an infinite-dimensional Hilbert space.³⁹

The quantum state is an abstract concept, but it contains all the information about the system. Observables are Hermitian operators, which take real eigenvalues only. A wave function is associated with a state, whereas a space function is not necessary a state. An operator acting on a ket produces another ket. However, the result of an operator on a state is not necessary a state, it may be a space function.^{35,44} In our case, a rotation operator converts an old state into a new state because rotation operators are unitary operators.

One of the key benefits of Dirac notation² is that operators, kets, and bras are independent of any representation basis. Very often it is convenient to use some less abstract representations of states and operators to get numerical results.

In finite-dimensional Hilbert space, we expand any ket as a linear combination of the eigen kets of an observable.⁴⁵ If Q is such an observable in a 2-D vector space with eigen kets $\{|i\rangle, |j\rangle\}$, then an arbitrary state $|\Phi\rangle$ can be expressed as a linear combination of $\{|i\rangle, |j\rangle\}$. These two eigen kets are basis vectors in an orthonormal coordinate system. That is,

$$|\Phi\rangle = a_i|i\rangle + a_j|j\rangle. \quad (21)$$

The components are given by $\langle i | \Phi \rangle = a_i$ and $\langle j | \Phi \rangle = a_j$.

Therefore, the state Φ may be written as an abstract ket state $|\Phi\rangle$, a superposition of ket basis vectors (Eq. (21)), or a set of numbers (expansion coefficients $\langle i | \Phi \rangle = a_i$ and $\langle j | \Phi \rangle = a_j$ in Eq. (21)). The three kets $|\Phi\rangle$, $|i\rangle$, and $|j\rangle$ belong to the same Hilbert space. The set of components $\{a_i, a_j\}$ of $|\Phi\rangle$ along the eigen kets of Q completely describe $|\Phi\rangle$. They are called the Q representation of $|\Phi\rangle$.^{29,45} Changing representations does not change the state ket. The ket state $|\Phi\rangle$ itself is representation-free. Similarly, the scalar product is also representation-free.^{35,46}

When we take a scalar product in quantum mechanics, we use a common basis in both states.

A scalar product or a bra-ket pair can be interpreted in two ways.³⁹ First, a bra-ket pair corresponds to a vector projection. The projection of $|\Phi\rangle$ onto the eigen ket $|i\rangle$ is $\langle i | \Phi \rangle$, that on $|j\rangle$ is $\langle j | \Phi \rangle$. Therefore, Eq. (21) can be written as

$$|\Phi\rangle = \langle i | \Phi \rangle |i\rangle + \langle j | \Phi \rangle |j\rangle = \sum_{a=i,j} |a\rangle \langle a | \Phi \rangle, \quad (22)$$

because the closure relation $\sum_{a=i,j} |a\rangle \langle a| = 1$ is available.

Second, the quantity $\langle \Psi | \Phi \rangle$ represents the probability amplitude that the system's ket state $|\Phi\rangle$ before a measurement will be found to be in another ket state $|\Psi\rangle$ after the measurement.

Some Hilbert spaces are of infinite number of dimensions, where the observables can take on an infinite number of possible values. The typical examples are function spaces where vectors are functions. In quantum mechanics, wave functions are often space functions.^{32,43} For states with continuous eigenvalues, such as two wave functions $\Psi_1(\mathbf{r})$ and $\Psi_2(\mathbf{r})$, the scalar product is defined by integral^{33,47}

$$\langle \Psi_1 | \Psi_2 \rangle = \int \Psi_1^*(\mathbf{r}) \Psi_2(\mathbf{r}) d^3\mathbf{r}. \quad (23)$$

In other words, $\langle \Psi_1 | \Psi_2 \rangle$ corresponds to the integral of $\Psi_1^*(\mathbf{r}) \Psi_2(\mathbf{r})$.⁴⁶ As we mentioned above, the scalar product $\langle \Psi_1 | \Psi_2 \rangle$ is the projection of $|\Psi_2\rangle$ onto $|\Psi_1\rangle$. However, the more general interpretation of $\langle \Psi_1 | \Psi_2 \rangle$, independent of representation, is that it represents the probability amplitude for the ket state $|\Psi_2\rangle$ to be found in the ket state $|\Psi_1\rangle$;²⁶ operators are not explicitly involved in this case.

If an observable $\mathbf{N}$ is involved, we are interested in calculating the mean value $\langle \Psi | \mathbf{N} | \Psi \rangle$, which can be checked by performed the same experiment on the same state many times. The state Ψ appears as both a bra and a ket. $\langle \Psi | \mathbf{N} | \Psi \rangle$ is also called expectation value.

4.2 | Position representation

We focus on the position representation corresponding to measuring position operator R for a spinless particle in 3-D space. The eigen kets of R are $|\mathbf{r}\rangle$ with corresponding eigenvalues $\mathbf{r}$,²⁶ the position vectors of the particle. The eigen kets are labeled by the eigenvalues. That is,

$$R|\mathbf{r}\rangle = \mathbf{r}|\mathbf{r}\rangle. \quad (24)$$

These eigenvalues are continuous as every value of position is measurable. The position representation may be defined by the continuous set of ket position basis $|\mathbf{r}\rangle$. So we have

$$\text{Ket position basis: } |\mathbf{r}\rangle, \quad \forall \mathbf{r} \in \mathbf{R}^3. \quad (25)$$

In Eq. (21), the ket state is expressed in a countable basis, identified by an integer. On the other hand, the position basis is uncountable, identified by real numbers.

The ket position bases verify^{26,28,39} the closure relation

$$\int |\mathbf{r}\rangle \langle \mathbf{r}| d^3\mathbf{r} = 1, \quad (26)$$

and the orthonormality condition

$$\langle \mathbf{r}' | \mathbf{r} \rangle = \delta(\mathbf{r} - \mathbf{r}'), \quad (27)$$

the latter being the highly localized Dirac delta function^{5,28,33,44,48} defined by

$$f(\mathbf{r}) = \int \delta(\mathbf{r} - \mathbf{r}') f(\mathbf{r}') d^3\mathbf{r}' \quad (28)$$

for any function f that is continuous at $\mathbf{r}$. Suppose the particle is at position $\mathbf{r}_0$. The corresponding ket is $|\mathbf{r}_0\rangle$. The position representation of $|\mathbf{r}_0\rangle$ ^{35,49} or its wave function is $\delta(\mathbf{r} - \mathbf{r}_0)$.

The norm of the continuous ket position bases is infinite.^{29,39} Therefore, the kets $|\mathbf{r}\rangle$ are not square integrable.^{28,39} As Hilbert space admits only vectors of finite norm,²⁹ the kets $|\mathbf{r}\rangle$ are not elements of the particle's Hilbert space^{34,39,49} but remain a valid basis that spans the particle's Hilbert space.^{28,39}

The scalar product $\langle \mathbf{r} | \Phi \rangle$ of $|\mathbf{r}\rangle$ with an arbitrary state ket $|\Phi\rangle$ is a square-integrable function of $\mathbf{r}$, $\Phi(\mathbf{r})$.⁴⁹ The result of an operator L on $|\Phi\rangle$ is $L|\Phi\rangle$. Its position representation is $\langle \mathbf{r} | L | \Phi \rangle$.

4.3 | Wave function

Space function $\Psi(\mathbf{r})$ of a particle in 3-D space is defined by^{24,25}

$$\Psi(\mathbf{r}) = \langle \mathbf{r} | \Psi \rangle, \quad (29)$$

which is not an equation in the usual sense. $\Psi(\mathbf{r})$ is also known as normalized Schrödinger wave function for ket state $|\Psi\rangle$ ^{14,28,39,47} with

$$|\Psi\rangle = \int_{\text{all space}} |\mathbf{r}'\rangle \langle \mathbf{r}' | \Psi \rangle d^3\mathbf{r}' = \int_{\text{all space}} |\mathbf{r}'\rangle \Psi(\mathbf{r}') d^3\mathbf{r}'. \quad (30)$$

A particle's wave function defines not only its position but also all the spatial properties of the particle. The product of the wave function with its complex conjugate is the density probability^{25,44} for finding the particle at position $\mathbf{r}$.

Equation (29) relates the conventional notation of the abstract wave function Ψ in position representation with

Dirac notation of the wave function.⁴⁶ It shows that the wave function is the projection of the ket state $|\Psi\rangle$ onto the bra position base $\langle \mathbf{r} |$.^{39,50}

The use of the position eigenstates as basis states to represent operators and states is referred to as the position representation. Equation (30) is the expansion of an arbitrary ket state $|\Psi\rangle$ in terms of the ket position bases $|\mathbf{r}'\rangle$, where the expansion coefficient is the wave function in position representation. The summation over the index of a complete set of eigenvalues in Eq. (22) becomes an integral over continuous eigenvalues in Eq. (30). $\Psi(\mathbf{r})$ is also the probability amplitude^{13,33,44,51} for finding a particle at position $\mathbf{r}$ in an orthonormal basis of 3-D space.

Therefore, the symbol $\Psi(\mathbf{r})$ has two different meanings in different contexts.⁴⁴

1. The first meaning is $\Psi(\mathbf{r}) = |\Psi\rangle$, $\Psi(\mathbf{r})$ means a mathematical function of $\mathbf{r}$, the whole function without being explicit the actual value of $\mathbf{r}$. It is the position representation of the abstract ket state $|\Psi\rangle$. As the list of components of a vector in a basis of 3-D vector space is a particular representation of that vector, $\Psi(\mathbf{r})$ and $|\Psi\rangle$ are similar to the components of a vector in a particular basis and the vector, respectively. Similarly, $\Psi(\mathbf{p}) = |\Psi\rangle$ is the momentum representation of the abstract ket state $|\Psi\rangle$, but $\Psi(\mathbf{p})$ is the Fourier transform of $\Psi(\mathbf{r})$.²⁶ It is important to note that the mathematical expression of $\Psi(\mathbf{r})$ differs with that of $\Psi(\mathbf{p})$.
2. The second meaning of $\Psi(\mathbf{r})$ is Eq. (29), that is, the probability amplitude $\Psi(\mathbf{r})$ for finding the particle in the state $|\Psi\rangle$ at the some specific position $\mathbf{r}$,⁵² or more generally the value $\Psi(\mathbf{r})$ of the space function Ψ at some specific position $\mathbf{r}$,³¹ not the whole function. A scalar product is a number, and $\langle \mathbf{r} | \Psi \rangle$ is the value of Ψ at the position $\mathbf{r}$. If $\langle \mathbf{r} | \Psi \rangle = 0$, it does not mean $|\Psi\rangle$ and $|\mathbf{r}\rangle$ are orthogonal because they do not belong to the same Hilbert space. It just means the value of the wave function Ψ at the specific position $\mathbf{r}$ is zero.

A particle in state $|\mathbf{r}\rangle$ is located at position $\mathbf{r}$. In contrast, a particle in state $|\Psi\rangle$ can be found at different positions with corresponding probability amplitudes. The action of an operator L on a space function is related to its action on the abstract vector space by the rule²⁹ $L\Psi(\mathbf{r}) = \langle \mathbf{r} | L | \Psi \rangle$ with $\Psi(\mathbf{r}) = \langle \mathbf{r} | \Psi \rangle$.

4.4 | Active rotation of space function in one coordinate system

Consider the right-handed active rotation^{9,11,22,32,34,38,40,53} about z -axis by angle α of the space function in the space-fixed coordinate system (O, x, y, z) . The rotation operator is denoted by $R_A(\alpha, z)$.

Before the rotation, the physical system is described by the ket state $|\Psi\rangle$, whose space function $\Psi(\mathbf{r})$ is the $\mathbf{r}$ -position representation of $|\Psi\rangle$ in (O, x, y, z) . $\Psi(\mathbf{r})$ is a mathematical function of $\mathbf{r}$, the first meaning (1) of a space function. After the rotation, the physical system is described by the new ket state $|\Psi'_A\rangle = R_A(\alpha, z)|\Psi\rangle$, whose space function $\Psi'_A(\mathbf{r})$ is the $\mathbf{r}$ -position representation of $|\Psi'_A\rangle$ in the same coordinate system (O, x, y, z) . As whole functions, the mathematical expression of $\Psi(\mathbf{r})$ differs with that of $\Psi'_A(\mathbf{r})$, that is, $\Psi(\mathbf{r}) \neq \Psi'_A(\mathbf{r})$.

As the rotation operator $R_A(\alpha, z)$ is a unitary operator, the value $\Psi'_A(\mathbf{r})$ of the space function at the position $\mathbf{r}$ is equal to the value $\Psi(\mathbf{r}_1)$ of the space function before rotation at the position $\mathbf{r}_1$ (Figure 6A):

$$\Psi'_A(\mathbf{r}) = \Psi(\mathbf{r}_1). \quad (31)$$

The second meaning (2) of space functions $\Psi(\mathbf{r})$ and $\Psi'_A(\mathbf{r})$ is used in Eq. (31).

The two positions $\mathbf{r}_1$ and $\mathbf{r}$ in (O, x, y, z) are related³ by the right-handed active rotation matrix $A_z(\alpha)$:

$$\mathbf{r} = A_z(\alpha)\mathbf{r}_1 = \begin{pmatrix} \cos \alpha & -\sin \alpha & 0 \\ \sin \alpha & \cos \alpha & 0 \\ 0 & 0 & 1 \end{pmatrix} \mathbf{r}_1. \quad (32)$$

Formally, we can introduce the right-handed passive rotation matrix $P_z(\alpha)$:³

$$\mathbf{r}_1 = A_z(-\alpha)\mathbf{r} = P_z(\alpha)\mathbf{r}. \quad (33)$$

Equation (33) relates the components of position vectors using rotation matrices.

Equation (33) does not mean the two positions $\mathbf{r}$ and $\mathbf{r}_1$ are the same position vector viewed in two different coordinate systems. It suggests that the two positions $\mathbf{r}$ and $P_z(\alpha)\mathbf{r}$ (Figure 6B) are viewed in two different coordinate systems, that of $\mathbf{r}$ is (O, x, y, z) and that of $P_z(\alpha)\mathbf{r}$ is (O, x', y', z') . The latter is generated by the left-handed rotation of (O, x, y, z) about z -axis by angle α . Notice that we use the same symbol α for two rotation angles of opposite signs. In other words, the components of position $\mathbf{r}$ in (O, x, y, z) are identical to those of position $P_z(\alpha)\mathbf{r}$ in (O, x', y', z') .

The left-handed rotation of coordinate system is related to the fact that the position $\mathbf{r}_1 = P_z(\alpha)\mathbf{r}$ is deduced from the position $\mathbf{r}$ by a left-handed rotation. As a result, $P_z(\alpha)$ may be either a right-handed passive rotation matrix or a left-handed passive rotation matrix, depending on the circumstance.

We illustrate this property of $P_z(\alpha)$ with Figure 7. Figure 7A shows the space function $\Psi(y)$ in the fixed coordinate system (O, x, y, z) . The action of a right-handed active rotation of $\Psi(y)$ about z -axis by angle $\alpha = \frac{\pi}{2}$ is shown in Figure 7B where the space function becomes $\Psi'_A(-x)$. The action of $P_z(\alpha = \frac{\pi}{2})$ on $\mathbf{r}$ is

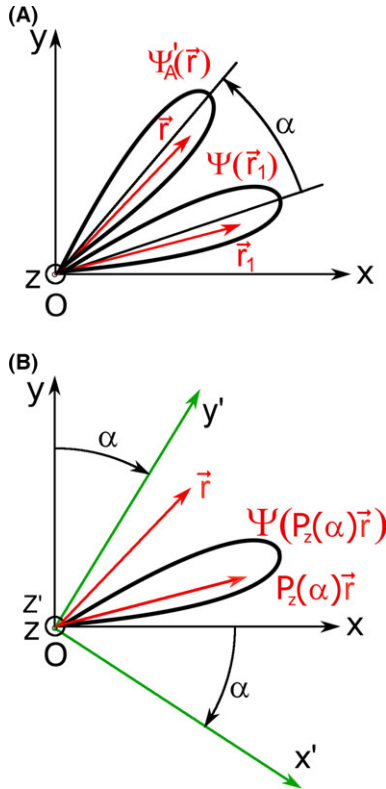


FIGURE 6 (A) Right-handed active rotation of space function about z -axis by angle α shown in a single coordinate system (O, x, y, z) . $\Psi(\mathbf{r}_1)$ is the initial space function before rotation and $\Psi'_A(\mathbf{r})$ is the rotated space function. (B) Equivalent left-handed rotation of coordinate system from (O, x, y, z) to (O, x', y', z') . Position vector $\mathbf{r}$ is attached to (O, x, y, z) and position vector $P_z(\alpha)\mathbf{r}$ is attached to (O, x', y', z')

$$P_z(\alpha = \frac{\pi}{2})\mathbf{r} = \begin{pmatrix} \cos(\alpha = \frac{\pi}{2}) & \sin(\alpha = \frac{\pi}{2}) & 0 \\ -\sin(\alpha = \frac{\pi}{2}) & \cos(\alpha = \frac{\pi}{2}) & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} y \\ -x \\ z \end{pmatrix}. \quad (34)$$

In fact, the position vector $\mathbf{r}$ represents the coordinate system. That is, x - and y -axes become y - and $-x$ -axes, respectively. In Figure 7C, the original x - and y -axes are black lines and the rotated axes are green lines. The green coordinate system is deduced from the black one by a left-handed rotation about z -axis by angle $\alpha = \frac{\pi}{2}$. The space function becomes $\Psi(-x)$ in the green coordinate system like the space function in Figure 7B.

Equation (31) becomes²⁴

$$\Psi'_A(\mathbf{r}) = \Psi(\mathbf{r}_1) = \Psi(P_z(\alpha)\mathbf{r}). \quad (35)$$

The position $P_z(\alpha)\mathbf{r}$ is described in the left-hand rotated coordinate system (O, x', y', z') .

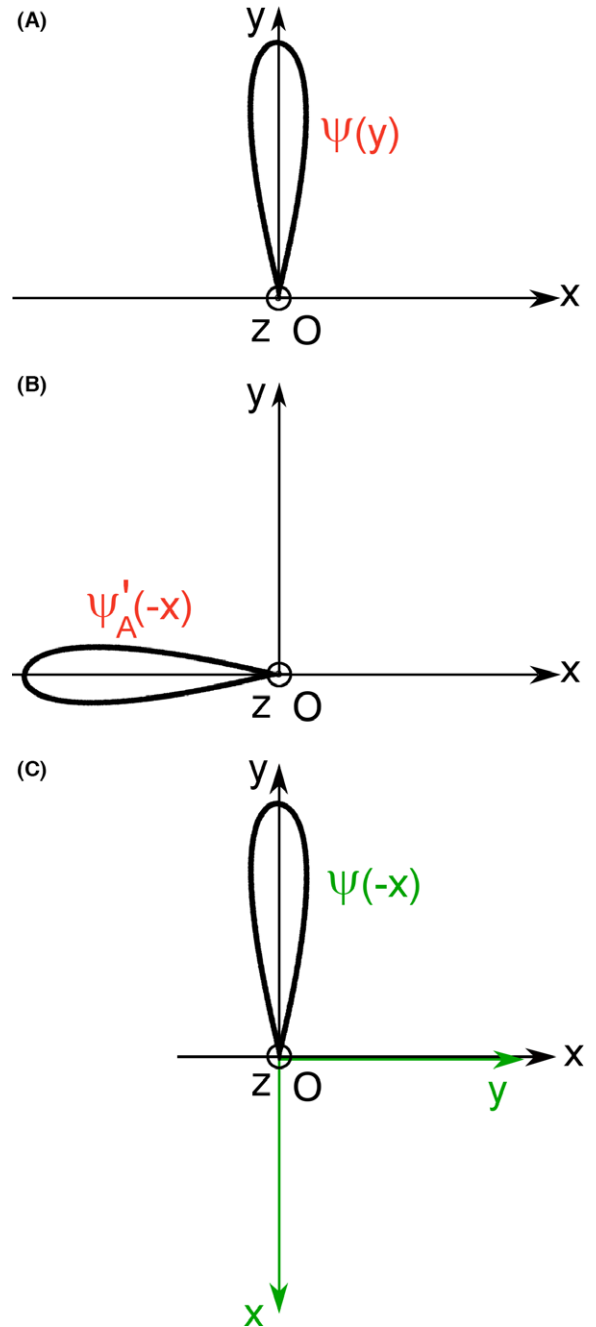


FIGURE 7 Equivalence between right-handed active rotation of space function about z -axis by angle $\alpha = \pi/2$ transforming the space function $\Psi(y)$ in (A) to the space function $\Psi'_A(-x)$ in (B) and left-handed rotation of coordinate system about z -axis by angle $\alpha = \pi/2$ transforming black (O, x, y, z) to green (O, x, y, z) in (C); the space function is $\Psi(y)$ in black (O, x, y, z) and $\Psi(-x)$ in green (O, x, y, z)

The space function $\Psi(\mathbf{r}')$ is the $\mathbf{r}'$ -position representation of the initial ket state $|\Psi\rangle$ in (O, x', y', z') . The same space function Ψ designates the initial space function in (O, x, y, z) and that in (O, x', y', z') . This may confuse us, but it is correct, because the ket state $|\Psi\rangle$ is viewed in two coordinate systems. Its space function is $\Psi(\mathbf{r})$ in $(O, x, y,$

z) and $\Psi(\mathbf{r}')$ in (O, x', y', z') . As whole functions, the mathematical expression of $\Psi(\mathbf{r}')$ differs with that of $\Psi(\mathbf{r})$.

We deduce from Eq. (35) that the value $\Psi'_A(\mathbf{r})$ of the right-hand rotated space function at position $\mathbf{r}$ in the fixed coordinate system (O, x, y, z) (Figure 6A) is identical to the value $\Psi(\mathbf{P}_z(\alpha)\mathbf{r})$ of the initial space function at position $\mathbf{P}_z(\alpha)\mathbf{r}$ in the left-hand rotated coordinate system (O, x', y', z') (Figure 6B). In other words, a right-handed active rotation of space function in a fixed coordinate system (Figure 6A) is equivalent to a left-handed rotation of coordinate system keeping the space function fixed (Figure 6B).

Introducing the operator of right-handed active rotation about z -axis by angle α denoted by^{1,40,53,54}

$$R_A(\alpha, z) = \exp(-i\alpha L_z), \quad (36)$$

Eq. (35) becomes^{11,29,32,34,40}

$$\Psi'_A(\mathbf{r}) \stackrel{1}{=} R_A(\alpha, z)\Psi(\mathbf{r}) \stackrel{2}{=} \Psi(\mathbf{r}_1) \stackrel{3}{=} \Psi(\mathbf{P}_z(\alpha)\mathbf{r}). \quad (37)$$

Two interpretations of the action of $R_A(\alpha, z)$ are possible:⁴⁰

1. By definition, the action of right-handed operator $R_A(\alpha, z)$ upon the space function $\Psi(\mathbf{r})$ must give us a new function $\Psi'_A(\mathbf{r})$ of same argument.³² The first equality denoted by $\stackrel{1}{=}$ describes a right-handed active rotation of the space function from Ψ to Ψ'_A , their arguments $\mathbf{r}$ being the same. As the argument $\mathbf{r}$ of the space function also represents the coordinate system, the right-handed operator $R_A(\alpha, z)$ rotates the space function from Ψ to Ψ'_A , keeping the coordinate system fixed. We may write Eq. (37) as

$$\Psi'_A(\mathbf{r}) \stackrel{1}{=} [R_A(\alpha, z)\Psi](\mathbf{r}) \stackrel{2}{=} \Psi(\mathbf{r}_1) \stackrel{3}{=} \Psi(\mathbf{P}_z(\alpha)\mathbf{r}). \quad (38)$$

2. In contrast, the equality denoted by $\stackrel{3}{=}$ in Eq. (37) describes the action of $R_A(\alpha, z)$ as a left-handed rotation of coordinate system from $\mathbf{r}$, which is associated with (O, x, y, z) , to $\mathbf{P}_z(\alpha)\mathbf{r}$, which is associated with (O, x', y', z') , keeping the space function Ψ fixed.

In quantum mechanics, an active rotation operator $R_A(\alpha, z)$ is a unitary transformation, that is,

$$[R_A(\alpha, z)]^\dagger = [R_A(\alpha, z)]^{-1} = R_A(-\alpha, z) = R_P(\alpha, z). \quad (39)$$

The operator $R_P(\alpha, z)$ will be introduced in Section 4.6. The definition of a space function in Eq. (29) allows us to write

$$\begin{aligned} [R_A(\alpha, z)\Psi](\mathbf{r}) &= \langle \mathbf{r} | R_A(\alpha, z)\Psi \rangle = \langle \mathbf{r} | R_A(\alpha, z) | \Psi \rangle \\ &= \left\langle [R_A(\alpha, z)]^\dagger \mathbf{r} \middle| \Psi \right\rangle = \langle R_A(-\alpha, z)\mathbf{r} | \Psi \rangle \\ &= \langle R_P(\alpha, z)\mathbf{r} | \Psi \rangle \stackrel{3}{=} \Psi(\mathbf{P}_z(\alpha)\mathbf{r}). \end{aligned} \quad (40)$$

Equation (38) written in Dirac notation becomes

$$\begin{aligned} \langle \mathbf{r} | \Psi'_A \rangle &\stackrel{1}{=} \langle \mathbf{r} | R_A(\alpha, z) | \Psi \rangle \stackrel{2}{=} \langle \mathbf{r}_1 | \Psi \rangle \stackrel{3}{=} \Psi(\mathbf{P}_z(\alpha)\mathbf{r}) \\ &= \langle R_P(\alpha, z)\mathbf{r} | \Psi \rangle. \end{aligned} \quad (41)$$

The operator $R_A(\alpha, z)$ defined in Eq. (36) is the right-handed counter-clockwise active rotation operator for space function. In $\langle \mathbf{r} | R_A(\alpha, z) | \Psi \rangle$, it behaves as a right-handed active rotation (Figure 2A) operator when it is applied to the ket state $R_A(\alpha, z)|\Psi\rangle = |R_A(\alpha, z)\Psi\rangle$ or as a left-handed passive rotation (Figure 2A) operator when it is applied to the bra position basis $\langle \mathbf{r} | R_A(\alpha, z) = \langle \mathbf{r} | [R_P(\alpha, z)]^\dagger$.

We have introduced right-handed and left-handed types of rotation in our discussions. The coordinate system in Dirac notations is expressed by bra position basis $\langle \mathbf{r} |$ in $\langle \mathbf{r} | R_A(\alpha, z) | \Psi \rangle$. If we only use right-handed rotations, we will say: The operator $R_A(\alpha, z)$ in $\langle \mathbf{r} | R_A(\alpha, z) | \Psi \rangle$ behaves as a counter-clockwise active rotation operator (Figure 4B) when it is applied to the ket state or as a clockwise passive rotation operator (Figure 4A) when it is applied to the bra position basis. In this sentence, we may replace counter-clockwise by positive and clockwise by negative.

4.5 | Active rotation of space function in two coordinate systems—canonical transformation

The two coordinate systems are the space-fixed coordinate system (O, x, y, z) in Figure 8 and the rotated body-attached coordinate system (O, x', y', z') in Figure 8B. The space function and its body-attached coordinate system rotate together as a whole.

Figure 8A is identical to Figure 6A. It shows the space functions $\Psi(\mathbf{r})$ and $\Psi'_A(\mathbf{r})$ of the initial ket state $|\Psi\rangle$ and the right-hand rotated ket state $|\Psi'_A\rangle = R_A(\alpha, z)|\Psi\rangle$ in (O, x, y, z) , respectively. Equations deduced in the previous subsection remain valid here. Therefore, we have (see Eq. (37))

$$\Psi'_A(\mathbf{r}) \stackrel{1}{=} R_A(\alpha, z)\Psi(\mathbf{r}) \stackrel{2}{=} \Psi(\mathbf{r}_1) \quad \text{with} \quad \mathbf{r}_1 = \mathbf{P}_z(\alpha)\mathbf{r}. \quad (42)$$

Figure 8B shows the rotated ket state $|\Psi'_A\rangle$ in two coordinate systems. Its $\mathbf{r}$ -position representation [the first meaning (1) of space function] is the space function $\Psi'_A(\mathbf{r})$ in (O, x, y, z) . Its $\mathbf{r}'$ -position representation should be the space function $\Psi'_A(\mathbf{r}')$ in (O, x', y', z') . As whole functions, the mathematical expression of $\Psi'_A(\mathbf{r})$ differs with that of $\Psi'_A(\mathbf{r}')$, that is, $\Psi'_A(\mathbf{r}) \neq \Psi'_A(\mathbf{r}')$.

It is important to note that in Figure 8B we have used the space function $\Psi(\mathbf{r}')$ associated with the initial ket state $|\Psi\rangle$ to denote the right-hand rotated space function in its body-attached coordinate system. We have used the property that the rotated space function as a whole function in its body-attached coordinate system remains the same as that before rotation $\Psi(\mathbf{r})$, but its argument is $\mathbf{r}'$ in $(O, x', y',$

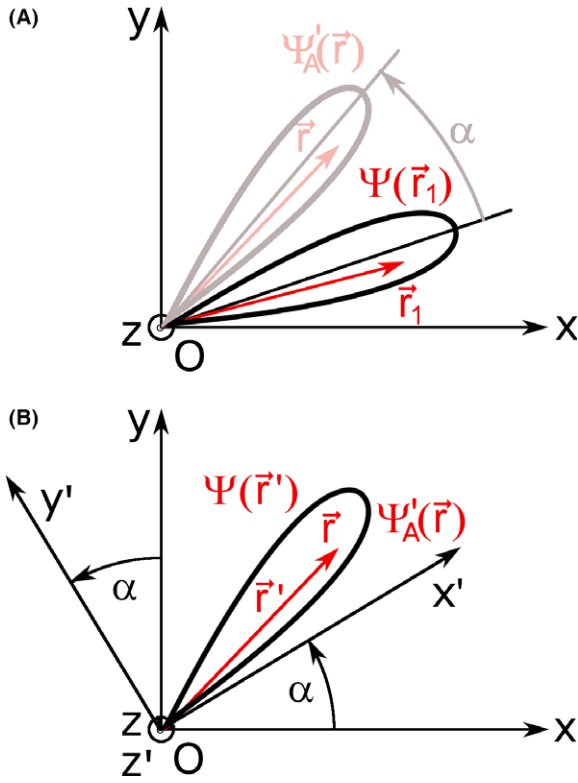


FIGURE 8 Canonical transformation (or active rotation) of space function about z -axis by angle α in two coordinate systems, the space-fixed coordinate system (O, x, y, z) and the body-attached coordinate system (O, x', y', z') . (A) Before rotation: $\Psi(\mathbf{r}_1)$ is the space function; (O, x, y, z) and (O, x', y', z') coincide. (B) After rotation: $\Psi'_A(\mathbf{r})$ is the rotated space function in the space-fixed coordinate system and $\Psi(\mathbf{r}')$ is the rotated space function in its body-attached coordinate system

z'). As whole functions, the mathematical expression of $\Psi'_A(\mathbf{r})$ differs with that of $\Psi(\mathbf{r}')$, that is, $\Psi'_A(\mathbf{r}) \neq \Psi(\mathbf{r}')$.

The angle α describes the rotation of (O, x', y', z') in Figure 8B, whereas it describes the rotation of the space function in Figure 8A when one coordinate system is used. As the rotated ket state $|\Psi'_A\rangle$ in Figure 8B is viewed in two coordinate systems, the value $\Psi'_A(\mathbf{r})$ of the rotated space function Ψ'_A at the rotated position $\mathbf{r}$ in (O, x, y, z) is equal to the value $\Psi(\mathbf{r}')$ of the rotated space function Ψ at the position $\mathbf{r}'$ in the rotated body-attached coordinate system (O, x', y', z') :³⁶

$$\Psi'_A(\mathbf{r}) = \Psi(\mathbf{r}'). \quad (43)$$

The second meaning (2) of space function is used in Eq. (43), where the positions $\mathbf{r}$ and $\mathbf{r}'$ are those shown in Figure 8B.

Equation (43) differs with Eq. (31). In Eq. (43) the argument of the space function Ψ is the rotated position $\mathbf{r}'$ in the rotated body-attached coordinate system (O, x', y', z') , whereas in Eq. (31) it is the initial position $\mathbf{r}_1$ in the fixed coordinate system (O, x, y, z) .⁵⁵

The positions $\mathbf{r}'$ and $\mathbf{r}$ are identical in Figure 8B, but they are viewed in two coordinate systems, $\mathbf{r}'$ in (O, x', y', z') and $\mathbf{r}$ in (O, x, y, z) . Therefore,³

$$\mathbf{r}' = \mathbf{P}_z(\alpha)\mathbf{r}. \quad (44)$$

Equation (44) relates the components of position vectors using rotation matrix.

Substituting Eq. (44) into Eq. (43) yields

$$\Psi'_A(\mathbf{r}) = \Psi(\mathbf{r}') = \Psi(\mathbf{P}_z(\alpha)\mathbf{r}). \quad (45)$$

Combining Eqs. (42) and (45) yields

$$\Psi'_A(\mathbf{r}) \stackrel{1}{=} R_A(\alpha, z)\Psi(\mathbf{r}) \stackrel{4}{=} \Psi(\mathbf{r}') \stackrel{3}{=} \Psi(\mathbf{P}_z(\alpha)\mathbf{r}). \quad (46)$$

Furthermore, the space function is motionless in its body-attached coordinate system. We have an obvious expression concerning the values of space function, which is not always provided in the literature:

$$\Psi(\mathbf{r}') \stackrel{2}{=} \Psi(\mathbf{r}_1), \quad (47)$$

$\mathbf{r}_1$ being the initial position vector in (O, x, y, z) before rotation of the body-attached coordinate system and $\mathbf{r}'$ the corresponding position vector in (O, x', y', z') after rotation of the body-attached coordinate system. This corresponds to the canonical transformation. Equation (47) means the space function is described in its body-attached coordinate system.

The active rotations of a space function in one and two coordinate systems are equivalent. This is supported by the same series of equalities in Eqs. (37) and (46). The equality $\stackrel{4}{=}$ in Eq. (46) is due to the implication of the body-attached coordinate system. Van de Wiele⁵⁶ and Devanathan⁵⁷ also use two coordinate systems.

Equations (46) and (47) may be written in Dirac notation:

$$\begin{aligned} \langle \mathbf{r} | \Psi'_A \rangle &\stackrel{1}{=} \langle \mathbf{r} | R_A(\alpha, z) | \Psi \rangle \stackrel{4}{=} \langle \mathbf{r}' | \Psi \rangle \\ &\stackrel{3}{=} \langle \mathbf{P}_z(\alpha)\mathbf{r} | \Psi \rangle = \langle R_P(\alpha, z)\mathbf{r} | \Psi \rangle, \end{aligned} \quad (48)$$

and

$$\langle \mathbf{r}' | \Psi \rangle \stackrel{2}{=} \langle \mathbf{r}_1 | \Psi \rangle. \quad (49)$$

The comments for the active rotation of space function in one coordinate system remains valid: The right-handed counter-clockwise active rotation operator for space function $R_A(\alpha, z)$ in $\langle \mathbf{r} | R_A(\alpha, z) | \Psi \rangle$ behaves as a right-handed active rotation (Figure 2B) operator when it is applied to the ket state $R_A(\alpha, z) | \Psi \rangle = | R_A(\alpha, z) \Psi \rangle$ or as a left-handed passive rotation (Figure 2A) operator when it is applied to the bra position basis $\langle \mathbf{r} | R_A(\alpha, z) = \langle \mathbf{r} | [R_P(\alpha, z)]^\dagger$.

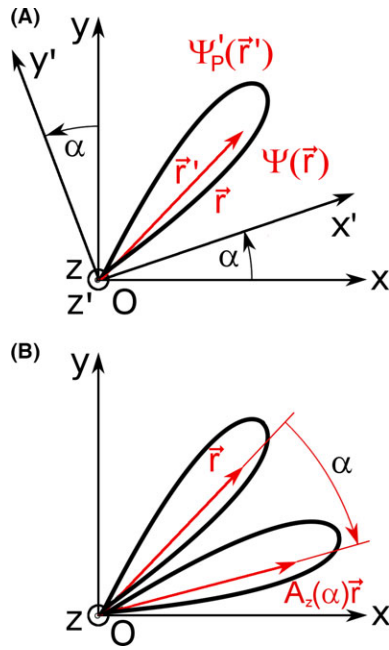


FIGURE 9 (A) Right-handed passive rotation of space function (or rotation of coordinate system) about z-axis by angle α . The space function is viewed in two coordinate systems. $\Psi(\mathbf{r})$ is the space function in the space-fixed coordinate system (O, x, y, z) and $\Psi'_p(\mathbf{r}')$ is the space function in the rotated coordinate system (O, x', y', z') . (B) Equivalent left-handed active rotation of space function from position vector $\mathbf{r}$ to position vector $A_z(\alpha)\mathbf{r}$ in the space-fixed coordinate system (O, x, y, z)

4.6 | Passive rotation of space function

Contrary to the active rotation of space function, which can be described in one and in two coordinate systems, two coordinate systems are naturally involved in the passive rotation of space function. Figure 9A shows these two coordinate systems related by a right-handed rotation about z-axis by angle α : the space-fixed coordinate system (O, x, y, z) and the rotated one (O, x', y', z') . The operator for right-handed passive rotation of space function is denoted by $R_p(\alpha, z)$.

Under passive rotation, the key state $|\Psi\rangle$ remains unchanged as we mentioned in Section 3, but its space function as a whole function depends on the coordinate system. It is tempting to define the whole function of its space function in (O, x, y, z) by $\Psi(\mathbf{r})$, the $\mathbf{r}$ -position representation of $|\Psi\rangle$, and that in (O, x', y', z') by $\Psi(\mathbf{r}')$, the $\mathbf{r}'$ -position representation of $|\Psi\rangle$. These two space functions only differ by their arguments. We already met a similar definition of space functions in the above subsection where the rotated coordinate system is the rotated body-attached coordinate system. This is not the case here; (O, x', y', z') in Figure 9A is not the rotated body-attached coordinate system.

We have to denote the space function by $\Psi(\mathbf{r})$ in (O, x, y, z) and by $\Psi'_p(\mathbf{r}')$ in (O, x', y', z') . The first meaning (1)

of space function is used: these two space functions $\Psi(\mathbf{r})$ and $\Psi'_p(\mathbf{r}')$ represent the components of the ket state $|\Psi\rangle$ in (O, x, y, z) and (O, x', y', z') , respectively. As whole functions, the mathematical expression of $\Psi(\mathbf{r})$ differs with that of $\Psi'_p(\mathbf{r}')$, that is, $\Psi(\mathbf{r}) \neq \Psi'_p(\mathbf{r}')$.

As the ket state $|\Psi\rangle$ remains unchanged under passive rotation, whose operator is a unitary operator, we have⁴⁰

$$\Psi'_p(\mathbf{r}') = \Psi(\mathbf{r}). \quad (50)$$

The second meaning (2) of space function is used in Eq. (50): the value $\Psi'_p(\mathbf{r}')$ of the space function after passive rotation at the position $\mathbf{r}'$ in (O, x', y', z') is identical to the value $\Psi(\mathbf{r})$ of the space function before passive rotation at the position $\mathbf{r}$ in (O, x, y, z) . These two identical positions $\mathbf{r}$ and $\mathbf{r}'$ are those shown in Figure 9A.

The components of $\mathbf{r}'$ in (O, x', y', z') and those of $\mathbf{r}$ in (O, x, y, z) are related by the right-handed passive rotation matrix $P_z(\alpha)$:³

$$\mathbf{r}' = P_z(\alpha)\mathbf{r}. \quad (51)$$

Formally, we can introduce the right-handed active rotation matrix $A_z(\alpha)$:³

$$\begin{aligned} \mathbf{r} &= (P_z(\alpha))^{-1}\mathbf{r}' = P_z(-\alpha)\mathbf{r}' = A_z(\alpha)\mathbf{r}' \\ &= \begin{pmatrix} \cos \alpha & -\sin \alpha & 0 \\ \sin \alpha & \cos \alpha & 0 \\ 0 & 0 & 1 \end{pmatrix} \mathbf{r}'. \end{aligned} \quad (52)$$

Equation (52) relates the components of position vectors using rotation matrices.

Equation (52) does not mean the two positions $\mathbf{r}$ and $\mathbf{r}'$ in Figure 9A are related by an active rotation. It suggests that the two positions $\mathbf{r}'$ and $A_z(\alpha)\mathbf{r}'$ are related by a left-handed active rotation about z-axis by angle α in (O, x', y', z') . The left-handed active rotation of position vector is suggested by the fact that the position $P_z(-\alpha)\mathbf{r}'$ is deduced from the position $\mathbf{r}'$ by a left-handed rotation. As $\mathbf{r}'$ and $\mathbf{r}$ represent the same position vector viewed in two coordinate systems, it follows that the two positions $\mathbf{r}$ and $A_z(\alpha)\mathbf{r}$ in Figure 9B are also related by a left-handed active rotation about z-axis by angle α in (O, x, y, z) . Notice that we use the same symbol α for two rotation angles of opposite signs. As a result, $A_z(\alpha)$ may be either a right-handed active rotation matrix or a left-handed active rotation matrix, depending on the circumstance. In other words, $\mathbf{r}$ and $A_z(\alpha)\mathbf{r}$ are equivalent to $\mathbf{r}'$ and $A_z(\alpha)\mathbf{r}'$. Equation (50) becomes²⁴

$$\Psi'_p(\mathbf{r}') = \Psi(\mathbf{r}) \stackrel{3}{=} \Psi(A_z(\alpha)\mathbf{r}'). \quad (53)$$

Equation (53) relates the values of space functions at different position vectors. In particular, the equality

$\Psi(\mathbf{r}) \stackrel{3}{=} \Psi(\mathbf{A}_z(\alpha)\mathbf{r}')$ is equivalent to $\Psi(\mathbf{r}) \stackrel{3}{=} \Psi(\mathbf{A}_z(\alpha)\mathbf{r})$. This suggests that the space function is expressed in its body-attached coordinate system, $\Psi(\mathbf{r})$ before the left-handed rotation and $\Psi(\mathbf{A}_z(\alpha)\mathbf{r}')$ after the left-handed rotation of the space function and its body-attached coordinate system. In other words, the equality $\Psi(\mathbf{r}) \stackrel{3}{=} \Psi(\mathbf{A}_z(\alpha)\mathbf{r}')$ describes a left-handed active rotation of space function in two coordinate systems, whereas the above subsection describes a right-handed active rotation of space function in two coordinate systems. As an active rotation of space function in one coordinate system and in two coordinate systems are equivalent, the equality $\Psi(\mathbf{r}) \stackrel{3}{=} \Psi(\mathbf{A}_z(\alpha)\mathbf{r}')$ also suggests a left-handed active rotation of a space function in the fixed coordinate system (O, x, y, z).

We deduce from Eq. (53) that the value $\Psi'_P(\mathbf{r}')$ of the space function at the position $\mathbf{r}'$ in the rotated coordinate system (Figure 9A) is equal to the value $\Psi(\mathbf{A}_z(\alpha)\mathbf{r}')$ of the left-hand rotated space function Ψ at the position $\mathbf{A}_z(\alpha)\mathbf{r}$ in the fixed coordinate system (Figure 9B). In other words, a right-handed rotation of coordinate system keeping the space function fixed (Figure 9A) is equivalent to a left-handed active rotation of space function in a fixed coordinate system (Figure 9B).

The right-handed counter-clockwise passive rotation operator $R_P(\alpha, z')$ about z' -axis by angle α for a space function^{40,58} is

$$R_P(\alpha, z') = \exp(i\alpha L_{z'}). \quad (54)$$

The z' - and z -axes, which are parallel, are the rotation axis in (O, x', y', z') and (O, x, y, z) , respectively. Wolf⁴⁰ established the passive rotation operator about fixed axes for space function involving Euler angles.

Weissbluth⁵⁹ like many authors^{58,60,61} chooses z instead of z' for rotation axis:

$$R_P(\alpha, z) = \exp(i\alpha L_z). \quad (55)$$

In this article, we also choose this notation. Therefore,

$$\Psi'_P(\mathbf{r}') = R_P(\alpha, z)\Psi(\mathbf{r}'). \quad (56)$$

As a result, the right-handed counter-clockwise active rotation operator in Eq. (36) and the right-handed counter-clockwise passive rotation operator in Eq. (55) differ only by the sign of the rotation angle.

Putting Eqs. (53) and (56) together yields^{29,32}

$$\Psi'_P(\mathbf{r}') \stackrel{1}{=} R_P(\alpha, z)\Psi(\mathbf{r}') \stackrel{2}{=} \Psi(\mathbf{r}) \stackrel{3}{=} \Psi(\mathbf{A}_z(\alpha)\mathbf{r}'). \quad (57)$$

As with the active rotation of space function, two interpretations of Eq. (57) are possible:⁴⁰

1. The first equality denoted by $\stackrel{1}{=}$ describes a right-handed passive rotation of space function from Ψ to Ψ'_P , their arguments $\mathbf{r}'$ being the same.

2. In contrast, the equality denoted by $\stackrel{3}{=}$ in Eq. (57) describes the action of $R_P(\alpha, z)$ as a left-handed active rotation of space function in fixed coordinate system.

It is worth noting that Eqs. (37) and (57) have the same structure. Figure 8B about the active rotation of space function described in two coordinate systems and Figure 9A about the passive rotation of space function also in two coordinate systems look similar, but the space functions are different. In Figure 8B, the space function $\Psi'_A(\mathbf{r})$ is expressed in the fixed coordinate system and $\Psi(\mathbf{r}')$ in the rotated body-attached coordinate system. It is the opposite in Figure 9A. The space function $\Psi'_P(\mathbf{r}')$ is expressed in the rotated coordinate system and $\Psi(\mathbf{r})$ in the fixed coordinate system.

In quantum mechanics, a passive rotation operator $R_P(\alpha, z)$ is a unitary transformation, that is,

$$[R_P(\alpha, z)]^\dagger = [R_P(\alpha, z)]^{-1} = R_A(\alpha, z). \quad (58)$$

Equation (57) written in Dirac notation becomes

$$\begin{aligned} \langle \mathbf{r}' | \Psi'_P \rangle &\stackrel{1}{=} \langle \mathbf{r}' | R_P(\alpha, z) | \Psi \rangle \stackrel{2}{=} \langle \mathbf{r} | \Psi \rangle \\ &\stackrel{3}{=} \Psi(\mathbf{A}_z(\alpha)\mathbf{r}') = \langle R_A(\alpha, z)\mathbf{r}' | \Psi \rangle. \end{aligned} \quad (59)$$

In $\langle \mathbf{r}' | R_P(\alpha, z) | \Psi \rangle$, $R_P(\alpha, z)$ behaves as a right-handed passive rotation operator (Figure 3A) when it is applied to the bra

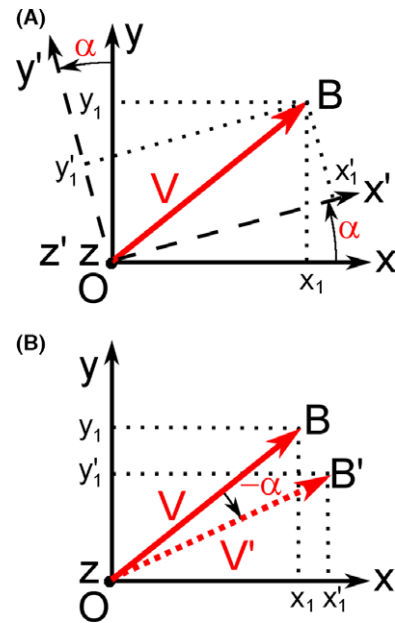


FIGURE 10 Two equivalent points of view for a rotation of axes by an angle α in a plane: (A) the vector $\mathbf{V}$ is fixed in the plane while the axes are right-hand rotated about z -axis by a positive angle α in passive point of view; (B) the axes are fixed, whereas the vector $\mathbf{V}$ is right-hand rotated to a new position $\mathbf{V}'$ about z -axis by a negative angle $-\alpha$ in active point of view

position basis ($\langle \mathbf{r}' | R_P(\alpha, z) | \Psi \rangle$) and as a left-handed active rotation operator (Figure 3B) when it is applied to the ket state:

$$\langle \mathbf{r}' | (R_P(\alpha, z) | \Psi \rangle) = \langle \mathbf{r}' | R_A(-\alpha, z) | \Psi \rangle. \quad (60)$$

If we only use right-handed rotations, we will say: The operator $R_P(\alpha, z)$ in $\langle \mathbf{r}' | R_P(\alpha, z) | \Psi \rangle$ behaves as a counter-clockwise passive rotation operator (Figure 10A) when it is applied to the bra position basis and as a clockwise active rotation operator (Figure 10B) when it is applied to the ket state (Eq. (60)). In this sentence, we may replace counter-clockwise by positive and clockwise by negative.

Equality $\stackrel{2}{=}$ in Eq. (59) provides us with

$$\langle \mathbf{r}' | R_P(\alpha, z) = \langle \mathbf{r} |. \quad (61)$$

Although the two positions $\mathbf{r}'$ and $\mathbf{r}$ are identical, the two bra position bases $\langle \mathbf{r}' |$ and $\langle \mathbf{r} |$ are different. It is interesting to note that the initial bra position basis $\langle \mathbf{r} |$ is deduced from the final bra position basis $\langle \mathbf{r}' |$ using the passive rotation operator $R_P(\alpha, z)$. The components of the two positions $\mathbf{r}'$ and $\mathbf{r}$ are related by Eq. (51).

Equation (61) may be rewritten as

$$\langle \mathbf{r}' | = \langle \mathbf{r} | R_A(\alpha, z). \quad (62)$$

In words, the passive rotation of a space function using the passive rotation operator $R_P(\alpha, z)$ is visualized by an active rotation of the bra position basis from $\langle \mathbf{r} |$ to $\langle \mathbf{r}' |$ or by an active rotation of coordinate system from (O, x, y, z) to (O, x', y', z') .

5 | ROTATION OF SPACE FUNCTION IN TERMS OF EULER ANGLES

Several ways to parameterize the rotation matrix for the orientation of a rigid body in a coordinate system or the relative orientation of two coordinate systems are available. Some of them are: direction cosine matrix,⁶² Euler angles,^{3,24,55,63} angle-axis of rotation^{24,55,62–64} denoted by $(\theta, \mathbf{n})$, the four Cayley-Klein parameters,^{63,65} and quaternions.^{25,64} Siemens et al.⁶⁶ discussed in details the benefits of using angle-axis of rotation parametrization over that of Euler angles in NMR. In contrast, we focus on Euler angle parametrization, which is extensively used in the literature other than that about NMR. We want to clarify its implications in active and passive rotations by exploring the equivalence between the active rotation of a physical quantity in one direction and the rotation of the coordinate system in the opposite direction. In particular, we emphasize on which Euler angle, α or γ , is the first rotation angle.

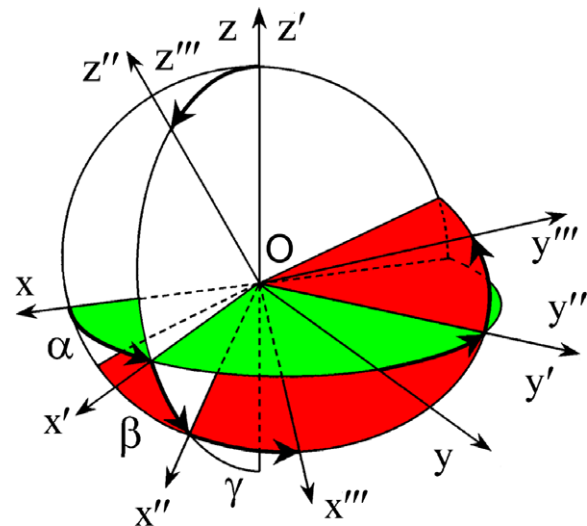


FIGURE 11 Euler angles are traditionally defined with rotated coordinate systems

In Section 4, we show that right- and left-handed rotations of coordinate system about z -axis by angle α are expressed mathematically by the application of the operators $R_P(\alpha, z)$ and $R_A(\alpha, z)$ to the bra position basis, respectively. In contrast, right- and left-handed active rotations of space function about z -axis by angle α are expressed by the application of $R_A(\alpha, z)$ and $R_P(\alpha, z)$ to the ket space function, respectively. We extend these rules to rotation operators defined with Euler angles. As three rotation axes are involved, we need to distinguish rotations about rotated axes with those about fixed axes.

5.1 | Active rotation operator about rotated axes

We already provided the right-handed active rotation operator about axes of rotated body-attached coordinate system and about fixed axes in terms of Euler angles.¹ We simply recall the main results written in Dirac notations.

The coordinate systems shown in Figure 11 are the body-attached coordinate system of the space function. The first rotation about the z -axis by angle α transforms the coordinate system (O, x, y, z) into a new coordinate system (O, x', y', z') . The second rotation about the y' -axis by angle β transforms (O, x', y', z') into a new coordinate system (O, x'', y'', z'') . The third rotation about the z'' -axis by angle γ transforms (O, x'', y'', z'') into a new coordinate system (O, x''', y''', z''') . This is the traditional way^{14,37,67–71} to introduce Euler angles. The successive rotations are made about rotated axes.

We denoted the operator for right-handed active rotation of space function about rotated axes of body-attached coordinate system by^{9,14,25,28,29,34,36,38,39,47,52,55,57,61,72–74}

$$R_A^{\text{rot}}(\gamma, \beta, \alpha) = \exp(-i\gamma L_{z''}) \exp(-i\beta L_{y'}) \exp(-i\alpha L_z). \quad (63)$$

The order of Euler angles in the arguments of $R_A^{\text{rot}}(\gamma, \beta, \alpha)$ follows that of Euler angles in the three elementary active rotation operators. This notation is not universal. The first rotation angle α is the right-hand side argument of $R_A^{\text{rot}}(\gamma, \beta, \alpha)$ because this operator is applied to a ket state $|\Psi\rangle$. Therefore, we have the generalization of Eq. (41) for one coordinate system:

$$\begin{aligned} \langle \mathbf{r} | \Psi_A^{\text{rot}} \rangle &\stackrel{1}{=} \langle \mathbf{r} | R_A^{\text{rot}}(\gamma, \beta, \alpha) | \Psi \rangle \stackrel{2}{=} \langle \mathbf{r}_1 | \Psi \rangle \\ &\stackrel{3}{=} \Psi [P_{\text{rotatedZ3Y2Z1}}(\gamma, \beta, \alpha) \mathbf{r}], \end{aligned} \quad (64)$$

and of Eq. (48) for two coordinate systems:

$$\begin{aligned} \langle \mathbf{r} | \Psi_A^{\text{rot}} \rangle &\stackrel{1}{=} \langle \mathbf{r} | R_A^{\text{rot}}(\gamma, \beta, \alpha) | \Psi \rangle \stackrel{4}{=} \langle \mathbf{r}''' | \Psi \rangle \\ &\stackrel{3}{=} \Psi [P_{\text{rotatedZ3Y2Z1}}(\gamma, \beta, \alpha) \mathbf{r}], \end{aligned} \quad (65)$$

$P_{\text{rotatedZ3Y2Z1}}(\gamma, \beta, \alpha)$ being the passive rotation matrix.^{1,3}

5.2 | Active rotation operator about fixed axes

We¹ manipulated the expression of $R_A^{\text{rot}}(\gamma, \beta, \alpha)$ defined in Eq. (63), which depends on angular momentum operators of successively rotated body-attached coordinate systems, so that the expression depends on angular momentum operators of fixed coordinate system. The operator $R_A^{\text{fixed}}(\alpha, \beta, \gamma)$ for the right-handed active rotation of space function about fixed axes is^{9,11,14,22,24,25,28,29,34,36,38,39,42,47,52,56, 57,60,61,67,71–77}

$$R_A^{\text{fixed}}(\alpha, \beta, \gamma) = \exp(-i\alpha L_z) \exp(-i\beta L_{y'}) \exp(-i\gamma L_{z''}). \quad (66)$$

The order of Euler angles in the arguments of $R_A^{\text{fixed}}(\alpha, \beta, \gamma)$ follows that of elementary active rotation operators about fixed axes. The notation is not universal. The Euler angle for the first rotation is γ because this operator is applied to a ket state $|\Psi\rangle$. This order is the reverse of that in $R_A^{\text{rot}}(\gamma, \beta, \alpha)$. Equation (64) for one coordinate system becomes²⁹

$$\begin{aligned} \langle \mathbf{r} | \Psi_A^{\text{rot}} \rangle &\stackrel{1}{=} \langle \mathbf{r} | R_A^{\text{fixed}}(\alpha, \beta, \gamma) | \Psi \rangle \stackrel{2}{=} \langle \mathbf{r}_1 | \Psi \rangle \\ &\stackrel{3}{=} \Psi [P_{\text{fixedZ1Y2Z3}}(\gamma, \beta, \alpha) \mathbf{r}], \end{aligned} \quad (67)$$

$P_{\text{fixedZ1Y2Z3}}(\gamma, \beta, \alpha)$ being the passive rotation matrix.^{1,3} Equation (65) for two coordinate systems (or canonical transformation) becomes^{9,14,36}

$$\begin{aligned} \langle \mathbf{r} | \Psi_A^{\text{rot}} \rangle &\stackrel{1}{=} \langle \mathbf{r} | R_A^{\text{fixed}}(\alpha, \beta, \gamma) | \Psi \rangle \stackrel{4}{=} \langle \mathbf{r}''' | \Psi \rangle \\ &\stackrel{3}{=} \Psi [P_{\text{fixedZ1Y2Z3}}(\gamma, \beta, \alpha) \mathbf{r}]. \end{aligned} \quad (68)$$

The equality $\langle \mathbf{r} | \Psi_A^{\text{rot}} \rangle \stackrel{4}{=} \langle \mathbf{r}''' | \Psi \rangle$ in Eq. (68) means the rotated state $|\Psi_A^{\text{rot}}\rangle$ appears in the fixed coordinate system $\langle \mathbf{r} |$ exactly as $|\Psi\rangle$ does in the rotated body-attached coordinate system $\langle \mathbf{r}''' |$.¹⁴

The two passive rotation matrices $P_{\text{rotatedZ3Y2Z1}}(\gamma, \beta, \alpha)$ and $P_{\text{fixedZ1Y2Z3}}(\gamma, \beta, \alpha)$ are identical.^{1,3} When active rotations are performed with body-attached coordinate systems, the first rotation angle is α . When active rotations are performed in fixed coordinate system, the first rotation angle is γ . This matrix^{3,67} is

$$\begin{aligned} P_{\text{fixedZ1Y2Z3}}(\gamma, \beta, \alpha) &= P_{\text{rotatedZ3Y2Z1}}(\gamma, \beta, \alpha) \\ &= \begin{pmatrix} C\alpha C\beta C\gamma - S\alpha S\gamma & S\alpha C\beta C\gamma + C\alpha S\gamma & -S\beta C\gamma \\ -C\alpha C\beta S\gamma - S\alpha C\gamma & -S\alpha C\beta S\gamma + C\alpha C\gamma & S\beta S\gamma \\ C\alpha S\beta & S\alpha S\beta & C\beta \end{pmatrix}. \end{aligned} \quad (69)$$

For simplicity, we have replaced cos and sin by C and S in Eq. (69).

We mention that the active rotation operator about fixed axes $R_A^{\text{fixed}}(\theta, \mathbf{n})$ in angle-axis of rotation parametrization^{24–26,34,36,39,47,55,56,76} is

$$R_A^{\text{fixed}}(\theta, \mathbf{n}) = \exp(-i\theta \mathbf{n} \cdot \mathbf{L}). \quad (70)$$

Note that $R_A^{\text{fixed}}(\theta, \mathbf{n}) \equiv R_A^{\text{fixed}}(\alpha, \beta, \gamma)$.

5.3 | Example V.1

In Section 4, we have checked that right-handed active rotation of space function about z -axis by angle α is equivalent to left-handed rotation of coordinate system about z -axis by angle α . We extend this rule to rotation about rotated axes of body-attached coordinate system and to rotation about fixed axes by Euler angles with simple examples.

5.3.1 | Active rotation about rotated axes

Right-handed active rotation of space function about rotated axes of its body-attached coordinate system is formulated as

$$R_A^{\text{rot}}(\gamma, \beta, \alpha) |\Psi\rangle = \exp(-i\gamma L_{z''}) \exp(-i\beta L_{y'}) \exp(-i\alpha L_z) |\Psi\rangle. \quad (71)$$

The first, second, and third right-handed active rotations of the space function are about z -axis by angle α , about y' -axis by angle β , and about z'' -axis by angle γ , respectively.

The same result can be obtained with left-handed rotation of coordinate system about rotated axes as

$$\langle \mathbf{r} | R_A^{\text{rot}}(\gamma, \beta, \alpha) = \langle \mathbf{r} | \exp(-i\gamma L_{z''}) \exp(-i\beta L_{y'}) \exp(-i\alpha L_{z''}). \quad (72)$$

We have to rename the rotation axes. This is a reason why rotation operators about rotated axes should not be used. The first, second, and third left-handed rotations of coordinate system are about z -axis by angle γ , about y' -axis by angle β , and about z'' -axis by angle α , respectively.

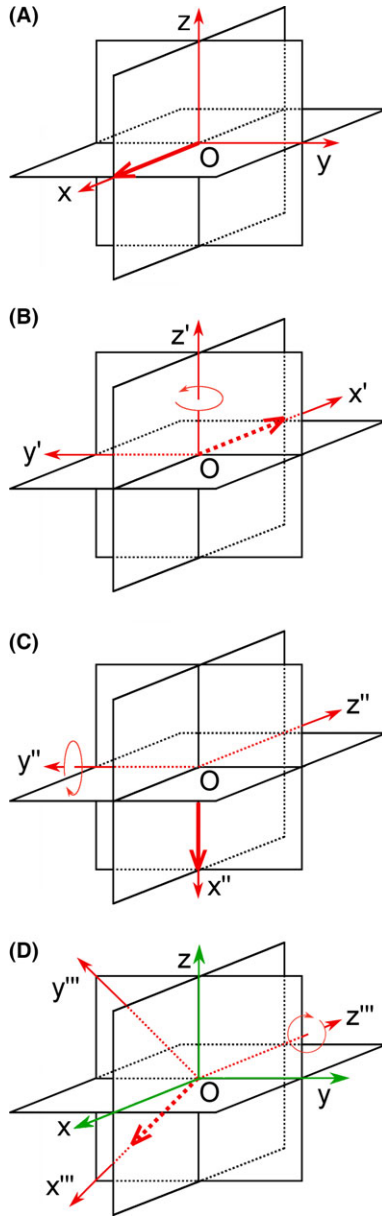


FIGURE 12 Right-handed active rotations of space function $\Psi(x, y, z)=p_x$ (represented by an arrow for simplicity) about axes of its body-attached coordinate system: (A) initial configuration; the first (B), second (C), and third (D) rotations of the space function are about z -axis by angle $\alpha=\pi$, about y' -axis by angle $\beta=\pi/2$, and about z'' -axis by angle $\gamma=\pi/4$, respectively. In (D), the rotated space function lies in the $\{y, z\}$ plane

The active rotation operator $R_A^{\text{rot}}(\gamma, \beta, \alpha)$ has two meanings: (a) When it is applied to space function or ket state as in Eq. (71), it is the right-handed active rotation operator. (b) When it is applied to coordinate system via bra position basis $\langle \mathbf{r} |$ as in Eq. (72), it is the left-handed passive rotation operator.

Consider the right-handed active rotation of the space function $\Psi(x, y, z) = p_x$ -orbital about rotated axes of its body-attached coordinate system (Figure 12). This atomic

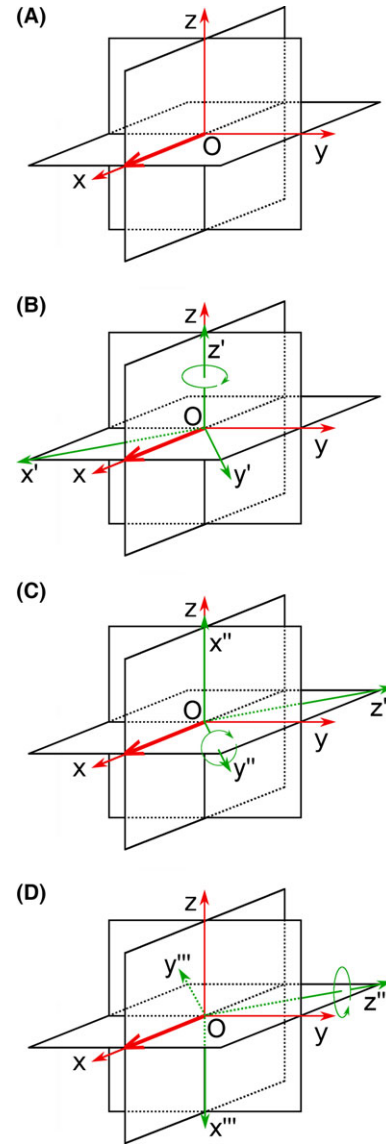


FIGURE 13 Left-handed rotations of coordinate system about axes of rotated coordinate systems, the space function $\Psi(x, y, z)=p_x$ remains fixed: (A) initial configuration; the first (B), second (C), and third (D) rotations of the coordinate system are about z -axis by angle $\gamma=\pi/4$, about y' -axis by angle $\beta=\pi/2$, and about z'' -axis by angle $\alpha=\pi$, respectively

orbital has quantum numbers $n=2$, $\ell=1$, and $m=1$. It is related to spherical harmonics by⁷¹

$$p_x = \frac{1}{\sqrt{2}} (Y_{1,-1} - Y_{1,1}). \quad (73)$$

Its two lobes extend along the x -axis. The space function is represented by an arrow for simplicity. The first (Figure 12B), second (Figure 12C), and third (Figure 12D) right-handed active rotations of the space function are about z -axis by angle $\alpha=\pi$, about y' -axis by angle $\beta=\pi/2$, and about z'' -axis by angle $\gamma=\pi/4$, respectively. In its body-attached coordinate system (O, x''', y''', z''') , the space

function $\Psi(x, y, z) = p_x$ lies on the x''' -axis by definition. Figure 12D shows that the right-hand actively rotated space function lies in the $\{y, z\}$ plane of the fixed coordinate system (O, x, y, z) .

We should obtain the same result with left-handed rotation of coordinate system about rotated axes (Figure 13), keeping fixed the space function $\Psi(x, y, z) = p_x$. The first (Figure 13B), second (Figure 13C), and third (Figure 13D) left-handed rotations of coordinate system are about z -axis by angle $\gamma = \pi/4$, about y' -axis by angle $\beta = \pi/2$, and about z'' -axis by angle $\alpha = \pi$, respectively. Figure 13D shows that the space function $\Psi(x, y, z) = p_x$ lies in the $\{y''', z'''\}$ plane of left-hand rotated coordinate system (O, x''', y''', z''') , in agreement with Figure 12D.

We have checked that right-handed active rotation of space function about rotated axes of its body-attached coordinate system by Euler angles (α, β, γ) is equivalent to left-handed rotation of coordinate system about rotated axes by Euler angles (γ, β, α) . The standard formulation is:⁷⁷ right-handed active rotation of space function about rotated axes of its body-attached coordinate system by Euler angles (α, β, γ) is equivalent to right-handed rotation of coordinate system about rotated axes by Euler angles $(-\gamma, -\beta, -\alpha)$.

5.3.2 | Active rotation about fixed axes

Right-handed active rotation of space function about fixed axes is formulated as

$$R_A^{\text{fixed}}(\gamma, \beta, \alpha)|\Psi\rangle = \exp(-i\alpha L_z) \exp(-i\beta L_y) \exp(-i\gamma L_x)|\Psi\rangle. \quad (74)$$

The first, second, and third right-handed active rotations of the space function are about z -axis by angle γ , about y -axis by angle β , and about x -axis by angle α , respectively.

The same result can be obtained with left-handed rotation of coordinate system about fixed axes as

$$\langle \mathbf{r} | R_A^{\text{fixed}}(\gamma, \beta, \alpha) = \langle \mathbf{r} | \exp(-i\alpha L_z) \exp(-i\beta L_y) \exp(-i\gamma L_x). \quad (75)$$

We do not need to rename the fixed rotation axes. The first, second, and third left-handed rotations of coordinate system are about z -axis by angle α , about y -axis by angle β , and about x -axis by angle γ , respectively.

The active rotation operator $R_A^{\text{fixed}}(\alpha, \beta, \gamma)$ has two meanings: (a) When it is applied to space function or ket state as in Eq. (74), it is the right-handed active rotation operator. (b) When it is applied to coordinate system via bra position basis $\langle \mathbf{r} |$ as in Eq. (75), it is the left-handed passive rotation operator.⁷⁷

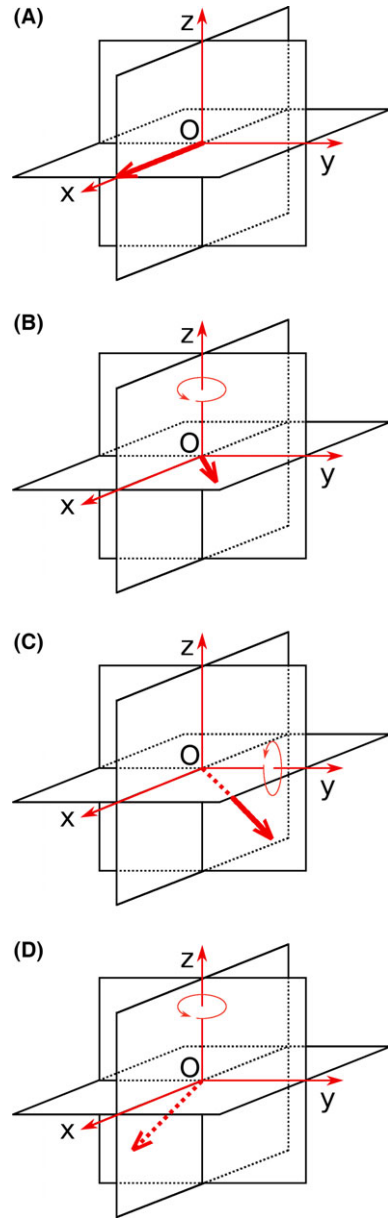


FIGURE 14 Right-handed active rotations of space function $\Psi(x, y, z) = p_x$ about axes of the fixed coordinate system (O, x, y, z) : (A) initial configuration; the first (B), second (C), and third (D) rotations of the space function are about z -axis by angle $\gamma = \pi/4$, about y -axis by angle $\beta = \pi/2$, and about x -axis by angle $\alpha = \pi$, respectively. In (D), the rotated space function lies in the $\{y, z\}$ plane

Consider the right-handed active rotation of the space function $\Psi(x, y, z) = p_x$ about fixed axes (Figure 14). The space function is represented by an arrow for simplicity. The first (Figure 14B), second (Figure 14C), and third (Figure 14D) right-handed active rotations of the space function are about z -axis by angle $\gamma = \pi/4$, about y -axis by angle $\beta = \pi/2$, and about x -axis by angle $\alpha = \pi$, respectively. Figure 14D shows that the right-hand actively rotated space function of $\Psi(x, y, z) = p_x$ lies in the $\{y, z\}$ plane of the fixed coordinate system (O, x, y, z) .

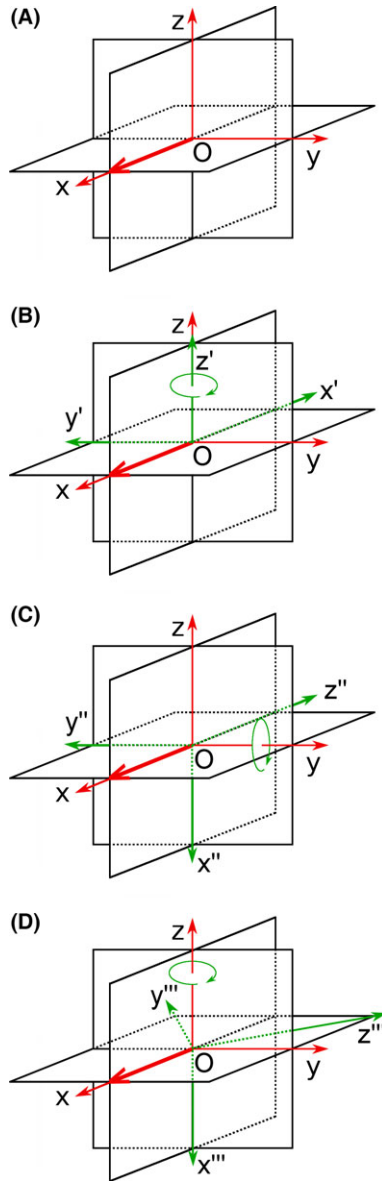


FIGURE 15 Left-handed rotations of coordinate system about axes of the fixed coordinate system (O, x, y, z), the space function $\Psi(x, y, z) = p_x$ remains fixed: (A) initial configuration; the first (B), second (C), and third (D) rotations of the coordinate system are about z -axis by angle $\alpha = \pi$, about y -axis by angle $\beta = \pi/2$, and about z -axis by angle $\gamma = \pi/4$, respectively

Right-handed active rotation of space function about rotated axes of its body-attached coordinate system (Figure 12D) agrees with that about fixed axes (Figure 14D).

We should obtain the same result with left-handed rotations of coordinate system (Figure 15), keeping fixed the space function $\Psi(x, y, z) = p_x$. The first (Figure 15B), second (Figure 15C), and third (Figure 15D) rotations of the coordinate system are about z -axis by angle $\alpha = \pi$, about y -axis by angle $\beta = \pi/2$, and about z -axis by angle $\gamma = \pi/4$, respectively. Figure 15D shows that the space function

$\Psi(x, y, z) = p_x$ lies in the $\{y''', z'''\}$ plane of its left-hand rotated coordinate system (O, x''', y''', z'''), in agreement with Figure 14D.

We have checked that right-handed active rotation of space function about fixed axes by Euler angles (γ, β, α) is equivalent to left-handed rotation of coordinate system about fixed axes by Euler angles (α, β, γ) . The standard formulation is:⁷⁷ right-handed active rotation of space function about fixed axes by Euler angles (γ, β, α) is equivalent to right-handed rotation of coordinate system about fixed axes by Euler angles $(-\alpha, -\beta, -\gamma)$.

5.4 | Passive rotation operator about rotated axes

The first rotation about the z -axis by angle α transforms the coordinate system (O, x, y, z) into a new coordinate system (O, x', y', z') (Figure 11). This corresponds to the passive rotation of space function about a single axis. This transformation is described by Eq. (59):

$$\langle \mathbf{r}' | \Psi' \rangle \stackrel{1}{=} \langle \mathbf{r}' | R_P(\alpha, z) | \Psi \rangle \stackrel{2}{=} \langle \mathbf{r} | \Psi \rangle. \quad (76)$$

In fact, we apply the rotation operator to $\langle \mathbf{r}' |$.

Then, the second rotation about the y' -axis by angle β transforms the coordinate system (O, x', y', z') into a new coordinate system (O, x'', y'', z''). The right-handed passive rotation operator $R_P(\beta, y') = \exp(i\beta L_{y'})$ transforms Eq. (76) to

$$\langle \mathbf{r}'' | \Psi'' \rangle \stackrel{1}{=} \langle \mathbf{r}'' | R_P(\alpha, z) R_P(\beta, y') | \Psi \rangle \stackrel{2}{=} \langle \mathbf{r} | \Psi \rangle. \quad (77)$$

In fact, we apply the rotation operator to $\langle \mathbf{r}'' | R_P(\alpha, z)$.

Finally, the third rotation about the z'' -axis by angle γ transforms the coordinate system (O, x'', y'', z'') into a new coordinate system (O, x''', y''', z'''). The right-handed passive rotation operator $R_P(\gamma, z'') = \exp(i\gamma L_{z''})$ transforms Eq. (77) to

$$\langle \mathbf{r}''' | \Psi''' \rangle \stackrel{1}{=} \langle \mathbf{r}''' | R_P(\alpha, z) R_P(\beta, y') R_P(\gamma, z'') | \Psi \rangle \stackrel{2}{=} \langle \mathbf{r} | \Psi \rangle. \quad (78)$$

In fact, we apply the rotation operator to $\langle \mathbf{r}''' | R_P(\alpha, z) R_P(\beta, y')$.

We denote the right-handed passive rotation operator about rotated axes by¹²

$$R_P^{\text{rot}}(\alpha, \beta, \gamma) = \exp(i\alpha L_z) \exp(i\beta L_{y'}) \exp(i\gamma L_{z''}). \quad (79)$$

The order of Euler angles in the arguments of $R_P^{\text{rot}}(\alpha, \beta, \gamma)$ follows that of elementary passive rotation operators about rotated axes. This notation is not universal. This operator is similar to $R_A^{\text{rot}}(\gamma, \beta, \alpha)$, which involves angular momentum operators in successively rotated coordinate systems.

Silver⁵⁸ presented the passive rotation of a space function in the traditional way without Dirac notation and defined the passive rotation operator by

$$R_p^{\text{rot,Silver}}(\gamma, \beta, \alpha) = \exp(i\gamma L_{z''}) \exp(i\beta L_{y'}) \exp(i\alpha L_z). \quad (80)$$

The Euler angles and rotation axes differ with those in Eq. (79). As this passive rotation operator describes the transformation of a space function $\Psi(\mathbf{r})$, it becomes obviously that

$$\begin{aligned} R_p^{\text{rot,Silver}}(\gamma, \beta, \alpha) \Psi(\mathbf{r}''') \\ = \exp(i\gamma L_{z''}) \exp(i\beta L_{y'}) \exp(i\alpha L_z) \Psi(\mathbf{r}'''). \end{aligned} \quad (81)$$

The generalization of Eq. (59) to Euler angles is

$$\begin{aligned} \langle \mathbf{r}''' | \Psi_p''' \rangle &\stackrel{1}{=} \langle \mathbf{r}''' | R_p^{\text{rot}}(\alpha, \beta, \gamma) | \Psi \rangle \stackrel{2}{=} \langle \mathbf{r} | \Psi \rangle \\ &\stackrel{3}{=} \Psi[A_{\text{rotatedZ1Y2Z3}}(\alpha, \beta, \gamma) \mathbf{r}''']. \end{aligned} \quad (82)$$

5.5 | Passive rotation operator about fixed axes

We determine the right-handed passive rotation operator about fixed axes from that about rotated axes defined in Eq. (79).

First we express the angular momentum operator $L_{y'}$ in terms of angular momentum operator L_y (Figure 11). $L_{y'}$ is derived from an active rotation of L_y about z -axis by angle α (see Section 10 about rotation of vector operator):

$$L_{y'} = \exp(-i\alpha L_z) L_y \exp(i\alpha L_z). \quad (83)$$

Applying the following transformation formula^{1,74}

$$Uf(A)U^\dagger = f(UAU^\dagger) \quad (84)$$

to Eq. (83) yields

$$\exp(i\beta L_{y'}) = \exp(-i\alpha L_z) \exp(i\beta L_y) \exp(i\alpha L_z). \quad (85)$$

Equation (85) can be rewritten as

$$\exp(i\alpha L_z) \exp(i\beta L_{y'}) \exp(-i\alpha L_z) = \exp(i\beta L_y) \quad (86)$$

Similarly, we express the angular momentum operator $L_{z''}$ in terms of angular momentum operator L_z :

$$L_{z''} = \exp(-i\beta L_{y'}) L_z \exp(i\beta L_{y'}). \quad (87)$$

Applying the formula in Eq. (84) to Eq. (87) yields

$$\exp(i\gamma L_{z''}) = \exp(-i\beta L_{y'}) \exp(i\gamma L_z) \exp(i\beta L_{y'}). \quad (88)$$

Equation (88) can be rewritten as

$$\exp(i\beta L_{y'}) \exp(i\gamma L_{z''}) \exp(-i\beta L_{y'}) = \exp(i\gamma L_z). \quad (89)$$

Inserting $\exp(-i\beta L_{y'}) \exp(i\beta L_{y'})$ into the right-hand side of $R_p^{\text{rot}}(\alpha, \beta, \gamma)$ yields

$$\begin{aligned} R_p^{\text{rot}}(\alpha, \beta, \gamma) &= \exp(i\alpha L_z) \exp(i\beta L_{y'}) \exp(i\gamma L_{z''}) \\ &\quad \{ \exp(-i\beta L_{y'}) \exp(i\beta L_{y'}) \} = \exp(i\alpha L_z) \\ &\quad \{ \exp(i\beta L_{y'}) \exp(i\gamma L_{z''}) \exp(-i\beta L_{y'}) \} \exp(i\beta L_{y'}). \end{aligned} \quad (90)$$

Replacing the inner three elementary rotation operators in Eq. (90) by Eq. (89) yields

$$R_p^{\text{rot}}(\alpha, \beta, \gamma) = \exp(i\alpha L_z) \exp(i\gamma L_z) \exp(i\beta L_{y'}). \quad (91)$$

Inserting $\exp(i\gamma L_z) \exp(-i\gamma L_z)$ into Eq. (91) yields

$$\begin{aligned} R_p^{\text{rot}}(\alpha, \beta, \gamma) &= \{ \exp(i\gamma L_z) \exp(-i\gamma L_z) \} \exp(i\alpha L_z) \\ &\quad \exp(i\gamma L_z) \exp(i\beta L_{y'}) = \exp(i\gamma L_z) \\ &\quad \{ \exp(-i\gamma L_z) \exp(i\alpha L_z) \exp(i\gamma L_z) \} \exp(i\beta L_{y'}). \end{aligned} \quad (92)$$

The inner three elementary rotation operators in Eq. (92) commute, which yields

$$R_p^{\text{rot}}(\alpha, \beta, \gamma) = \exp(i\gamma L_z) \exp(i\alpha L_z) \exp(i\beta L_{y'}). \quad (93)$$

Inserting $\exp(-i\alpha L_z) \exp(i\alpha L_z)$ into Eq. (93) yields

$$\begin{aligned} R_p^{\text{rot}}(\gamma, \beta, \alpha) &= \exp(i\gamma L_z) \exp(i\alpha L_z) \exp(i\beta L_{y'}) \\ &\quad \{ \exp(-i\alpha L_z) \exp(i\alpha L_z) \} = \exp(i\gamma L_z) \\ &\quad \{ \exp(i\alpha L_z) \exp(i\beta L_{y'}) \exp(-i\alpha L_z) \} \exp(i\alpha L_z). \end{aligned} \quad (94)$$

Finally, substituting Eq. (86) into Eq. (94) yields the right-handed passive rotation operator about fixed axes^{12,42,56,58,67,70,75,76,78,79}

$$R_p^{\text{fixed}}(\gamma, \beta, \alpha) = \exp(i\gamma L_z) \exp(i\beta L_y) \exp(i\alpha L_z). \quad (95)$$

The orders of Euler angles in the two operators $R_p^{\text{rot}}(\alpha, \beta, \gamma)$ and $R_p^{\text{fixed}}(\gamma, \beta, \alpha)$ are in the reverse order as for $R_A^{\text{rot}}(\gamma, \beta, \alpha)$ and $R_A^{\text{fixed}}(\alpha, \beta, \gamma)$. We have manipulated the expression of $R_A^{\text{rot}}(\gamma, \beta, \alpha)$, so that it only depends on angular momentum operators of the fixed coordinate system without taking into account the space function or the coordinate system.

Although Silver⁵⁸ defined the passive rotation operator about rotated axes with Eq. (80), which differs with Eq. (79) used by us, he deduced for the passive rotation operator about fixed axes the same relation as Eq. (95). The same order of Euler angles appears in the two expressions of Silver (Eqs. (80) and (95)). This may generate conflicting results. This is another reason why rotation operators about rotated axes should not be used.

Equation (82) becomes

$$\begin{aligned} \langle \mathbf{r}''' | \Psi_p''' \rangle &\stackrel{1}{=} \langle \mathbf{r}''' | R_p^{\text{fixed}}(\gamma, \beta, \alpha) | \Psi \rangle \stackrel{2}{=} \langle \mathbf{r} | \Psi \rangle \\ &\stackrel{3}{=} \Psi[A_{\text{fixedZ3Y2Z1}}(\alpha, \beta, \gamma) \mathbf{r}'''], \end{aligned} \quad (96)$$

with^{3,67}

$$\begin{aligned} \mathbf{A}_{\text{rotatedZ1Y2Z3}}(\alpha, \beta, \gamma) &= \mathbf{A}_{\text{fixedZ3Y2Z1}}(\alpha, \beta, \gamma) \\ &= \begin{pmatrix} C\alpha C\beta C\gamma - S\alpha S\gamma & -C\alpha C\beta S\gamma - S\alpha C\gamma & C\alpha S\beta \\ S\alpha C\beta C\gamma + C\alpha S\gamma & -S\alpha C\beta S\gamma + C\alpha C\gamma & S\alpha S\beta \\ -S\beta C\gamma & S\beta S\gamma & C\beta \end{pmatrix}. \end{aligned} \quad (97)$$

Due to various expressions for rotation operators, it is recommended²⁴ to add A or P and fixed or rotated in their definitions to distinguish their developed forms in rotated and fixed coordinate systems.

We mention that the passive rotation operator about fixed axes $R_p^{\text{fixed}}(\theta, \mathbf{n})$ in angle-axis parametrization^{12,56,59,76,80} is

$$R_p^{\text{fixed}}(\theta, \mathbf{n}) = \exp(i\theta \mathbf{n} \cdot \mathbf{L}). \quad (98)$$

Note that $R_p^{\text{fixed}}(\theta, \mathbf{n}) \equiv R_p^{\text{fixed}}(\gamma, \beta, \alpha)$.

5.6 | Example V.2

In Section 4, we have checked that right-handed rotation of coordinate system about z -axis by angle α keeping the space function fixed is equivalent to left-handed active rotation of space function about z -axis by angle α in fixed coordinate system. We extend this rule to rotations about rotated axes and fixed axes by Euler angles with simple examples.

5.6.1 | Passive rotation about rotated axes

Right-handed rotation of coordinate system about rotated axes (Eq. (79)), keeping the space function fixed, is formulated as

$$\langle \mathbf{r}''' | R_p^{\text{rot}}(\alpha, \beta, \gamma) = \langle \mathbf{r}''' | \exp(i\alpha L_z) \exp(i\beta L_{y'}) \exp(i\gamma L_{z''}). \quad (99)$$

The first, second, and third right-handed rotations of coordinate systems are about z -axis by angle α , about y' -axis by angle β , and about z'' -axis by angle γ , respectively.

The same result can be obtained with left-handed active rotation of space function about rotated axes of its body-attached coordinate system as

$$R_p^{\text{rot}}(\alpha, \beta, \gamma) |\Psi\rangle = \exp(i\alpha L_{z''}) \exp(i\beta L_{y'}) \exp(i\gamma L_z) |\Psi\rangle. \quad (100)$$

We have to rename the rotation axes. This is another reason why rotation operators about rotated axes should not be used. The first, second, and third left-handed active rotations of space function are about z -axis by angle γ , about y' -axis by angle β , and about z'' -axis by angle α , respectively.

The passive rotation operator $R_p^{\text{rot}}(\alpha, \beta, \gamma)$ has two meanings: (a) When it is applied to coordinate system via bra position basis $\langle \mathbf{r}''' |$ as in Eq. (99), it is the right-handed

passive rotation operator about rotated axes. (b) When it is applied to space function or ket state as in Eq. (100), it is the left-handed active rotation operator about rotated axes.

Consider the right-handed rotations of coordinate system keeping fixed the space function $\Psi(x, y, z) = p_x$ (Figure 16). The space function is represented by an arrow for simplicity. The first (Figure 16B), second (Figure 16C), and third (Figure 16D) right-handed rotations of the coordinate system are about z -axis by angle $\alpha=\pi$, about y' -axis by angle $\beta=\pi/2$, and about z'' -axis by angle $\gamma=\pi/4$, respectively. Figure 16D shows that the space function $\Psi(x, y, z) = p_x$ lies on the $-z'''$ -axis of the rotated coordinate system (O, x''', y''', z''').

We should obtain the same result with left-handed active rotations of the space function $\Psi(x, y, z) = p_x$ (Figure 17) about rotated axes of its body-attached coordinate system. The first (Figure 17B), second (Figure 17C), and third (Figure 17D) left-handed rotations of the space function are about z -axis by angle $\gamma=\pi/4$, about y' -axis by angle $\beta=\pi/2$, and about z'' -axis by angle $\alpha=\pi$, respectively. Figure 17D shows that the rotated space function lies on the $-z$ -axis of the fixed coordinate system, in agreement with Figure 16D.

We have checked that right-handed rotation of coordinate system about rotated axes by Euler angles (α, β, γ) keeping the space function fixed is equivalent to left-handed active rotation of space function about rotated axes of its body-attached coordinate system by Euler angles (γ, β, α) . The standard formulation⁷⁷ is: right-handed rotation of coordinate system about rotated axes by Euler angles (α, β, γ) keeping the space function fixed is equivalent to right-handed active rotation of space function about rotated axes of its body-attached coordinate system by Euler angles $(-\gamma, -\beta, -\alpha)$.

5.6.2 | Passive rotation about fixed axes

Right-handed rotation of coordinate system about fixed axes keeping fixed the space function is formulated as

$$\langle \mathbf{r}''' | R_p^{\text{fixed}}(\gamma, \beta, \alpha) = \langle \mathbf{r}''' | \exp(i\gamma L_z) \exp(i\beta L_y) \exp(i\alpha L_x). \quad (101)$$

The first, second, and third right-handed rotations of coordinate system are about z -axis by angle γ , about y -axis by angle β , and about x -axis by angle α , respectively.

The same result can be obtained with left-handed active rotation of the space function about fixed axes as

$$R_p^{\text{fixed}}(\gamma, \beta, \alpha) |\Psi\rangle = \exp(i\gamma L_z) \exp(i\beta L_y) \exp(i\alpha L_x) |\Psi\rangle. \quad (102)$$

We do not need to rename the fixed rotation axes. The first, second, and third left-handed active rotations of the space function are about z -axis by angle α , about y -axis by angle β , and about x -axis by angle γ , respectively.

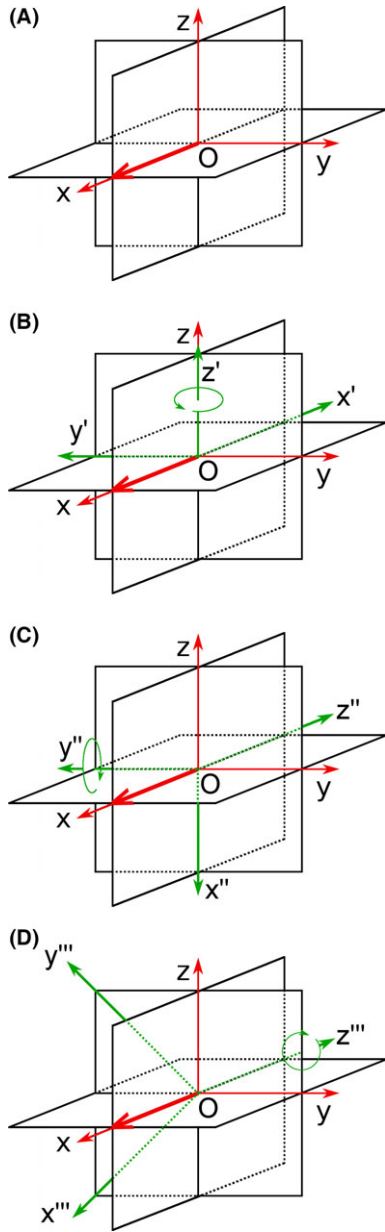


FIGURE 16 Right-handed rotations of coordinate system about axes of rotated coordinate systems, the space function $\Psi(x, y, z) = p_x$ remains fixed: (A) initial configuration; the first (B), second (C), and third (D) rotations of the coordinate system are about z -axis by angle $\alpha = \pi$, about y' -axis by angle $\beta = \pi/2$, and about z'' -axis by angle $\gamma = \pi/4$, respectively

The passive rotation operator $R_p^{\text{fixed}}(\gamma, \beta, \alpha)$ has two meanings: (a) When it is applied to coordinate system via bra position basis $\langle \mathbf{r}''' |$ as in Eq. (101), it is the right-handed passive rotation operator about fixed axes.⁷⁷ (b) When it is applied to space function or ket state as in Eq. (102), it is the left-handed active rotation operator about fixed axes.

Consider the right-handed rotations of coordinate system keeping fixed the space function $\Psi(x, y, z) = p_x$ (Figure 18). The space function is represented by an arrow for simplicity. The first (Figure 18B), second (Figure 18C),

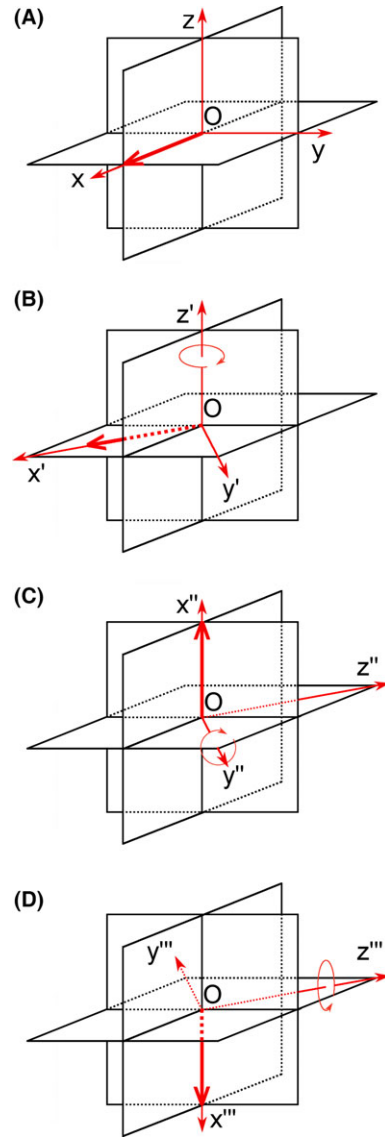


FIGURE 17 Left-handed active rotations of space function $\Psi(x, y, z) = p_x$ about rotated axes of its body-attached coordinate system: (A) initial configuration; the first (B), second (C), and third (D) rotations of the space function are about z -axis by angle $\gamma = \pi/4$, about y' -axis by angle $\beta = \pi/2$, and about z'' -axis by angle $\alpha = \pi$, respectively

and third (Figure 18D) right-handed rotations of the coordinate system are about z -axis by angle $\gamma = \pi/4$, about y -axis by angle $\beta = \pi/2$, and about z -axis by angle $\alpha = \pi$, respectively. Figure 18D shows that the space function $\Psi(x, y, z) = p_x$ lies on the $-z'''$ -axis of the rotated coordinate system (O, x''', y''', z''') .

Right-handed rotation of coordinate system about rotated axes (Figure 16D) agrees with that about fixed axes (Figure 18D).

We should obtain the same result when we perform left-handed active rotations of the space function $\Psi(x, y, z) = p_x$ about fixed axes (Figure 19). The first (Figure 19B), second (Figure 19C), and third (Figure 19D)

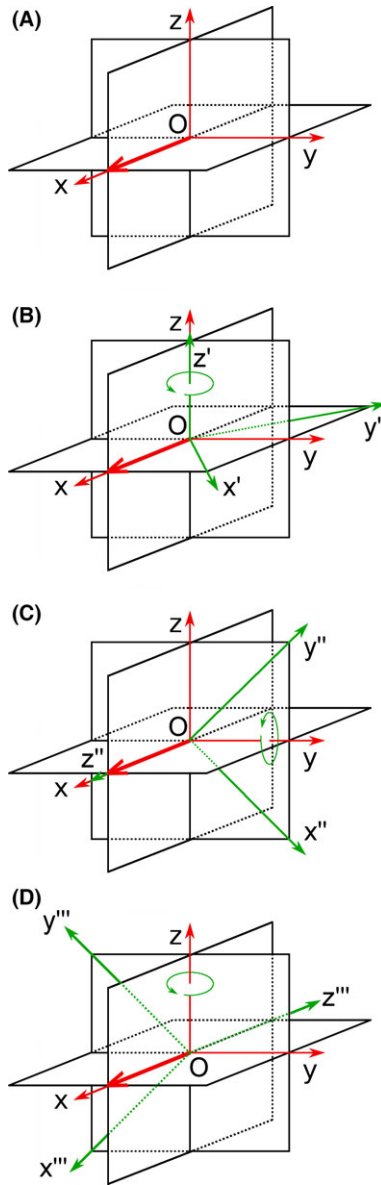


FIGURE 18 Right-handed rotations of coordinate system about axes of the fixed coordinate system (O, x, y, z), the space function $\Psi(x, y, z) = p_x$ remains fixed: (A) initial configuration; the first (B), second (C), and third (D) rotations of the coordinate system are about z -axis by angle $\gamma = \pi/4$, about y -axis by angle $\beta = \pi/2$, and about z -axis by angle $\alpha = \pi$, respectively

left-handed rotations of the space function are about z -axis by angle $\alpha = \pi$, about y -axis by angle $\beta = \pi/2$, and about z -axis by angle $\gamma = \pi/4$, respectively. Figure 19D shows that the rotated space function lies on the $-z$ -axis in the fixed coordinate system, in agreement with Figure 18D.

We have checked that right-handed rotation of coordinate system about fixed axes by Euler angles (γ, β, α) keeping the space function fixed is equivalent to left-handed active rotation of space function about fixed axes by Euler angles (α, β, γ) . The standard formulation⁷⁷ is:

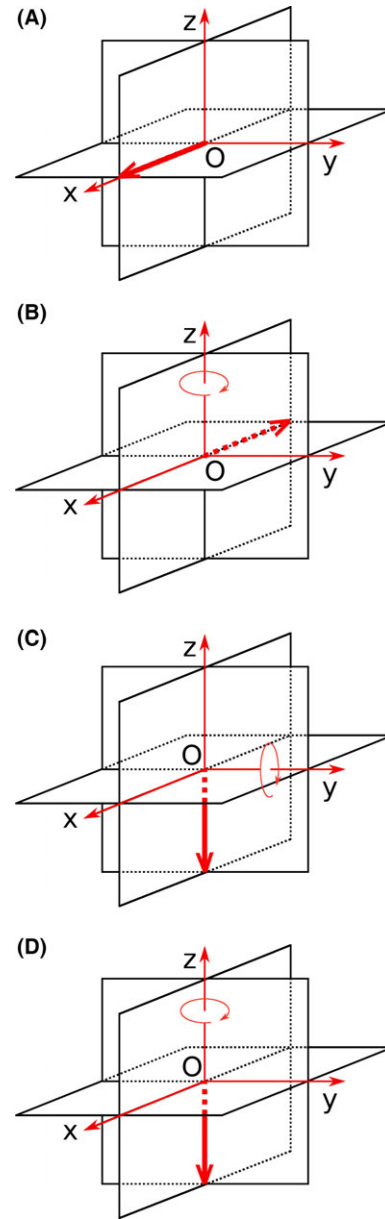


FIGURE 19 Left-handed active rotations of space function $\Psi(x, y, z) = p_x$ about axes of the fixed coordinate system (O, x, y, z): (A) initial configuration; the first (B), second (C), and third (D) rotations of the space function are about z -axis by angle $\alpha = \pi$, about y -axis by angle $\beta = \pi/2$, and about z -axis by angle $\gamma = \pi/4$, respectively

right-handed rotation of coordinate system about fixed axes by Euler angles (γ, β, α) keeping the space function fixed is equivalent to right-handed active rotation of space function about fixed axes by Euler angles $(-\alpha, -\beta, -\gamma)$.

6 | WHY ROTATION ABOUT FIXED AXES IS RECOMMENDED?

Consider a right-handed rotation about the Z -axis by angle ϕ of a fixed coordinate system (O, X, Y, Z). A new

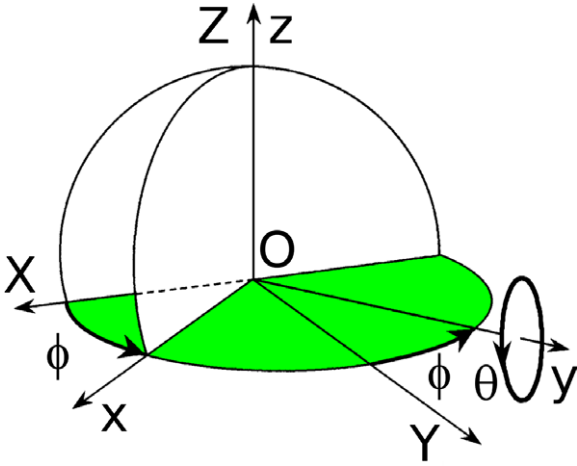


FIGURE 20 A rotation about Z-axis by angle ϕ is followed by a rotation about the rotated y-axis by angle θ

coordinate system (O, x, y, z) is generated (Figure 20). As the two axes Z and z are parallel, we can always write

$$\langle \mathbf{r}' | \exp(i\phi L_z) = \langle \mathbf{r}' | \exp(i\phi L_Z). \quad (103)$$

The bra position basis $\langle \mathbf{r}' |$ represents the rotated coordinate system (O, x, y, z) . Then we apply a right-handed rotation about the y-axis by angle θ to the rotated coordinate system (O, x, y, z) . A new coordinate system is generated, whose bra position basis is $\langle \mathbf{r}' |$. Equation (103) becomes

$$\langle \mathbf{r}' | \exp(i\phi L_z) \exp(i\theta L_y) = \langle \mathbf{r}' | \exp(i\phi L_Z) \exp(i\theta L_Y). \quad (104)$$

The left-hand side of Eq. (104) involves angular momentum operators about rotated axes, whereas the right-hand side involves angular momentum operators about fixed and rotated axes.

Figure 20 shows that L_y is deduced from a right-handed active rotation of L_Y about Z-axis by angle ϕ :

$$L_y = \exp(-i\phi L_Z) L_Y \exp(i\phi L_Z). \quad (105)$$

Applying the transformation formula in Eq. (84) to Eq. (105) yields

$$\exp(i\theta L_y) = \exp(-i\phi L_Z) \exp(i\theta L_Y) \exp(i\phi L_Z). \quad (106)$$

Replacing²⁸ $\exp(i\theta L_y)$ in Eq. (104) by that in Eq. (106) transforms its right-hand side so that only angular momentum operators about fixed axes are involved. Therefore, Eq. (104) becomes

$$\begin{aligned} \exp(i\phi L_z) \exp(i\theta L_y) &= \exp(i\phi L_Z) \{ \exp(-i\phi L_Z) \\ &\quad \exp(i\theta L_Y) \exp(i\phi L_Z) \} \\ &= \exp(i\theta L_Y) \exp(i\phi L_Z). \end{aligned} \quad (107)$$

Similarly, if we first apply a right-handed rotation of the fixed coordinate system (O, X, Y, Z) about the fixed Y-axis

by angle θ , then a rotation of the rotated coordinate system about the rotated z-axis by angle ϕ , we obtain

$$\exp(i\theta L_y) \exp(i\phi L_z) = \exp(i\phi L_Z) \exp(i\theta L_Y). \quad (108)$$

Subtracting Eq. (108) from Eq. (107), term by term, yields:

$$\begin{aligned} \exp(i\phi L_z) \exp(i\theta L_y) - \exp(i\theta L_y) \exp(i\phi L_z) \\ = \exp(i\theta L_Y) \exp(i\phi L_Z) - \exp(i\phi L_Z) \exp(i\theta L_Y). \end{aligned} \quad (109)$$

If the two angles ϕ and θ are small, Eq. (109) becomes

$$\begin{aligned} (1 + i\phi L_z)(1 + i\theta L_y) - (1 + i\theta L_y)(1 + i\phi L_z) \\ = (1 + i\theta L_Y)(1 + i\phi L_Z) - (1 + i\phi L_Z)(1 + i\theta L_Y). \end{aligned} \quad (110)$$

Expanding each product term of Eq. (110) yields

$$L_y L_z - L_z L_y = L_Z L_Y - L_Y L_Z. \quad (111)$$

That is,

$$[L_y, L_z] = [L_Z, L_Y]. \quad (112)$$

The angular momentum operators in fixed coordinate system and those in rotated one commute differently.^{55,77,81–84} Therefore, we focus on rotations about fixed axes in the remaining of the article.

7 | WIGNER ACTIVE AND PASSIVE ROTATION MATRICES

Wigner rotation matrices realize transformations of covariant components of any spherical tensor under coordinate rotations.⁵⁵ We distinguish between Wigner active $\mathbf{D}^{(\ell,A)}(\alpha, \beta, \gamma)$ and passive $\mathbf{D}^{(\ell,P)}(\gamma, \beta, \alpha)$ rotation matrices. However, they are related. Matrix elements with $m'=m=0$ are Legendre polynomials $P_\ell(\cos \theta)$.

7.1 | Wigner active rotation matrix

The Wigner active rotation matrix element $D_{m'm}^{(\ell,A)}(\alpha, \beta, \gamma)$ is defined by the right-handed active rotation operator about axes of fixed coordinate system^{9,11,22,29,30,34,37–39,61,63,71,73,85–87} provided by Eq. (66):

$$\begin{aligned} D_{m'm}^{(\ell,A)}(\alpha, \beta, \gamma) &= \langle \ell, m' | R_A^{\text{fixed}}(\alpha, \beta, \gamma) | \ell, m \rangle \\ &= \langle \ell, m' | \exp(-i\alpha L_z) \exp(-i\beta L_y) \\ &\quad \exp(-i\gamma L_z) | \ell, m \rangle = \exp(-i\alpha m') \langle \ell, m' | \\ &\quad \exp(-i\beta L_y) | \ell, m \rangle \exp(-i\gamma m) \\ &= \exp(-i\alpha m') d_{m'm}^{(\ell,A)}(\beta) \exp(-i\gamma m). \end{aligned} \quad (113)$$

The reduced matrix element $d_{m'm}^{(\ell,A)}(\beta)$ is defined by^{9,13,22,34,37,55,56,72,77,88–90}

$$d_{m'm}^{(\ell,A)}(\beta) = \sum_w (-1)^w \frac{[(\ell+m)! (\ell-m)! (\ell+m')! (\ell-m')!]^{\frac{1}{2}}}{(\ell+m'-w)! (\ell-m-w)! w! (w+m-m')!} \times \left(\cos \frac{\beta}{2}\right)^{2\ell-m+m'-2w} \left(\sin \frac{\beta}{2}\right)^{2w-m'+m}. \quad (114)$$

The number w runs over all integer values for which the factorial arguments are non-negative.

Another expression of $d_{m'm}^{(\ell,A)}(\beta)$ is also available:^{11,36,38,57,71,91}

$$d_{m'm}^{(\ell,A)}(\beta) = \sum_w (-1)^w \frac{[(\ell+m)! (\ell-m)! (\ell+m')! (\ell-m')!]^{\frac{1}{2}}}{(\ell-m'-w)! (\ell+m-w)! w! (w-m+m')!} \times \left(\cos \frac{\beta}{2}\right)^{2\ell+m-m'-2w} \left(-\sin \frac{\beta}{2}\right)^{2w+m'-m}. \quad (115)$$

The matrix $\mathbf{D}^{(1,A)}(\alpha, \beta, \gamma)$ where $\ell=1$ is^{9,22,24,34,36,38,54-57,71,87,91-93}

$$\mathbf{D}^{(1,A)}(\alpha, \beta, \gamma) = \begin{matrix} & |1\rangle & |0\rangle & |-1\rangle \\ \begin{matrix} \langle 1| \\ \langle 0| \\ \langle -1| \end{matrix} & \begin{pmatrix} \frac{1}{2}(1+\cos\beta)e^{-i(\alpha+\gamma)} & -\frac{1}{\sqrt{2}}\sin\beta e^{-i\alpha} & \frac{1}{2}(1-\cos\beta)e^{-i(\alpha-\gamma)} \\ \frac{1}{\sqrt{2}}\sin\beta e^{-i\gamma} & \cos\beta & -\frac{1}{\sqrt{2}}\sin\beta e^{i\gamma} \\ \frac{1}{2}(1-\cos\beta)e^{i(\alpha-\gamma)} & \frac{1}{\sqrt{2}}\sin\beta e^{i\alpha} & \frac{1}{2}(1+\cos\beta)e^{i(\alpha+\gamma)} \end{pmatrix} \end{matrix}. \quad (116)$$

The Wigner active rotation matrix $\mathbf{D}^{(2,A)}(\alpha, \beta, \gamma)$ is available.^{85-87,91,94,95} The reduced Wigner active rotation matrix $\mathbf{d}^{(4,A)}(\beta)$ is reported in Man.⁹⁶ Varshalovich et al.⁵⁵ tabulate $\mathbf{d}^{(\ell,A)}(\beta)$ from $\ell=1/2$ up to and including $\ell=5$.

We mention that Wigner active rotation matrix in angle-axis of rotation parametrization^{55,63} is defined by

$$D_{m'm}^{(\ell,A)}(\theta, \mathbf{n}) = \langle \ell, m' | R_A^{\text{fixed}}(\theta, \mathbf{n}) | \ell, m \rangle. \quad (117)$$

Explicit forms of $D_{m'm}^{(\ell,A)}(\theta, \mathbf{n})$ for $\ell=1$ and 2 are available.⁵⁵

Because the basis vectors $|\ell, m\rangle$ are orthonormal and remain so on rotation, the Wigner rotation matrices are unitary, that is, $[\mathbf{D}^{(\ell,A)}(\alpha, \beta, \gamma)]^\dagger = [\mathbf{D}^{(\ell,A)}(\alpha, \beta, \gamma)]^{-1}$. As a result,^{9,88}

$$\langle \ell, m' | \ell, m \rangle = \langle \ell, m' | [R_A^{\text{fixed}}(\alpha, \beta, \gamma)]^\dagger R_A^{\text{fixed}}(\alpha, \beta, \gamma) | \ell, m \rangle, \quad \delta_{m'm} = \sum_{m''} \langle \ell, m' | [R_A^{\text{fixed}}(\alpha, \beta, \gamma)]^\dagger | \ell, m'' \rangle \langle \ell, m'' | R_A^{\text{fixed}}(\alpha, \beta, \gamma) | \ell, m \rangle, \quad (118)$$

$$\delta_{m'm} = \sum_{m''} [D_{m''m'}^{(\ell,A)}(\alpha, \beta, \gamma)]^* D_{m''m}^{(\ell,A)}(\alpha, \beta, \gamma).$$

Similarly, we have^{9,22,88}

$$\langle \ell, m' | \ell, m \rangle = \langle \ell, m' | R_A^{\text{fixed}}(\alpha, \beta, \gamma) [R_A^{\text{fixed}}(\alpha, \beta, \gamma)]^\dagger | \ell, m \rangle, \quad (119)$$

$$\delta_{m'm} = \sum_{m''} \langle \ell, m' | R_A^{\text{fixed}}(\alpha, \beta, \gamma) | \ell, m'' \rangle \langle \ell, m'' | [R_A^{\text{fixed}}(\alpha, \beta, \gamma)]^\dagger | \ell, m \rangle, \quad \delta_{m'm} = \sum_{m''} D_{m''m'}^{(\ell,A)}(\alpha, \beta, \gamma) [D_{mm''}^{(\ell,A)}(\alpha, \beta, \gamma)]^*.$$

Equations (118) and (119) are orthogonality relations among Wigner rotation matrices.

7.2 | Wigner passive rotation matrix

The Wigner passive rotation matrix element $D_{m'm}^{(\ell,P)}(\gamma, \beta, \alpha)$ ^{40,65,70,79,97,98} is defined by the right-handed passive rotation operator about axes of fixed coordinate system provided by Eq. (95):

$$\begin{aligned} D_{m'm}^{(\ell,P)}(\gamma, \beta, \alpha) &= \langle \ell, m' | R_P^{\text{fixed}}(\gamma, \beta, \alpha) | \ell, m \rangle \\ &= \langle \ell, m' | \exp(i\gamma L_z) \exp(i\beta L_y) \exp(i\alpha L_z) | \ell, m \rangle \\ &= \exp(i\gamma m') \langle \ell, m' | \exp(i\beta L_y) | \ell, m \rangle \exp(i\alpha m) \\ &= \exp(i\gamma m') d_{m'm}^{(\ell,P)}(\beta) \exp(i\alpha m). \end{aligned} \quad (120)$$

Fano and Racah,⁷⁸ Fano and Rao,⁹⁹ and Schwinger¹² used the Euler angles Ψ , θ , and ϕ instead of γ , β , and α , respectively. Otherwise, their Wigner passive rotation matrix elements are identical to Eq. (120).

Wigner¹⁰⁰ and Weissbluth⁵⁹ exchanged the positions of α and γ . This means that the Euler angles defined with rotated coordinate systems are γ (the first rotation angle), β (the second rotation angle), and α (the third rotation angle). In other words, the Euler angles in fixed coordinate system are α (the first rotation angle), β (the second rotation angle), and γ (the third rotation angle). As a result, the Wigner passive rotation matrix described by Wigner¹⁰⁰ and Weissbluth⁵⁹ has the following expression:

$$\begin{aligned} D_{m'm}^{(\ell,P,\text{Wigner})}(\alpha, \beta, \gamma) &= \langle \ell, m' | \exp(i\alpha L_z) \exp(i\beta L_y) \exp(i\gamma L_z) | \ell, m \rangle \\ &= \exp(i\alpha m') d_{m'm}^{(\ell,P)}(\beta) \exp(i\gamma m). \end{aligned} \quad (121)$$

The reduced Wigner passive rotation matrix $\mathbf{d}^{(\ell,P)}(\beta)$ is given by Wigner,¹⁰⁰ Fano and Racah,⁷⁸ Weissbluth,⁵⁹ Scheck,⁹⁸ and Fano and Rau.⁹⁹

$$\begin{aligned} d_{m'm}^{(\ell,P)}(\beta) &= \sum_w (-1)^w \frac{[(\ell+m)! (\ell-m)! (\ell+m')! (\ell-m')!]^{\frac{1}{2}}}{(\ell-m'-w)! (\ell+m-w)! w! (w-m+m')!} \\ &\times \left(\cos \frac{\beta}{2}\right)^{2\ell+m-m'-2w} \left(\sin \frac{\beta}{2}\right)^{2w+m'-m}. \end{aligned} \quad (122)$$

It differs with Eq. (115) by a minus sign for the sinus function.

In Eqs. [43.8], [43.12], and [43.13] of Davydov,³² the two indices of Wigner passive rotation matrix element $D_{mm'}^{(\ell,P,\text{Davydov})}(\gamma, \beta, \alpha)$ are exchanged. But the matrix elements

remain identical those defined in Eq. (120). In other words, the matrix elements $D_{mm'}^{(\ell,P,Davydov)}(\gamma, \beta, \alpha)$ are the transposes of $D_{m'm}^{(\ell,P)}(\gamma, \beta, \alpha)$:

$$\begin{aligned} D_{mm'}^{(\ell,P,Davydov)}(\gamma, \beta, \alpha) &= \langle \ell, m' | \exp(i\gamma L_z) \exp(i\beta L_y) \exp(i\alpha L_z) | \ell, m \rangle \\ &= \exp(i\gamma m') \langle \ell, m' | \exp(i\beta L_y) | \ell, m \rangle \exp(i\alpha m) \\ &= \exp(i\gamma m') d_{mm'}^{(\ell,P,Davydov)}(\beta) \exp(i\alpha m). \end{aligned} \quad (123)$$

The Wigner passive rotation matrix $\mathbf{D}^{(1,P)}(\gamma, \beta, \alpha)$ for $\ell=1$ is^{56,58,65,70}

$$\begin{aligned} \mathbf{D}^{(1,P)}(\gamma, \beta, \alpha) &= \begin{matrix} & |1\rangle & |0\rangle & |-1\rangle \\ \begin{matrix} \langle 1| \\ \langle 0| \\ \langle -1| \end{matrix} & \begin{pmatrix} \frac{1}{2}(1+\cos\beta)e^{i(\alpha+\gamma)} & \frac{1}{\sqrt{2}}\sin\beta e^{i\gamma} & \frac{1}{2}(1-\cos\beta)e^{-i(\alpha-\gamma)} \\ -\frac{1}{\sqrt{2}}\sin\beta e^{i\alpha} & \cos\beta & \frac{1}{\sqrt{2}}\sin\beta e^{-i\alpha} \\ \frac{1}{2}(1-\cos\beta)e^{i(\alpha-\gamma)} & -\frac{1}{\sqrt{2}}\sin\beta e^{-i\gamma} & \frac{1}{2}(1+\cos\beta)e^{-i(\alpha+\gamma)} \end{pmatrix} \end{matrix} \end{aligned} \quad (124)$$

As Weissbluth⁵⁹ defined the first Euler angle with γ and the third Euler angle with α , his Wigner passive rotation matrix is $\mathbf{D}^{(1,P)}(\alpha, \beta, \gamma)$, exchanging the positions of γ and α in the matrix of Eq. (124). It is worth noting that Wigner¹⁰⁰ altered not only the Euler angles (like Weissbluth) but also the order of $|m\rangle$ in the passive rotation matrix:

$$\begin{aligned} \mathbf{D}^{(1,P,Wigner)}(\alpha, \beta, \gamma) &= \begin{matrix} & |-1\rangle & |0\rangle & |1\rangle \\ \begin{matrix} \langle -1| \\ \langle 0| \\ \langle 1| \end{matrix} & \begin{pmatrix} \frac{1}{2}(1+\cos\beta)e^{-i(\alpha+\gamma)} & -\frac{1}{\sqrt{2}}\sin\beta e^{-i\alpha} & \frac{1}{2}(1-\cos\beta)e^{-i(\alpha-\gamma)} \\ \frac{1}{\sqrt{2}}\sin\beta e^{-i\gamma} & \cos\beta & -\frac{1}{\sqrt{2}}\sin\beta e^{i\gamma} \\ \frac{1}{2}(1-\cos\beta)e^{i(\alpha-\gamma)} & \frac{1}{\sqrt{2}}\sin\beta e^{i\alpha} & \frac{1}{2}(1+\cos\beta)e^{i(\alpha+\gamma)} \end{pmatrix} \end{matrix} \end{aligned} \quad (125)$$

The Wigner passive rotation matrix $\mathbf{D}^{(2,P)}(\gamma, \beta, \alpha)$ for $\ell=2$ is available in Refs.^{101–103} Reduced matrices $\mathbf{d}^{(\ell,A)}(\beta)$ and $\mathbf{d}^{(\ell,P)}(\beta)$ are related:^{36,97,104}

$$\begin{aligned} \left\{ \mathbf{d}^{(\ell,A)}(\beta) \right\}^T &= \mathbf{d}^{(\ell,A)}(-\beta) = \mathbf{d}^{(\ell,P)}(\beta), \\ \left\{ \mathbf{d}^{(\ell,P)}(\beta) \right\}^T &= \mathbf{d}^{(\ell,P)}(-\beta) = \mathbf{d}^{(\ell,A)}(\beta). \end{aligned} \quad (126)$$

7.3 | Some properties of Wigner rotation matrices

The matrix elements of Wigner rotation matrices are as follows:

$$D_{m'm}^{(\ell,A)}(\alpha, \beta, \gamma) = \exp(-i\alpha m') d_{m'm}^{(\ell,A)}(\beta) \exp(-i\gamma m), \quad (127)$$

and

$$D_{m'm}^{(\ell,P)}(\gamma, \beta, \alpha) = \exp(i\gamma m') d_{m'm}^{(\ell,P)}(\beta) \exp(i\alpha m). \quad (128)$$

It follows that the complex conjugate of Wigner active rotation matrix is the transpose of Wigner passive rotation matrix:⁹⁷

$$\begin{aligned} \left\{ D_{m'm}^{(\ell,A)}(\alpha, \beta, \gamma) \right\}^* &= \exp(i\alpha m') d_{m'm}^{(\ell,A)}(\beta) \exp(i\gamma m) \\ &= \exp(i\gamma m) d_{m'm}^{(\ell,P)}(\beta) \exp(i\alpha m') \\ &= D_{m'm}^{(\ell,P)}(\gamma, \beta, \alpha). \end{aligned} \quad (129)$$

For inverse rotation that is accomplished by performing the rotations through negative Euler angles about the same axes but in opposite order, Wigner active rotation matrix becomes

$$\begin{aligned} D_{m'm}^{(\ell,A)}[(\alpha, \beta, \gamma)^{-1}] &= D_{m'm}^{(\ell,A)}(-\gamma, -\beta, -\alpha) \\ &= \exp(i\gamma m') d_{m'm}^{(\ell,A)}(-\beta) \exp(i\alpha m) \\ &= \exp(i\gamma m') d_{m'm}^{(\ell,P)}(\beta) \exp(i\alpha m) \\ &= D_{m'm}^{(\ell,P)}(\gamma, \beta, \alpha). \end{aligned} \quad (130)$$

Equations (129) and (130) yield

$$D_{m'm}^{(\ell,A)}(-\gamma, -\beta, -\alpha) = \left\{ D_{m'm}^{(\ell,A)}(\alpha, \beta, \gamma) \right\}^*. \quad (131)$$

Similarly, Wigner active rotation matrix is the complex conjugate and transpose of Wigner passive rotation matrix:

$$\left\{ D_{m'm}^{(\ell,P)}(\gamma, \beta, \alpha) \right\}^* = D_{m'm}^{(\ell,A)}(\alpha, \beta, \gamma). \quad (132)$$

Furthermore,

$$D_{m'm}^{(\ell,P)}(-\alpha, -\beta, -\gamma) = D_{m'm}^{(\ell,A)}(\alpha, \beta, \gamma), \quad (133)$$

and

$$D_{m'm}^{(\ell,P)}(-\alpha, -\beta, -\gamma) = \left\{ D_{m'm}^{(\ell,P)}(\gamma, \beta, \alpha) \right\}^*. \quad (134)$$

8 | SPHERICAL HARMONICS

As the formulation of spherical tensor is based on spherical harmonics, we begin with the presentation of spherical harmonics. The latter are extensively used in NMR.^{7,74,86,87,102,105} For example, the perturbed dipolar Hamiltonian for a single pair of identical spins can be written in the spherical tensor formalism as¹⁰⁶

$$(H_D)_{ij} = \sum_m (-1)^m F_{2,m}(\theta_{ij}, \phi_{ij}) T_{2,-m}, \quad (135)$$

$$F_{2,m}(\theta_{ij}, \phi_{ij}) = -\frac{\mu_0 \gamma^2 \hbar}{4\pi r_{ij}^3} \sqrt{\frac{24\pi}{5}} Y_{2,m}(\theta_{ij}, \phi_{ij}).$$

$Y_{2,m}(\theta_{ij}, \phi_{ij})$ are spherical harmonics of order 2 and component m , whereas $T_{2,-m}$ are products of spin operators.

Spherical harmonics are related to Wigner rotation matrices via simple relations. These relations allow us to determine the type (active or passive) of Wigner rotation matrix.

8.1 | Definition of spherical harmonics

Spherical harmonics $Y_{\ell,m}(\theta, \phi)$ normalized to unity are common eigen functions expressed in spherical polar coordinates of orbital angular momentum operator squared L^2 and L_z .^{31,34,41} They may be written as the product of two functions, one that depends only on the polar angle θ is a complex-valued function and the other that depends only on the azimuthal angle ϕ is a real-valued function.^{22,34,38,47,55}

$$Y_{\ell,m}(\theta, \phi) = \Theta_{\ell,m}(\theta)\Phi_m(\phi). \quad (136)$$

These two functions are

$$\Phi_m(\phi) = e^{im\phi}, \quad (137)$$

and for $m \geq 0$,

$$\Theta_{\ell,m}(\theta) = (-1)^m \sqrt{\frac{2\ell+1}{4\pi} \frac{(\ell-m)!}{(\ell+m)!}} P_{\ell,m}(\cos \theta). \quad (138)$$

In quantum mechanics, the phase factor $(-1)^m$ in the definition of spherical harmonics via Eq. (138) was introduced by Condon and Shortley.¹⁰⁷ Other conventions are available for spherical harmonics.^{49,61,108} As a result, this phase factor $(-1)^m$ does not appear in the associated Legendre functions^{11,34,38,54,57,61} defined by the Rodrigues' formula

$$P_{\ell,m}(\cos \theta) = \sin^m \theta \left[\frac{d}{d(\cos \theta)} \right]^m P_{\ell}(\cos \theta), \quad (139)$$

where

$$P_{\ell}(\cos \theta) = \frac{1}{2^{\ell} \ell!} \left[\frac{d}{d(\cos \theta)} \right]^{\ell} (\cos^2 \theta - 1)^{\ell} \quad (140)$$

are the ordinary Legendre polynomials of degree ℓ .^{11,34,38,54,57,109} The associated Legendre functions $P_{\ell,m}(\cos \theta)$ are real and depend only on $|m|$.

Table 1 presents some spherical harmonics^{1,31,34,70,110} in Condon and Shortley convention and covariant notation.^{55,111} They have negative phases for positive odd m , but positive phases for all other m . They are extensively used in NMR.

Table 2 presents some associated Legendre functions,^{11,54} but $P_{\ell,m}(\cos \theta)$ with $m=0$ are not reported because $P_{\ell,0}(\cos \theta) = P_{\ell}(\cos \theta)$. Furthermore,

$$P_{\ell-m}(\cos \theta) = (-1)^m \frac{(\ell-m)!}{(\ell+m)!} P_{\ell,m}(\cos \theta), \quad (141)$$

and

TABLE 1 First few normalized harmonic polynomials $r^{\ell} Y_{\ell,m}(x, y, z)$ and normalized spherical harmonics $Y_{\ell,m}(\theta, \phi)$ in Condon and Shortley phase convention and in covariant notation, with $x=r \sin \theta \cos \phi$, $y=r \sin \theta \sin \phi$, and $z=r \cos \theta$

ℓ	m	$r^{\ell} Y_{\ell,m}(x, y, z)$	$Y_{\ell,m}(\theta, \phi)$
0	0	$\sqrt{\frac{1}{4\pi}}$	$\sqrt{\frac{1}{4\pi}}$
1	0	$\sqrt{\frac{3}{4\pi}} z$	$\sqrt{\frac{3}{4\pi}} \cos \theta$
1	± 1	$\mp \sqrt{\frac{3}{8\pi}} (x \pm iy)$	$\mp \sqrt{\frac{3}{8\pi}} \sin \theta e^{\pm i\phi}$
2	0	$\sqrt{\frac{5}{4\pi}} \sqrt{\frac{1}{4}} (3z^2 - r^2)$	$\sqrt{\frac{5}{4\pi}} \sqrt{\frac{1}{4}} (3\cos^2 \theta - 1)$
2	± 1	$\mp \sqrt{\frac{5}{4\pi}} \sqrt{\frac{3}{2}} z (x \pm iy)$	$\mp \sqrt{\frac{5}{4\pi}} \sqrt{\frac{3}{2}} \cos \theta \sin \theta e^{\pm i\phi}$
2	± 2	$\sqrt{\frac{5}{4\pi}} \sqrt{\frac{3}{8}} (x \pm iy)^2$	$\sqrt{\frac{5}{4\pi}} \sqrt{\frac{3}{8}} \sin^2 \theta e^{\pm 2i\phi}$

TABLE 2 Associated Legendre functions $P_{\ell,m}(x)$ and $P_{\ell,m}(\cos \theta)$

ℓ	m	$P_{\ell,m}(x)$	$P_{\ell,m}(\cos \theta)$
1	1	$(1-x^2)^{1/2}$	$\sin \theta$
2	1	$3x(1-x^2)^{1/2}$	$3 \cos \theta \sin \theta$
	2	$3(1-x^2)$	$3 \sin^2 \theta$
3	1	$\frac{3}{2} (5x^2 - 1)(1-x^2)^{1/2}$	$\frac{3}{2} (5 \cos^2 \theta - 1) \sin \theta$
	2	$15x(1-x^2)$	$15 \cos \theta \sin^2 \theta$
	3	$15(1-x^2)^{3/2}$	$15 \sin^3 \theta$

TABLE 3 First six Legendre polynomials $P_{\ell}(x)$ of degree ℓ , $-1 \leq x \leq +1$

ℓ	$P_{\ell}(x)$
0	1
1	x
2	$\frac{1}{2} (3x^2 - 1)$
3	$\frac{1}{2} (5x^3 - 3x)$
4	$\frac{1}{8} (35x^4 - 30x^2 + 3)$
5	$\frac{1}{8} (63x^5 - 70x^3 + 15x)$

$$P_{\ell,m}(-\cos \theta) = (-1)^{\ell+m} P_{\ell,m}(\cos \theta). \quad (142)$$

Table 3 presents some ordinary Legendre polynomials $P_{\ell}(\cos \theta)$.^{11,34,54,57,61,109,110} These polynomials are either even or odd functions of $x=\cos \theta$ for even or odd degrees ℓ . Furthermore,

$$P_{\ell}(-\cos \theta) = (-1)^{\ell} P_{\ell}(\cos \theta). \quad (143)$$

The spherical harmonics satisfy the identity^{11,15,22,25,31,36,38,55}

$$\begin{aligned} (Y_{\ell,m}(\theta, \phi))^* &= Y_{\ell,m}(\theta, -\phi) = (-1)^m Y_{\ell,m}(-\theta, -\phi) \\ &= (-1)^m Y_{\ell,-m}(\theta, \phi). \end{aligned} \quad (144)$$

For the special case of $m=0$,^{15,22,31,38}

$$Y_{\ell,0}(\theta, \phi) = \Theta_{\ell,0}(\theta) = \sqrt{\frac{2\ell+1}{4\pi}} P_{\ell}(\cos \theta). \quad (145)$$

Because $P_{\ell m}(1)$ vanishes except for $m=0$, that is, when $\theta=0$,^{15,24,38,55,59}

$$Y_{\ell,m}(0, \phi) = \begin{cases} 0 & \text{for } m \neq 0 \\ \sqrt{\frac{2\ell+1}{4\pi}} & \text{for } m = 0. \end{cases} \quad (146)$$

This definition is rewritten as^{11,22,73}

$$Y_{\ell,m}(0, \phi) = \sqrt{\frac{2\ell+1}{4\pi}} \delta_{m,0}. \quad (147)$$

8.2 | Spherical harmonics as covariant components

The Cartesian components of a position vector $\mathbf{r}=(x, y, z)$ of length r , whose polar angles are θ and ϕ , are

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} r \sin \theta \cos \phi \\ r \sin \theta \sin \phi \\ r \cos \theta \end{pmatrix}. \quad (148)$$

The covariant spherical components of $\mathbf{r}$ are defined by^{1,28,57,58,112}

$$\begin{pmatrix} r_{1+1} \\ r_{10} \\ r_{1-1} \end{pmatrix} = \begin{pmatrix} -\frac{1}{\sqrt{2}}(x + iy) \\ z \\ \frac{1}{\sqrt{2}}(x - iy) \end{pmatrix}. \quad (149)$$

They are also known as the standard components.³⁴ Substituting Eq. (148) into Eq. (149) yields^{36,82,88}

$$\begin{aligned} \begin{pmatrix} -\frac{1}{\sqrt{2}}(x + iy) \\ z \\ \frac{1}{\sqrt{2}}(x - iy) \end{pmatrix} &= \begin{pmatrix} -\frac{1}{\sqrt{2}} r \sin \theta e^{i\phi} \\ r \cos \theta \\ \frac{1}{\sqrt{2}} r \sin \theta e^{-i\phi} \end{pmatrix} \\ &= \sqrt{\frac{4\pi}{3}} \begin{pmatrix} rY_{1,+1}(\theta, \phi) \\ rY_{1,0}(\theta, \phi) \\ rY_{1,-1}(\theta, \phi) \end{pmatrix}. \end{aligned} \quad (150)$$

This means $Y_{1,+1}(\theta, \phi)$, $Y_{1,0}(\theta, \phi)$, and $Y_{1,-1}(\theta, \phi)$ are also covariant spherical components of spherical harmonics with order $\ell=1$. They are³⁶

$$\begin{aligned} Y_{1,1}(\mathbf{r}) &= -\sqrt{\frac{3}{4\pi}} \frac{1}{\sqrt{2}} \frac{x+iy}{r}, \quad Y_{1,0}(\mathbf{r}) = \sqrt{\frac{3}{4\pi}} \frac{z}{r}, \\ Y_{1,-1}(\mathbf{r}) &= \sqrt{\frac{3}{4\pi}} \frac{1}{\sqrt{2}} \frac{x-iy}{r}. \end{aligned} \quad (151)$$

We can express them as

$$\begin{aligned} \sqrt{\frac{3}{4\pi}} \frac{x}{\sqrt{2}r} &= \frac{1}{2} (Y_{1,-1}(\mathbf{r}) - Y_{1,1}(\mathbf{r})), \\ \sqrt{\frac{3}{4\pi}} \frac{z}{r} &= Y_{1,0}(\mathbf{r}), \\ \sqrt{\frac{3}{4\pi}} \frac{y}{\sqrt{2}r} &= \frac{i}{2} (Y_{1,-1}(\mathbf{r}) + Y_{1,1}(\mathbf{r})). \end{aligned} \quad (152)$$

The set of operator equivalent for normalized spherical harmonics is^{41,113}

$$T_{\ell,m} = \sqrt{\frac{4\pi}{2\ell+1}} Y_{\ell,m}(\theta, \phi). \quad (153)$$

This set is called Racah tensor of rank ℓ .

8.3 | Relations with Wigner active rotation matrix

The relations between spherical harmonics and Wigner rotation matrices allow us to know how active or passive rotations are studied. Haeberlen¹⁰² and Chandrakumar and Subramanian¹⁰¹ use these relations in secular NMR Hamiltonians under passive rotations.

In Section 5 dealing with rotation of space function, we show that the quantity $\langle \mathbf{r} | R_A^{\text{fixed}}(\alpha, \beta, \gamma) | \Psi \rangle$ has two meanings: (a) right-handed active rotation of space function represented by $R_A^{\text{fixed}}(\alpha, \beta, \gamma) | \Psi \rangle$; (b) left-handed rotation of coordinate system represented by $\langle \mathbf{r} | R_A^{\text{fixed}}(\alpha, \beta, \gamma)$. In other words, the bra position basis $\langle \mathbf{r} |$ represents the coordinate system.

8.3.1 | First relation

Suppose an initial position vector $\mathbf{r}_1$ is along the z -axis of the fixed coordinate system (O, x, y, z) (Figure 21). We apply an active rotation on it such that the final position vector $\mathbf{r}$ is along some arbitrary direction specified by (θ, ϕ) . Two procedures are possible for this active rotation.

We rotate $\mathbf{r}_1$ first about the y -axis by angle $\beta=\theta$, then about the z -axis by angle $\alpha=\phi$. The polar angles of the actively rotated vector $\mathbf{r}$ in (O, x, y, z) are (θ, ϕ) . So the ket position vectors in this first procedure are related as²⁵

$$|\mathbf{r}\rangle = R_A^{\text{fixed}}(\alpha = \phi, \beta = \theta, \gamma = 0) |\mathbf{r}_1\rangle. \quad (154)$$

In contrast, if we rotate $\mathbf{r}_1$ first about the z -axis by angle ϕ ($\mathbf{r}_1$ remains unchanged), then about the y -axis by angle θ , the actively rotated vector $\mathbf{r}$ is in the $\{x, z\}$ plane. Its polar angles are θ and $\phi=0$. As one of polar angles is zero, we give up this second procedure.

We study the rotations of $|\mathbf{r}_1\rangle$ described by Eq. (154) and shown in Figure 21. We introduce the closure relation into Eq. (154):

$$|\mathbf{r}\rangle = \sum_m R_A^{\text{fixed}}(\phi, \theta, 0)|\ell, m\rangle\langle\ell, m|\mathbf{r}_1\rangle. \quad (155)$$

Then we multiply both sides of Eq. (155) by $\langle\ell, m'|\mathbf{r}\rangle$:

$$\begin{aligned} \langle\ell, m'|\mathbf{r}\rangle &= \sum_m \langle\ell, m'|R_A^{\text{fixed}}(\phi, \theta, 0)|\ell, m\rangle\langle\ell, m|\mathbf{r}_1\rangle \\ &= \sum_m D_{m'm}^{(\ell, A)}(\phi, \theta, 0)\langle\ell, m|\mathbf{r}_1\rangle. \end{aligned} \quad (156)$$

As spherical harmonic is defined by

$$Y_{\ell, m'}(\theta, \phi) = \langle\mathbf{r}|\ell, m'\rangle = \langle\theta, \phi|\ell, m'\rangle, \quad (157)$$

we deduce from Figure 21 that $\langle\ell, m|\mathbf{r}_1\rangle$ is $[Y_{\ell, m}(\theta, \phi)]^*$ evaluated at $\theta=0$ and ϕ undetermined.^{25,36,59}

$$\begin{aligned} \langle\ell, m|\mathbf{r}_1\rangle &= [Y_{\ell, m}(\theta=0, \phi)]^* = [Y_{\ell, m}(\theta=0, \phi=0)]^* \delta_{m,0} \\ &= \sqrt{\frac{2\ell+1}{4\pi}} \delta_{m,0}. \end{aligned} \quad (158)$$

Therefore,^{22,38}

$$Y_{\ell, m}(\theta=0, \phi) = Y_{\ell, m}(\theta=0, \phi=0) \delta_{m,0} = \sqrt{\frac{2\ell+1}{4\pi}} \delta_{m,0}. \quad (159)$$

As a result,^{25,37,38,52,56,73,114} Eq. (156) becomes the first relation connecting spherical harmonic with Wigner active rotation matrix:

$$[Y_{\ell, m'}(\theta, \phi)]^* = \sqrt{\frac{2\ell+1}{4\pi}} D_{m'0}^{(\ell, A)}(\phi, \theta, 0). \quad (160)$$

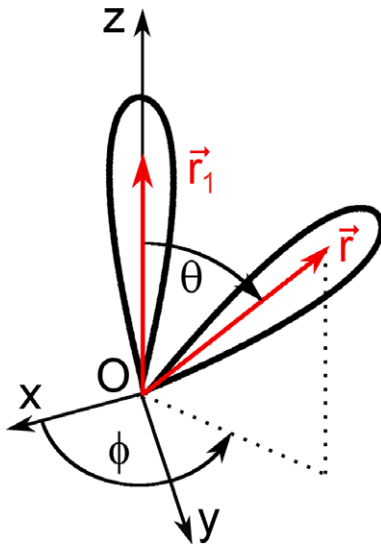


FIGURE 21 Right-handed active rotations of position vector from $\mathbf{r}_1$ to $\mathbf{r}$ in a single coordinate system: vector $\mathbf{r}_1$ is first rotated about the fixed y -axis by angle $\beta=\theta$, then about the fixed z -axis by angle $\alpha=\phi$

By extension, the first relation can be rewritten as:^{11,22,24,25,30,34,36,38,39,47,52,55–57,60,61,73,87,88,90,91,111,115,116}

$$[Y_{\ell, m'}(\beta, \alpha)]^* = \sqrt{\frac{2\ell+1}{4\pi}} D_{m'0}^{(\ell, A)}(\alpha, \beta, \gamma), \text{ (independent of } \gamma\text{)}. \quad (161)$$

An example of Eq. (161) with $\ell=m'=1$, $\mathbf{D}^{(1, A)}$ in Eq. (116), and $Y_{1,1}(\beta, \alpha)$ in Table 1 is

$$\begin{aligned} \sqrt{\frac{3}{4\pi}} D_{10}^{(1, A)}(\alpha, \beta, \gamma) &= -\sqrt{\frac{3}{8\pi}} \sin \beta e^{-i\alpha} = \left(-\sqrt{\frac{3}{8\pi}} \sin \beta e^{i\alpha} \right)^* \\ &= [Y_{1,1}(\beta, \alpha)]^*. \end{aligned} \quad (162)$$

8.3.2 | Second relation

Using Eqs. (126) and (127), it is easy to show that

$$[D_{m0}^{(\ell, A)}(-\phi, -\theta, 0)]^* = D_{0m}^{(\ell, A)}(0, \theta, \phi). \quad (163)$$

The first relation defined in Eq. (160) and the identity in Eq. (144) yield

$$\begin{aligned} [D_{m0}^{(\ell, A)}(-\phi, -\theta, 0)]^* &= \sqrt{\frac{4\pi}{2\ell+1}} Y_{\ell, m}(-\theta, -\phi) \\ &= \sqrt{\frac{4\pi}{2\ell+1}} Y_{\ell, -m}(\theta, \phi). \end{aligned} \quad (164)$$

Therefore, the second relation connecting spherical harmonics with Wigner active rotation matrix is

$$Y_{\ell, -m}(\theta, \phi) = \sqrt{\frac{2\ell+1}{4\pi}} D_{0m}^{(\ell, A)}(0, \theta, \phi). \quad (165)$$

By extension, the second relation can be rewritten as:^{11,22,24,38,55,56,60,61,111}

$$Y_{\ell, -m}(\beta, \gamma) = \sqrt{\frac{2\ell+1}{4\pi}} D_{0m}^{(\ell, A)}(\alpha, \beta, \gamma), \text{ (independent of } \alpha\text{)}, \quad (166)$$

or^{34,116}

$$[Y_{\ell, m}(\beta, \gamma)]^* = (-1)^m \sqrt{\frac{2\ell+1}{4\pi}} D_{0m}^{(\ell, A)}(\alpha, \beta, \gamma), \text{ (independent of } \alpha\text{)}. \quad (167)$$

An example of Eq. (167) with $\ell=m=1$, $\mathbf{D}^{(1, A)}$ in Eq. (116), and $Y_{1,1}(\beta, \gamma)$ in Table 1 is

$$\begin{aligned}
 -\sqrt{\frac{3}{4\pi}} D_{01}^{(1,A)}(\alpha, \beta, \gamma) &= -\sqrt{\frac{3}{8\pi}} \sin \beta e^{-i\gamma} = \left(-\sqrt{\frac{3}{8\pi}} \sin \beta e^{i\gamma} \right)^* \\
 &= \left[Y_{1,1}(\beta, \gamma) \right]^*.
 \end{aligned} \tag{168}$$

Wigner active rotation matrix elements $D_{m'm}^{(\ell,A)}(\alpha, \beta, \gamma)$ with $m'=0$ (Eq. (167)) or $m=0$ (Eq. (161)) are proportional to the complex conjugate of normalized spherical harmonics $Y_{\ell,m}(\beta, \gamma)$ and $Y_{\ell,m'}(\beta, \alpha)$ in Condon and Shortley convention and covariant notation, respectively.

8.4 | Relations with Wigner passive rotation matrix

In Section 5 dealing with rotation of space function, we show that the quantity $\langle \mathbf{r}''' | R_P^{\text{fixed}}(\gamma, \beta, \alpha) | \Psi \rangle$ has two meanings: (a) right-handed rotation of coordinate system represented by $\langle \mathbf{r}''' | R_P^{\text{fixed}}(\gamma, \beta, \alpha) | \Psi \rangle$; (b) left-handed active rotation of space function represented by $R_P^{\text{fixed}}(\gamma, \beta, \alpha) | \Psi \rangle$. In other words, the bra position basis $\langle \mathbf{r}''' |$ represents the rotated coordinate system.¹²

8.4.1 | First relation

Suppose the position vector $\mathbf{r}$ is along the z -axis in the fixed coordinate system (O, x, y, z) . We perform a right-handed rotation of coordinate system that transforms (O, x, y, z) into (O, x', y', z') . The position vector in (O, x', y', z') is $\mathbf{r}'$. This corresponds to a passive rotation of the position vector, which is viewed in the fixed coordinate system (O, x, y, z) and in the rotated coordinate system (O, x', y', z') . The two bra position bases are related by (see Eq. (96))⁵⁶

$$\langle \mathbf{r}' | R_P^{\text{fixed}}(\gamma, \beta, \alpha) = \langle \mathbf{r} |. \tag{169}$$

Conversely, the two ket position vectors are related by⁵⁶

$$|\mathbf{r}'\rangle = R_P^{\text{fixed}}(\gamma, \beta, \alpha) |\mathbf{r}\rangle. \tag{170}$$

Contrary to the transformation $R_P^{\text{fixed}}(\gamma, \beta, \alpha) | \Psi \rangle$ where $R_P^{\text{fixed}}(\gamma, \beta, \alpha)$ is left-handed active rotation operator for ket state as mentioned above, now the transformation $R_P^{\text{fixed}}(\gamma, \beta, \alpha) |\mathbf{r}\rangle$ is right-handed passive rotation operator applied to ket position vector. Two procedures are possible for this right-handed passive rotation of position vector.

We rotate (O, x, y, z) first about the fixed y -axis by angle $\beta=\theta$, then about the rotated z' -axis by angle $\gamma=\phi$ (Figure 22). As usual, the Euler angles are defined with rotated axes. The passive rotation operator about rotated axes $R_P^{\text{rot}}(\alpha=0, \beta=\theta, \gamma=\phi)$ is provided by Eq. (79). The bra position bases in this first procedure are related by

$$\langle \mathbf{r}' | = \langle \mathbf{r}' | R_P^{\text{rot}}(\alpha=0, \beta=\theta, \gamma=\phi). \tag{171}$$

Conversely, the ket position vectors are related by

$$|\mathbf{r}'\rangle = R_P^{\text{rot}}(\alpha=0, \beta=\theta, \gamma=\phi) |\mathbf{r}\rangle. \tag{172}$$

The polar angles of the position vector in the rotated coordinate system (O, x', y', z') are $(-\theta, -\phi)$. We replace the passive rotation operator about rotated axes by the passive rotation operator about fixed axes in Eq. (172), which becomes

$$|\mathbf{r}'\rangle = R_P^{\text{fixed}}(\gamma=\phi, \beta=\theta, \alpha=0) |\mathbf{r}\rangle. \tag{173}$$

In contrast, if we rotate (O, x, y, z) first about the fixed z -axis by angle $\alpha=\phi$, then about rotated y' -axis by angle $\beta=\theta$ (Figure 23), the passively rotated vector $\mathbf{r}'$ is in the $\{x', z'\}$ plane. The polar angles of $\mathbf{r}'$ in the rotated coordinate system (O, x', y', z') are $(-\theta, \phi=0)$. As one of the polar angles is zero, we give up this second procedure.

We focus on rotations shown in Figure 22 and Eq. (173) from the first procedure. We introduce the closure relation in Eq. (173):

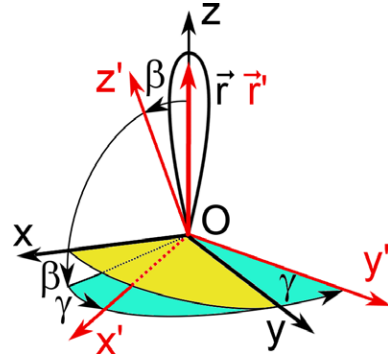


FIGURE 22 Right-handed rotations of coordinate system from (O, x, y, z) to (O, x', y', z') : (O, x, y, z) is first rotated about the fixed y -axis by angle $\beta=\theta$, then about the rotated z' -axis by angle $\gamma=\phi$

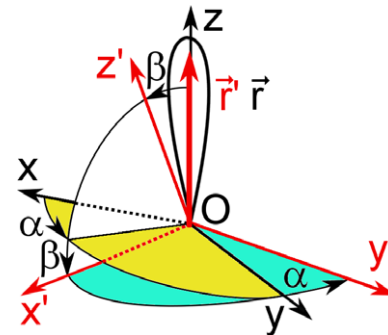


FIGURE 23 Right-handed rotations of coordinate system from (O, x, y, z) to (O, x', y', z') : (O, x, y, z) is first rotated about the fixed z -axis by angle $\alpha=\phi$, then about the rotated y' -axis by angle $\beta=\theta$

$$|\mathbf{r}'\rangle = \sum_m R_p^{\text{fixed}}(\gamma = \phi, \beta = \theta, \alpha = 0) |\ell, m\rangle \langle \ell, m | \mathbf{r} \rangle. \quad (174)$$

We multiply both sides of Eq. (174) by $\langle \ell, m' |$:

$$\langle \ell, m' | \mathbf{r}' \rangle = \sum_m \langle \ell, m' | R_p^{\text{fixed}}(\gamma = \phi, \beta = \theta, \alpha = 0) |\ell, m\rangle \langle \ell, m | \mathbf{r} \rangle. \quad (175)$$

By definition of spherical harmonics,

$$\{\langle \mathbf{r}' | \ell, m' \rangle\}^* = \sum_{\mathcal{D}} \langle \ell, m' | R_p^{\text{fixed}}(\gamma = \phi, \beta = \theta, \alpha = 0) |\ell, m\rangle \{\langle \mathbf{r} | \ell, m \rangle\}^*. \quad (176)$$

In the rotated coordinate system (O, x', y', z') represented by $\langle \mathbf{r}' |$, the polar angles of $\mathbf{r}'$ are $(-\theta, -\phi)$. In the fixed coordinate system (O, x, y, z) represented by $\langle \mathbf{r} |$, the polar angles of $\mathbf{r}$ are $\theta=0$ and ϕ undetermined. We deduce from Eq. (176) that

$$\begin{aligned} [Y_{\ell, m'}(-\theta, -\phi)]^* &= \sum_m D_{m' m}^{(\ell, P)}(\gamma = \phi, \beta = \theta, \\ &\alpha = 0) \sqrt{\frac{2\ell+1}{4\pi}} \delta_{m, 0} \\ &= D_{m' 0}^{(\ell, P)}(\phi, \theta, 0) \sqrt{\frac{2\ell+1}{4\pi}}. \end{aligned} \quad (177)$$

Using Eq. (144), the latter becomes the first relation connecting spherical harmonic with Wigner passive rotation matrix:

$$(-1)^{m'} Y_{\ell, m'}(\theta, \phi) = D_{m' 0}^{(\ell, P)}(\phi, \theta, 0) \sqrt{\frac{2\ell+1}{4\pi}}. \quad (178)$$

By extension, the first relation can be rewritten as^{56,58,97,102}

$$Y_{\ell, m'}(\beta, \gamma) = (-1)^{m'} \sqrt{\frac{2\ell+1}{4\pi}} D_{m' 0}^{(\ell, P)}(\gamma, \beta, \alpha), \text{ (independent of } \alpha). \quad (179)$$

In Eq. [43.17] of Davydov,³² the two indices m' and 0 in $D_{m' 0}^{(\ell, P)}(\gamma, \beta, \alpha)$ are exchanged.

An example of Eq. (179) with $\ell=m'=1$, $\mathbf{D}^{(1, P)}$ in Eq. (124), and $Y_{1,1}(\beta, \gamma)$ in Table 1 is

$$-\sqrt{\frac{3}{4\pi}} D_{10}^{(1, P)}(\gamma, \beta, \alpha) = -\sqrt{\frac{3}{8\pi}} \sin \beta e^{i\gamma} = Y_{1,1}(\beta, \gamma). \quad (180)$$

8.4.2 | Second relation

Using Eqs. (126) and (128), it is easy to show that

$$[D_{m0}^{(\ell, P)}(-\phi, -\theta, 0)]^* = D_{0m}^{(\ell, P)}(0, \theta, \phi). \quad (181)$$

The first relation defined in Eq. (178) and the identity in Eq. (144) yield

$$\begin{aligned} [D_{m0}^{(\ell, P)}(-\phi, -\theta, 0)]^* &= \left[(-1)^m \sqrt{\frac{4\pi}{2\ell+1}} Y_{\ell, m}(-\theta, -\phi) \right]^* \\ &= \sqrt{\frac{4\pi}{2\ell+1}} Y_{\ell, m}(\theta, \phi). \end{aligned} \quad (182)$$

Therefore, the second relation connecting spherical harmonics with Wigner passive rotation matrix¹² is

$$Y_{\ell, m}(\theta, \phi) = \sqrt{\frac{2\ell+1}{4\pi}} D_{0m}^{(\ell, P)}(0, \theta, \phi). \quad (183)$$

By extension, the second relation can be rewritten as^{56,58,80,97,102}

$$Y_{\ell, m}(\beta, \alpha) = \sqrt{\frac{2\ell+1}{4\pi}} D_{0m}^{(\ell, P)}(\gamma, \beta, \alpha), \text{ (independent of } \gamma). \quad (184)$$

In Eq. [43.17] of Davydov,³² the two indices 0 and m in $D_{0m}^{(\ell, P)}(\gamma, \beta, \alpha)$ are exchanged.

An example of Eq. (184) with $\ell=m'=1$, $\mathbf{D}^{(1, P)}$ in Eq. (124), and $Y_{1,1}(\beta, \alpha)$ in Table 1 is

$$\sqrt{\frac{3}{4\pi}} D_{01}^{(1, P)}(\gamma, \beta, \alpha) = -\sqrt{\frac{3}{8\pi}} \sin \beta e^{i\alpha} = Y_{1,1}(\beta, \alpha). \quad (185)$$

Wigner passive rotation matrix elements $D_{m' m}^{(\ell, P)}(\gamma, \beta, \alpha)$ with $m'=0$ (Eq. (184)) or $m=0$ (Eq. (179)) are proportional to normalized spherical harmonics $Y_{\ell, m}(\beta, \alpha)$ and $Y_{\ell, m'}(\beta, \gamma)$ in Condon and Shortley convention and covariant notation, respectively.

9 | ROTATION OF SPHERICAL HARMONIC AND SPHERICAL TENSOR

An application of Wigner active rotation matrix is the transformation of spherical harmonics induced by an active rotation of the physical system. This rotation may occurred in the same coordinate system or in two coordinate systems.⁶¹

In the configuration of one coordinate system, the active rotation of physical system is described by the Euler angles (α, β, γ) . In the configuration of two coordinate systems, the second coordinate system is attached to the physical system and rotates with it. It is called body-attached coordinate system. Before rotation, the two coordinate systems coincide. The relative orientation of these two coordinate systems after rotation is described by the Euler angles.

The spherical harmonics, eigen functions of orbital angular momentum, are the coordinate representation of the angular momentum eigenket vectors $|\ell, m\rangle$ with integer values of ℓ and m . The actively rotated eigenket vectors $|\ell, m\rangle'$ and the fixed eigenket vectors $|\ell, m\rangle$ are related:^{11,14,15,29,36,47}

$$\begin{aligned} |\ell, m\rangle' &= R_A^{\text{fixed}}(\alpha, \beta, \gamma)|\ell, m\rangle \\ &= \sum_{m'=-\ell}^{+\ell} |\ell, m'\rangle \langle \ell, m'| R_A^{\text{fixed}}(\alpha, \beta, \gamma) |\ell, m\rangle \\ &= \sum_{m'=-\ell}^{+\ell} |\ell, m'\rangle D_{m'm}^{(\ell, A)}(\alpha, \beta, \gamma). \end{aligned} \quad (186)$$

The eigenket vectors are in row matrices.

The passive rotation of spherical harmonics or the rotation of coordinate system associated with spherical harmonics is more subtle than the active rotation of spherical harmonics. We provide simple examples to support our results.

Finally, we rely on properties deduced from rotations of spherical harmonics to define the rotation properties of spherical tensor.

9.1 | Right-handed active rotation of spherical harmonic in one coordinate system

Consider the first configuration dealing with the right-handed active rotation of spherical harmonics in a fixed

coordinate system (O, x, y, z) . The initial position vector is named $\mathbf{r}_1$ and the final or right-hand actively rotated one is $\mathbf{r}$ in (O, x, y, z) as shown in Figure 24A,B. The corresponding ket position vectors are related by

$$|\mathbf{r}\rangle = R_A^{\text{fixed}}(\alpha, \beta, \gamma)|\mathbf{r}_1\rangle. \quad (187)$$

Conversely, the bra position bases are related by (see Eq. (64))

$$\langle \mathbf{r}_1| = \langle \mathbf{r}| R_A^{\text{fixed}}(\alpha, \beta, \gamma). \quad (188)$$

Multiplying each member of Eq. (188) by $|\ell, m\rangle$ and including the closure relation yield

$$\begin{aligned} \langle \mathbf{r}_1| \ell, m\rangle &= \langle \mathbf{r}| R_A^{\text{fixed}}(\alpha, \beta, \gamma) |\ell, m\rangle \\ &= \langle \mathbf{r}| \sum_{m'=-\ell}^{+\ell} |\ell, m'\rangle \langle \ell, m'| R_A^{\text{fixed}}(\alpha, \beta, \gamma) |\ell, m\rangle \\ &= \sum_{m'=-\ell}^{+\ell} \langle \mathbf{r}| \ell, m'\rangle D_{m'm}^{(\ell, A)}(\alpha, \beta, \gamma). \end{aligned} \quad (189)$$

The polar angles of the initial position vector $\mathbf{r}_1$ and those of the rotated one $\mathbf{r}$ in (O, x, y, z) are (θ_1, ϕ_1) and (θ, ϕ) , respectively. These angles allow us to rewrite Eq. (189) as

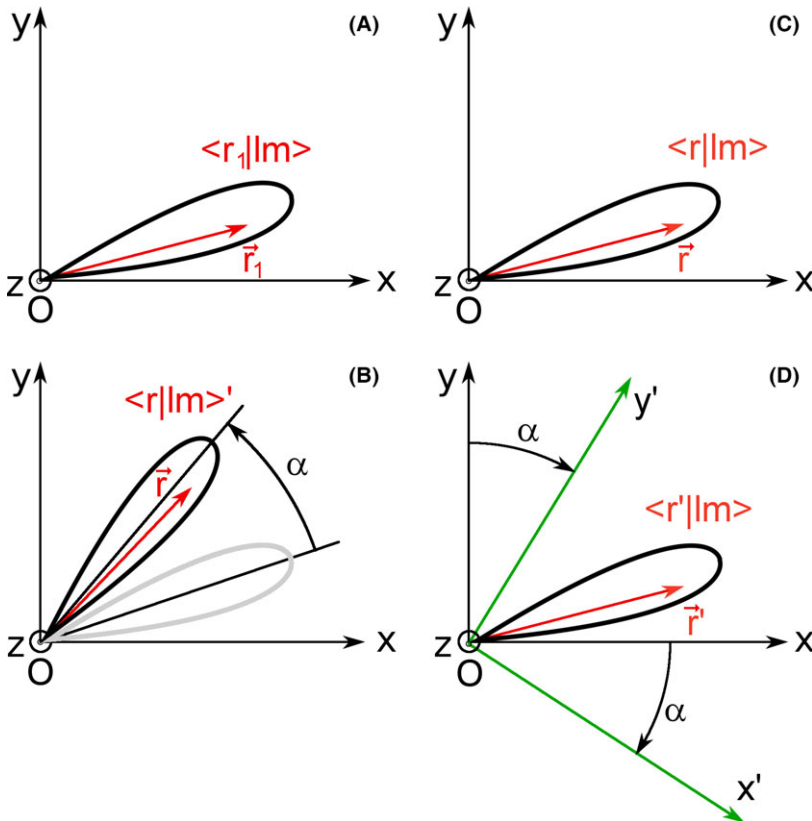


FIGURE 24 (A, B) Right-handed active rotation of spherical harmonics from $\langle \mathbf{r}_1| \ell, m\rangle$ to $\langle \mathbf{r}| \ell, m\rangle'$ in a single coordinate system (O, x, y, z) ; (C, D) left-handed rotation of coordinate system from (O, x, y, z) to (O, x', y', z) , the same spherical harmonics is called $\langle \mathbf{r}| \ell, m\rangle$ in (O, x, y, z) and $\langle \mathbf{r}'| \ell, m\rangle$ in (O, x', y', z)

$$\langle \theta_1, \phi_1 | \ell, m \rangle = \sum_{m'=-\ell}^{+\ell} \langle \theta, \phi | \ell, m' \rangle D_{m'm}^{(\ell, A)}(\alpha, \beta, \gamma). \quad (190)$$

Writing this result in terms of spherical harmonics yields^{11,15,37,56}

$$Y_{\ell, m}(\theta_1, \phi_1) \stackrel{5}{=} \sum_{m'=-\ell}^{+\ell} Y_{\ell, m'}(\theta, \phi) D_{m'm}^{(\ell, A)}(\alpha, \beta, \gamma). \quad (191)$$

The spherical harmonics $Y_{\ell, m}(\theta_1, \phi_1)$ whose arguments are the polar angles of the initial position vector $\mathbf{r}_1$ are expressed in terms of $Y_{\ell, m'}(\theta, \phi)$ whose arguments are the polar angles of the final or rotated position vector $\mathbf{r}$. The spherical harmonics in the two terms are identical but their arguments are different.

Although it remains uncommon, we may include the vector and its polar angles as arguments of spherical harmonics:

$$Y_{\ell, m}[\mathbf{r}_1(\theta_1, \phi_1)] = \sum_{m'=-\ell}^{+\ell} Y_{\ell, m'}[\mathbf{r}(\theta, \phi)] D_{m'm}^{(\ell, A)}(\alpha, \beta, \gamma). \quad (192)$$

These two vectors $\mathbf{r}_1$ and $\mathbf{r}$ are in the same coordinate system.

By extension, including the definition of the right-handed active rotation of space function yields

$$\begin{aligned} Y'_{\ell, m}(\theta, \phi) &\stackrel{1}{=} R_A^{\text{fixed}}(\alpha, \beta, \gamma) Y_{\ell, m}(\theta, \phi) \stackrel{2}{=} Y_{\ell, m}(\theta_1, \phi_1) \\ &\stackrel{5}{=} \sum_{m'=-\ell}^{+\ell} Y_{\ell, m'}(\theta, \phi) D_{m'm}^{(\ell, A)}(\alpha, \beta, \gamma). \end{aligned} \quad (193)$$

Sometimes, we need the reverse expression of Eq. (191), which expresses $Y_{\ell, m}(\theta, \phi)$ with respect to $Y_{\ell, m'}(\theta_1, \phi_1)$. We multiply both sides of Eq. (187) by $\langle \ell, m |$ and include the closure relation in the right-hand side member:

$$\langle \ell, m | \mathbf{r} \rangle = \sum_{m'=-\ell}^{+\ell} \langle \ell, m | R_A^{\text{fixed}}(\alpha, \beta, \gamma) | \ell, m' \rangle \langle \ell, m' | \mathbf{r}_1 \rangle, \quad (194)$$

which leads to^{1,39}

$$[Y_{\ell, m}(\theta, \phi)]^* = \sum_{m'=-\ell}^{+\ell} D_{mm'}^{(\ell, A)}(\alpha, \beta, \gamma) [Y_{\ell, m'}(\theta_1, \phi_1)]^*. \quad (195)$$

The complex conjugates of spherical harmonics are in column matrices. It is tempting to write Eq. (195) as follows:^{24,26,29,39,75}

$$Y_{\ell, m}(\theta, \phi) = \sum_{m'=-\ell}^{+\ell} [D_{mm'}^{(\ell, A)}(\alpha, \beta, \gamma)]^* Y_{\ell, m'}(\theta_1, \phi_1). \quad (196)$$

The right-hand actively rotated spherical harmonics in a fixed coordinate system are expressed as a linear

combination of spherical harmonics of the same quantum number ℓ before rotation.

Bear in mind that the two vectors $\mathbf{r}_1(\theta_1, \phi_1)$ and $\mathbf{r}(\theta, \phi)$ are in a single coordinate system, we may use Eq. (187) to reformulate Eq. (196) as⁷³

$$Y_{\ell, m}(R_A^{\text{fixed}}(\alpha, \beta, \gamma) \mathbf{r}_1) = \sum_{m'=-\ell}^{+\ell} [D_{mm'}^{(\ell, A)}(\alpha, \beta, \gamma)]^* Y_{\ell, m'}(\mathbf{r}_1). \quad (197)$$

Applying Eq. (129) to Eq. (196) yields

$$Y_{\ell, m}(\theta, \phi) = \sum_{m'=-\ell}^{+\ell} Y_{\ell, m'}(\theta_1, \phi_1) D_{m'm}^{(\ell, P)}(\gamma, \beta, \alpha). \quad (198)$$

The notation suggests a passive rotation even though we are studying active rotations. We prefer Eqs. (195) and (196) to Eq. (198).

9.2 | Example IX.1

Example 1 from Man¹ is again used to illustrate Eq. (196). Consider a position vector $\mathbf{A}$ in a 3-D Cartesian coordinate system (O, x, y, z) with an orthonormal basis $\{\mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z\}$. The Cartesian components of $\mathbf{A}$ in this basis are (a_x, a_y, a_z) .

We apply a right-handed active rotation about the z -axis by Euler angles $\alpha = \beta = 0$ and $\gamma = \frac{\pi}{2}$ to $\mathbf{A}$ (Figure 25A). The Cartesian components (a'_x, a'_y, a'_z) of the rotated vector $\mathbf{A}'$ is given by the direct product of the Cartesian active rotation matrix with the column component matrix of $\mathbf{A}$:³

$$\begin{aligned} \begin{pmatrix} a'_x \\ a'_y \\ a'_z \end{pmatrix} &= \begin{pmatrix} \cos \frac{\pi}{2} & -\sin \frac{\pi}{2} & 0 \\ \sin \frac{\pi}{2} & \cos \frac{\pi}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} a_x \\ a_y \\ a_z \end{pmatrix} \\ &= \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} a_x \\ a_y \\ a_z \end{pmatrix} = \begin{pmatrix} -a_y \\ a_x \\ a_z \end{pmatrix}. \end{aligned} \quad (199)$$

There is a second way to solve this problem. We can relate the Cartesian components of $\mathbf{A}$ to the spherical harmonics of order $l=1$:

$$\begin{aligned} Y_{1,1}(\theta_1, \phi_1) &= -\sqrt{\frac{3}{4\pi}} \frac{a_x + ia_y}{d\sqrt{2}}, \\ Y_{1,0}(\theta_1, \phi_1) &= \sqrt{\frac{3}{4\pi}} \frac{a_z}{d}, \\ Y_{1,-1}(\theta_1, \phi_1) &= \sqrt{\frac{3}{4\pi}} \frac{a_x - ia_y}{d\sqrt{2}}, \quad d = \|\mathbf{A}\|. \end{aligned} \quad (200)$$

In our case, $\mathbf{D}^{(1, A)}(\alpha, \beta, \gamma)$ defined in Eq. (116) becomes

$$\mathbf{D}^{(1,A)}(\alpha=0, \beta=0, \gamma=\frac{\pi}{2}) = \begin{pmatrix} -i & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & +i \end{pmatrix}. \quad (201)$$

Replacing covariant spherical harmonics in Eq. (196) by covariant spherical components of $\mathbf{A}$ and $\mathbf{A}'$ yields

$$\begin{pmatrix} -\frac{a'_x + ia'_y}{\sqrt{2}} \\ a'_z \\ \frac{a'_x - ia'_y}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} +i & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -i \end{pmatrix} \begin{pmatrix} -\frac{a_x + ia_y}{\sqrt{2}} \\ a_z \\ \frac{a_x - ia_y}{\sqrt{2}} \end{pmatrix}. \quad (202)$$

It follows that

$$a'_x = -a_y, \quad a'_y = a_x, \quad a'_z = a_z, \quad (203)$$

in agreement with the direct Cartesian rotation in Eq. (199).

9.3 | Left-handed rotation of coordinate system

The right-handed active rotation of spherical harmonics discussed above is equivalent to a left-handed rotation of coordinate system keeping the spherical harmonics fixed. Figure 24A,B shows the right-handed active rotation of spherical harmonics and (C, D) the left-handed rotation of coordinate system all about z -axis by angle α . The position vectors are $\mathbf{r}_1$ and $\mathbf{r}$ in Figure 24A,B; they are $\mathbf{r}$ and $\mathbf{r}'$ in Figure 24C,D. We explore the left-handed rotation of coordinate system with the passive point view of $R_A^{\text{fixed}}(\alpha, \beta, \gamma)$.

As $R_A^{\text{fixed}}(\alpha, \beta, \gamma)$ allows us to describe a left-handed rotation of a coordinate system from $\langle \mathbf{r} |$ to $\langle \mathbf{r}' |$, the ket position vectors in passive point of view of $R_A^{\text{fixed}}(\alpha, \beta, \gamma)$ are related by

$$|\mathbf{r}'\rangle = R_A^{\text{fixed}}(\alpha, \beta, \gamma)|\mathbf{r}\rangle. \quad (204)$$

Conversely, the bra position bases are related by

$$\langle \mathbf{r} | = \langle \mathbf{r}' | R_A^{\text{fixed}}(\alpha, \beta, \gamma). \quad (205)$$

These bra position bases are related (see Eq. (96)) by

$$\langle \mathbf{r} | = \langle \mathbf{r}' | R_P^{\text{fixed}}(\gamma, \beta, \alpha) \quad (206)$$

in a right-handed rotation of a coordinate system from $\langle \mathbf{r} |$ to $\langle \mathbf{r}' |$. In rotation of coordinate system (Eqs. (205) and (206)), the application of rotation operator to the rotated bra position basis $\langle \mathbf{r}' |$ yields the fixed bra position basis $\langle \mathbf{r} |$.

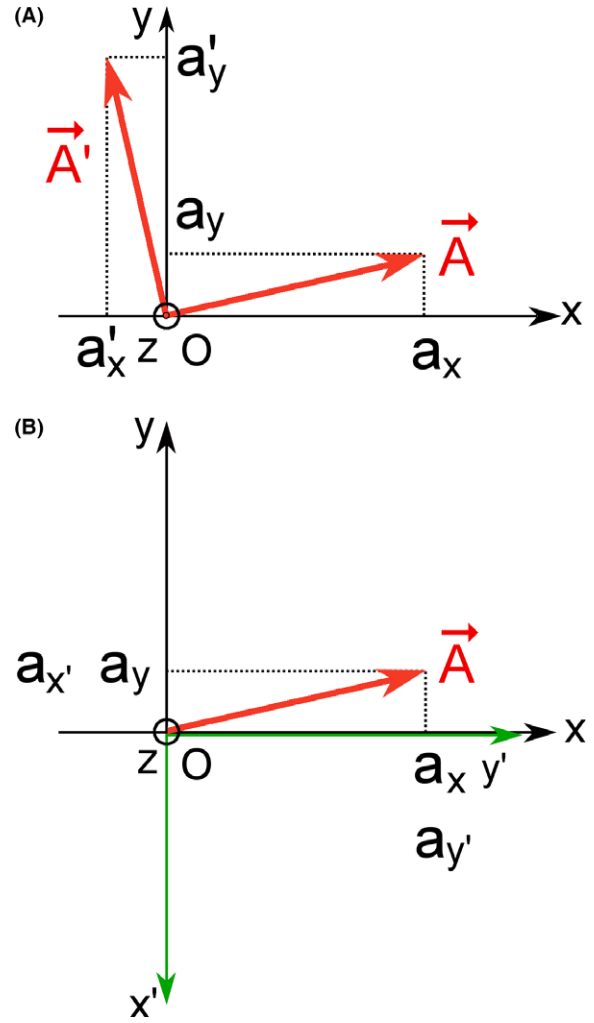


FIGURE 25 (A) Right-handed active rotation of vector from $\mathbf{A}$ to $\mathbf{A}'$ about the z -axis by Euler angles $\alpha=\beta=0$ and $\gamma=\pi/2$ in a single coordinate system (O, x, y, z) is equivalent to (B) left-handed rotation of coordinate system from (O, x, y, z) to (O, x', y', z) about the z -axis by Euler angles $\alpha=\beta=0$ and $\gamma=\pi/2$, $\mathbf{A}$ remains fixed

Multiplying each member of Eq. (205) by $|\ell, m\rangle$ and including the closure relation yield

$$\begin{aligned} \langle \mathbf{r} | \ell, m \rangle &= \langle \mathbf{r}' | R_A^{\text{fixed}}(\alpha, \beta, \gamma) | \ell, m \rangle \\ &= \sum_{m'=-\ell}^{+\ell} \langle \mathbf{r}' | \ell, m' \rangle D_{m'm}^{(\ell,A)}(\alpha, \beta, \gamma). \end{aligned} \quad (207)$$

In spherical harmonics notation, we have

$$Y_{\ell,m}(\theta, \phi) \stackrel{S}{=} \sum_{m'=-\ell}^{+\ell} Y_{\ell,m'}(\theta', \phi') D_{m'm}^{(\ell,A)}(\alpha, \beta, \gamma). \quad (208)$$

The spherical harmonics are in row matrices. Equation (208) describes the left-handed rotation of coordinate system despite the presence of Wigner active rotation matrix, whereas Eq. (191) describes the right-handed active rotation of spherical harmonics in a single coordinate system. They are two equivalent descriptions.

By extension, introducing the definition of left-handed rotation of coordinate system $R_A^{\text{fixed}}(\alpha, \beta, \gamma)Y_{\ell,m}(\theta', \phi')$ in Eq. (96) yields

$$Y'_{\ell,m}(\theta', \phi') \stackrel{1}{=} R_A^{\text{fixed}}(\alpha, \beta, \gamma)Y_{\ell,m}(\theta', \phi') \stackrel{2}{=} Y_{\ell,m}(\theta, \phi) \stackrel{5}{=} \sum_{m'=-\ell}^{+\ell} Y_{\ell,m'}(\theta', \phi') D_{mm'}^{(\ell,A)}(\alpha, \beta, \gamma). \quad (209)$$

In other words, the operator $R_A^{\text{fixed}}(\alpha, \beta, \gamma)$ in the equality $\stackrel{1}{=}$ expresses either the right-handed active rotation of spherical harmonics in a single coordinate system (Eq. (193)) or the left-handed rotation of coordinate system keeping spherical harmonics fixed (Eq. (209)). Equation (209) can be deduced from Eq. (193) in which we replace the polar angles (θ, ϕ) by (θ', ϕ') and (θ_1, ϕ_1) by (θ, ϕ) .

The coordinate system is not explicit in the notation $R_A^{\text{fixed}}(\alpha, \beta, \gamma)Y_{\ell,m}(\theta', \phi')$. In contrast with Dirac notation $\langle \mathbf{r}' | R_A^{\text{fixed}}(\alpha, \beta, \gamma) | \ell, m \rangle$, the fixed and the rotated coordinate systems are represented by the bra position bases $\langle \mathbf{r} |$ and $\langle \mathbf{r}' |$, respectively.

We deduce from Eq. (208) the reverse expression:

$$[Y_{\ell,m}(\theta', \phi')]^* = \sum_{m'=-\ell}^{+\ell} D_{mm'}^{(\ell,A)}(\alpha, \beta, \gamma) [Y_{\ell,m'}(\theta, \phi)]^*. \quad (210)$$

$Y_{\ell,m'}(\theta, \phi)$ is the spherical harmonic in the fixed coordinate system, whereas $Y_{\ell,m}(\theta', \phi')$ is the same spherical harmonic in the left-handed rotated coordinate system. Equation (210) has the same structure as Eq. (195).

9.4 | Example IX.2

Consider the same vector $\mathbf{A}$ used in Example IX.1. Now we left-hand rotate the coordinate system (O, x, y, z) about z -axis by Euler angles $\alpha=\beta=0$ and $\gamma=\frac{\pi}{2}$ (Figure 25B).

We recall that we use both left- and right-handed rotations to visualize rotation of vector and that of coordinate system. But for computation we still use mathematical expressions deduced from right-handed rotation. In contrast, the expression of a rotation operator R remains unchanged. But, we explore its active point of view when it is applied to space function represented by a ket state as $R|\Psi\rangle$ or its passive point of view when it is applied to coordinate system represented by a bra position basis as $\langle \mathbf{r}' | R$. More precisely, $R_A^{\text{fixed}}(\alpha, \beta, \gamma)|\Psi\rangle$ means we carry a right-handed active rotation of space function, whereas $\langle \mathbf{r}' | R_A^{\text{fixed}}(\alpha, \beta, \gamma)$ means we carry a left-handed rotation of coordinate system. In contrast, $\langle \mathbf{r}' | R_P^{\text{fixed}}(\gamma, \beta, \alpha)$ means we carry a right-handed rotation of coordinate system, whereas $R_P^{\text{fixed}}(\gamma, \beta, \alpha)|\Psi\rangle$ means we carry a left-handed active rotation of space function.

The Cartesian components $(a_{x'}, a_{y'}, a_{z'})$ of $\mathbf{A}$ in the rotated coordinate system (O, x', y', z') are given by the direct product of the Cartesian passive rotation matrix with the column component matrix of $\mathbf{A}$. The left-handed passive rotation matrix is deduced from that of right-handed passive rotation by changing the sign of its rotation angle:

$$\begin{pmatrix} a_{x'} \\ a_{y'} \\ a_{z'} \end{pmatrix} = \begin{pmatrix} \cos \frac{\pi}{2} & -\sin \frac{\pi}{2} & 0 \\ \sin \frac{\pi}{2} & \cos \frac{\pi}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} a_x \\ a_y \\ a_z \end{pmatrix} = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} a_x \\ a_y \\ a_z \end{pmatrix} = \begin{pmatrix} -a_y \\ a_x \\ a_z \end{pmatrix}. \quad (211)$$

As we left-hand rotate a coordinate system, we are studying $\langle \mathbf{r}' | R_A^{\text{fixed}}(\alpha, \beta, \gamma)$. The rotation operator is $R_A^{\text{fixed}}(\alpha=0, \beta=0, \gamma=\frac{\pi}{2})$. In our case, $\mathbf{D}^{(1,A)}(\alpha, \beta, \gamma)$ defined in Eq. (116) becomes

$$\mathbf{D}^{(1,A)}(\alpha=0, \beta=0, \gamma=\frac{\pi}{2}) = \begin{pmatrix} -i & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & +i \end{pmatrix}. \quad (212)$$

Now we explore the complex conjugate of Eq. (210):

$$\begin{pmatrix} -\frac{a_{x'}+ia_{y'}}{\sqrt{2}} \\ a_{z'} \\ \frac{a_{x'}-ia_{y'}}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} +i & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -i \end{pmatrix} \begin{pmatrix} -\frac{a_x+ia_y}{\sqrt{2}} \\ a_z \\ \frac{a_x-ia_y}{\sqrt{2}} \end{pmatrix}. \quad (213)$$

It follows that

$$a_{x'} = -a_y, a_{y'} = a_x, a_{z'} = a_z, \quad (214)$$

in agreement with the direct Cartesian rotation in Eq. (211). The coordinates of $\mathbf{A}$ in the left-hand rotated coordinate system are identical to those in Eq. (203) of Example IX.1 concerning the right-handed active rotation of $\mathbf{A}$ in a fixed coordinate system. These two examples are equivalent.

9.5 | Right-handed active rotation of spherical harmonic in two coordinate systems—canonical transformation

Consider two coordinate systems.⁶⁰ Initially, the position vector $\mathbf{r}_1$ is in the fixed coordinate system (O, x, y, z) that coincides with its body-attached coordinate system (O, x', y', z') as shown in Figure 26A. The polar angles of $\mathbf{r}_1$ are (θ_1, ϕ_1) . We right-hand rotate the position vector and its body-attached coordinate system simultaneously by the Euler angles as shown in Figure 26C. The actively rotated position vector is named $\mathbf{r}$ in (O, x, y, z) and $\mathbf{r}'$ in (O, x', y', z') .

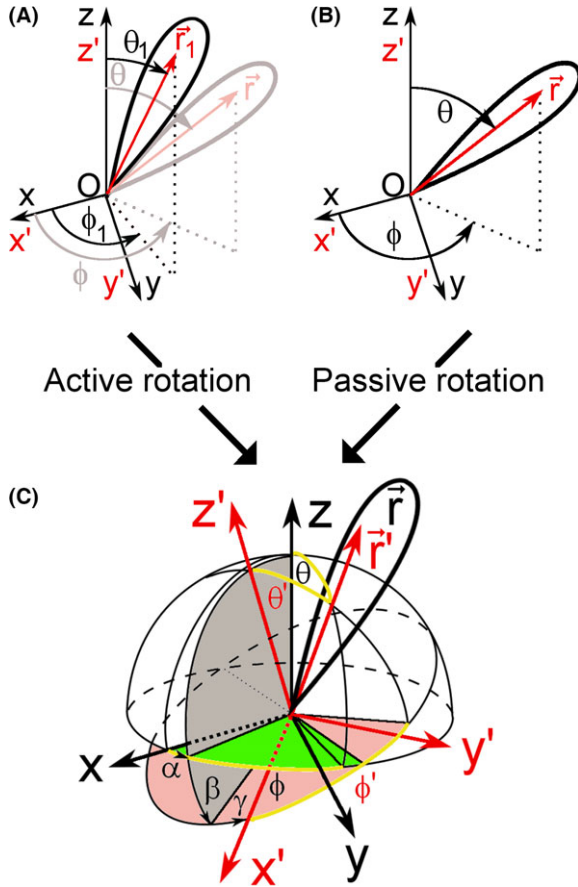


FIGURE 26 Similarities and differences between right-handed active rotations (or canonical transformation) of spherical harmonics and right-handed rotations of coordinate system from (O, x, y, z) to (O, x', y', z') , these two coordinate systems are related by Euler angles. (A) The position vector is $\mathbf{r}_1(\theta_1, \phi_1)$ before the right-handed active rotations of the spherical harmonics in a single coordinate system. (B) The position vector is $\mathbf{r}(\theta, \phi)$ before the right-handed rotations of coordinate system. (C) The rotated vector is also called $\mathbf{r}(\theta, \phi)$ in active rotation and $\mathbf{r}'(\theta', \phi')$ in rotation of coordinate system

$y', z')$.¹¹ This is an application of Eq. (68) about the active rotation of a space function. Now, the state ket $|\Psi\rangle$ is $|\ell, m\rangle$. Equations (68) and (186) allow us to write:

$$\begin{aligned} \langle \mathbf{r} | \ell, m \rangle' &= \langle \mathbf{r} | R_A^{\text{fixed}}(\alpha, \beta, \gamma) | \ell, m \rangle = \langle \mathbf{r}' | \ell, m \rangle \\ &= \sum_{m'=-\ell}^{+\ell} \langle \mathbf{r} | \ell, m' \rangle D_{m'm}^{(\ell, A)}(\alpha, \beta, \gamma). \end{aligned} \quad (215)$$

Therefore,

$$\langle \mathbf{r}' | \ell, m \rangle = \sum_{m'=-\ell}^{+\ell} \langle \mathbf{r} | \ell, m' \rangle D_{m'm}^{(\ell, A)}(\alpha, \beta, \gamma). \quad (216)$$

The polar angles of the same position vectors $\mathbf{r}$ and $\mathbf{r}'$ (Figure 26C) are (θ, ϕ) in (O, x, y, z) and (θ', ϕ') in (O, x', y', z') , respectively. These angles allow us to rewrite Eq. (216) as

$$\langle \theta', \phi' | \ell, m \rangle = \sum_{m'=-\ell}^{+\ell} \langle \theta, \phi | \ell, m' \rangle D_{m'm}^{(\ell, A)}(\alpha, \beta, \gamma). \quad (217)$$

Writing this result in terms of spherical harmonics, we obtain^{9,14,34,36,37,40,54,57,60,61,72,73,98,111,116,117}

$$Y_{\ell, m}(\theta', \phi') \stackrel{5}{=} \sum_{m'=-\ell}^{+\ell} Y_{\ell, m'}(\theta, \phi) D_{m'm}^{(\ell, A)}(\alpha, \beta, \gamma). \quad (218)$$

The spherical harmonics $Y_{\ell, m}(\theta', \phi')$ whose arguments are the polar angles of the position vector $\mathbf{r}'$ in its body-attached coordinate system are expressed in terms of $Y_{\ell, m'}(\theta, \phi)$ whose arguments are the polar angles of the rotated position vector $\mathbf{r}$ in the fixed coordinate system. The two position vectors $\mathbf{r}$ and $\mathbf{r}'$ in Figure 26C represent the same physical point.⁴⁷ As the position vector and its body-attached coordinate system rotate together, its polar angles (θ_1, ϕ_1) before rotation in the initial coordinate system are identical to those (θ', ϕ') after rotation in the rotated body-attached coordinate system:

$$(\theta', \phi') = (\theta_1, \phi_1). \quad (219)$$

The spherical harmonics on each side of Eq. (218) are identical but their arguments are different. We may include the vector and its polar angles in spherical harmonics¹¹⁸:

$$Y_{\ell, m}[\mathbf{r}(\theta', \phi')] \stackrel{5}{=} \sum_{m'=-\ell}^{+\ell} Y_{\ell, m'}[\mathbf{r}(\theta, \phi)] D_{m'm}^{(\ell, A)}(\alpha, \beta, \gamma). \quad (220)$$

The rotated position vector is viewed in two coordinate systems: $\mathbf{r}(\theta', \phi') = \mathbf{r}'(\theta', \phi')$ in its body-attached coordinate system and $\mathbf{r}(\theta, \phi)$ in the fixed coordinate system. The position vector before rotation is $\mathbf{r}_1(\theta_1, \phi_1)$ in the fixed coordinate system, which is understood in Eq. (218) due to Eq. (219). This corresponds to the equality denoted by $\stackrel{2}{=}$ in Eqs. (47) and (49). If we replace the polar angles (θ', ϕ') in Eq. (218) by those defined in Eq. (219), Eqs. (191) and (218) become identical. They follow the second interpretation of a rotation operator that only changes the arguments of spherical harmonics, leaving the spherical harmonics unchanged. The spherical harmonics transform among themselves with exactly the same matrix of coefficients as that for $2\ell+1$ angular momentum eigenket vectors $|\ell, m\rangle$ in Eq. (186). Equation (215) in spherical harmonic notation for canonical transformation becomes

$$\begin{aligned} Y'_{\ell, m}(\theta, \phi) &\stackrel{1}{=} R_A^{\text{fixed}}(\alpha, \beta, \gamma) Y_{\ell, m}(\theta, \phi) \stackrel{4}{=} Y_{\ell, m}(\theta', \phi') \\ &\stackrel{5}{=} \sum_{m'=-\ell}^{+\ell} Y_{\ell, m'}(\theta, \phi) D_{m'm}^{(\ell, A)}(\alpha, \beta, \gamma). \end{aligned} \quad (221)$$

9.6 | Right-handed rotation of coordinate system

This is an application of Eq. (96) about the passive rotation of space function about fixed axes. As shown in

Figure 27A,B, the position vector is named $\mathbf{r}$ with polar angles (θ, ϕ) in the fixed coordinate system (O, x, y, z) and $\mathbf{r}'$ with polar angles (θ', ϕ') in the rotated coordinate system (O, x', y', z) . The ket position vectors are related by the passive rotation operator as¹²

$$|\mathbf{r}'\rangle = R_P^{\text{fixed}}(\gamma, \beta, \alpha)|\mathbf{r}\rangle. \quad (222)$$

Therefore, the two bra position bases are related by¹²

$$\langle \mathbf{r}| = \langle \mathbf{r}'|R_P^{\text{fixed}}(\gamma, \beta, \alpha). \quad (223)$$

Equation (96) about the passive rotation of space function about fixed axes allows us to write

$$\begin{aligned} \langle \mathbf{r}|\ell, m\rangle &= \langle \mathbf{r}'|R_P^{\text{fixed}}(\gamma, \beta, \alpha)|\ell, m\rangle \\ &= \langle \mathbf{r}'|\sum_{m'=-\ell}^{+\ell} |\ell, m'\rangle \langle \ell, m'|R_P^{\text{fixed}}(\gamma, \beta, \alpha)|\ell, m\rangle \\ &= \langle \mathbf{r}'|\sum_{m'=-\ell}^{+\ell} |\ell, m'\rangle D_{m'm}^{(\ell, P)}(\gamma, \beta, \alpha). \end{aligned} \quad (224)$$

In spherical harmonic notation (Eq. (157)), we deduce from Eq. (224) that^{40,56,79,80}

$$Y_{\ell m}(\theta, \phi) = \sum_{m'=-\ell}^{+\ell} Y_{\ell m'}(\theta', \phi') D_{m'm}^{(\ell, P)}(\gamma, \beta, \alpha). \quad (225)$$

In right-handed rotation of coordinate system, Eq. (225) expresses the spherical harmonics in the fixed coordinate system as a linear combination of spherical harmonics of the same quantum number ℓ in the rotated coordinate system.⁵⁶

By extension, introducing the definition of right-handed rotation of coordinate system $R_P^{\text{fixed}}(\gamma, \beta, \alpha)Y_{\ell, m}(\theta', \phi')$ in Eq. (96) yields

$$\begin{aligned} Y'_{\ell, m}(\theta', \phi') &\stackrel{1}{=} R_P^{\text{fixed}}(\gamma, \beta, \alpha)Y_{\ell, m}(\theta', \phi') \stackrel{2}{=} Y_{\ell, m}(\theta, \phi) \\ &\stackrel{5}{=} \sum_{m'=-\ell}^{+\ell} Y_{\ell m'}(\theta', \phi') D_{m'm}^{(\ell, P)}(\gamma, \beta, \alpha). \end{aligned} \quad (226)$$

Equation (226) can be deduced from Eq. (209) about left-handed rotation of coordinate system by replacing the Euler angles α, β, γ by $-\gamma, -\beta, -\alpha$, respectively (Figure 28). Indeed, the equality $\stackrel{1}{=}$ in Eq. (209) becomes

$$\begin{aligned} R_A^{\text{fixed}}(\alpha \rightarrow -\gamma, \beta \rightarrow -\beta, \gamma \rightarrow -\alpha)Y_{\ell, m}(\theta', \phi') \\ = R_P^{\text{fixed}}(\gamma, \beta, \alpha)Y_{\ell, m}(\theta', \phi'). \end{aligned} \quad (227)$$

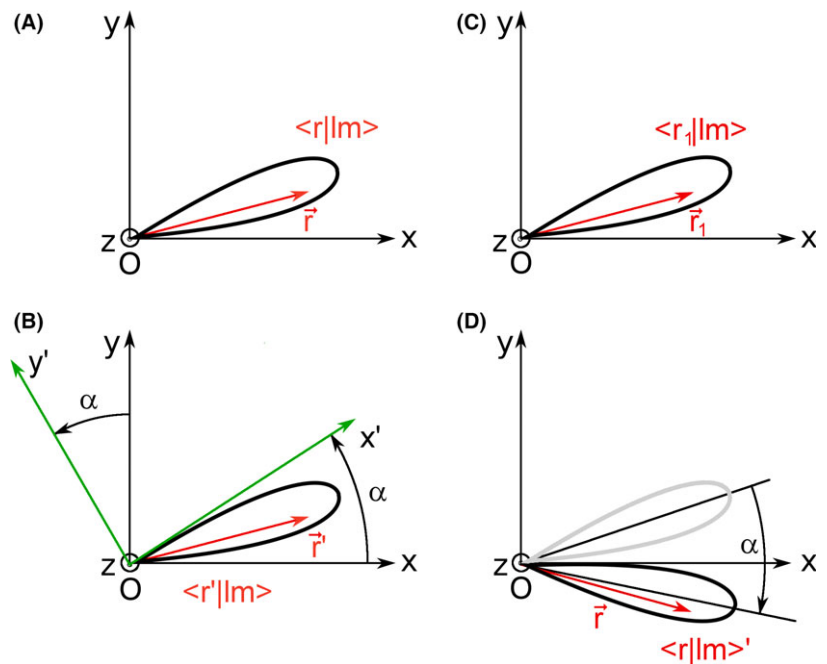
That is, the equality $\stackrel{1}{=}$ in Eq. (226). The equality $\stackrel{5}{=}$ in Eq. (209) becomes

$$\begin{aligned} \sum_{m'=-\ell}^{+\ell} Y_{\ell m'}(\theta', \phi') D_{m'm}^{(\ell, A)}(\alpha \rightarrow -\gamma, \beta \rightarrow -\beta, \gamma \rightarrow -\alpha) \\ = \sum_{m'=-\ell}^{+\ell} Y_{\ell m'}(\theta', \phi') D_{m'm}^{(\ell, P)}(\gamma, \beta, \alpha). \end{aligned} \quad (228)$$

That is, the equality $\stackrel{5}{=}$ in Eq. (226).

Equation (225) looks like Eq. (208) but they differ by Wigner rotation matrices. Equation (225) describes the right-handed passive rotation of spherical harmonics involving Wigner passive rotation matrix, whereas Eq. (208) describes

FIGURE 27 (A, B) Right-handed rotation of coordinate system from (O, x, y, z) to (O, x', y', z) about z -axis by angle α , the same spherical harmonics is called $\langle \mathbf{r}|\ell m\rangle$ in (O, x, y, z) and $\langle \mathbf{r}'|\ell m\rangle$ in (O, x', y', z) ; (C, D) left-handed active rotation of spherical harmonics from $\langle \mathbf{r}_1|\ell m\rangle$ to $\langle \mathbf{r}|\ell m\rangle'$ about z -axis by angle α in a single coordinate system (O, x, y, z)



the left-handed passive rotation of spherical harmonics involving Wigner active rotation matrix.

Sometimes, we need the reverse expression of Eq. (225), which expresses $Y_{\ell m}(\theta', \phi')$ with respect to $Y_{\ell m'}(\theta, \phi)$. A similar procedure that leading to Eq. (195) yields⁵⁶

$$[Y_{\ell m}(\theta', \phi')]^* = \sum_{m'=-\ell}^{+\ell} D_{mm'}^{(\ell, P)}(\gamma, \beta, \alpha) [Y_{\ell m'}(\theta, \phi)]^*, \quad (229)$$

or

$$Y_{\ell m}(\theta', \phi') = \sum_{m'=-\ell}^{+\ell} [D_{mm'}^{(\ell, P)}(\gamma, \beta, \alpha)]^* Y_{\ell m'}(\theta, \phi). \quad (230)$$

The spherical harmonics are in column matrices. The spherical harmonics in the right-hand rotated coordinate system are expressed as a linear combination of spherical harmonics of the same quantum number ℓ in the fixed coordinate system.

Figure 26 clarifies polar angle definitions. In active rotation (Figure 26A,C), (θ, ϕ) and (θ', ϕ') are the polar angles of the actively rotated vector in the fixed coordinate system and in its body-attached coordinate system, respectively. In its attached coordinate system, the actively rotated vector has the same polar angles, that is, $\theta' = \theta_1$ and $\phi' = \phi_1$, (θ_1, ϕ_1) being the polar angles of the vector in the fixed coordinate system before rotation (Figure 26A). In passive rotation (Figure 26B,C), the vector remains unchanged. The angles (θ, ϕ) and (θ', ϕ') are the polar angles of the vector in the fixed coordinate system and in the rotated coordinate system, respectively.

9.7 | Example IX.3

Consider the same vector $\mathbf{A}$ used in Example IX.1. Now we right-hand rotate the coordinate system (O, x, y, z) about z -axis by Euler angles $\alpha = \frac{\pi}{2}$ and $\beta = \gamma = 0$ (Figure 29A). The Cartesian components $(a_{x'}, a_{y'}, a_{z'})$ of $\mathbf{A}$ in the rotated coordinate system (O, x', y', z) are given by the direct product of the Cartesian passive rotation matrix with the column component matrix of $\mathbf{A}$:³

$$\begin{pmatrix} a_{x'} \\ a_{y'} \\ a_{z'} \end{pmatrix} = \begin{pmatrix} \cos \frac{\pi}{2} & \sin \frac{\pi}{2} & 0 \\ -\sin \frac{\pi}{2} & \cos \frac{\pi}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} a_x \\ a_y \\ a_z \end{pmatrix} \quad (231)$$

$$= \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} a_x \\ a_y \\ a_z \end{pmatrix} = \begin{pmatrix} a_y \\ -a_x \\ a_z \end{pmatrix}.$$

As we right-hand rotate a coordinate system, we are studying $\langle \mathbf{r}' | R_P^{\text{fixed}}(\gamma, \beta, \alpha)$. The rotation operator is $R_P^{\text{fixed}}(\gamma = 0, \beta = 0, \alpha = \frac{\pi}{2})$. In our case, $\mathbf{D}^{(1, P)}(\gamma, \beta, \alpha)$ defined in Eq. (124) becomes

$$\mathbf{D}^{(1, P)}(\gamma = 0, \beta = 0, \alpha = \frac{\pi}{2}) = \begin{pmatrix} +i & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -i \end{pmatrix}. \quad (232)$$

Numerical application of Eq. (230) is

$$\begin{pmatrix} -\frac{a_{x'} + ia_{y'}}{\sqrt{2}} \\ a_{z'} \\ \frac{a_{y'} - ia_{x'}}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} -i & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & +i \end{pmatrix} \begin{pmatrix} -\frac{a_x + ia_y}{\sqrt{2}} \\ a_z \\ \frac{a_x - ia_y}{\sqrt{2}} \end{pmatrix}. \quad (233)$$

It follows that

$$a_{x'} = a_y, a_{y'} = -a_x, a_{z'} = a_z, \quad (234)$$

in agreement with the direct Cartesian rotation in Eq. (231).

9.8 | Left-handed active rotation of spherical harmonic in one coordinate system

The right-handed rotation of coordinate system discussed above is equivalent to a left-handed active rotation of spherical harmonics in a fixed coordinate system. Figure 27A,B shows right-handed rotation of coordinate system about z -axis by angle α and (C, D) left-handed active rotation of spherical harmonics about z -axis by angle α . The position vectors are $\mathbf{r}$ and $\mathbf{r}'$ in Figure 27A,B; they are $\mathbf{r}_1$ and $\mathbf{r}$ in Figure 27C,D. For left-handed active rotation of spherical harmonics, we explore the left-handed active point view of $R_P^{\text{fixed}}(\gamma, \beta, \alpha)$. The ket position vectors are related by the left-handed active point view of $R_P^{\text{fixed}}(\gamma, \beta, \alpha)$:

$$|\mathbf{r}\rangle = R_P^{\text{fixed}}(\gamma, \beta, \alpha) |\mathbf{r}_1\rangle, \quad (235)$$

like in Eq. (187). Conversely,

$$\langle \mathbf{r}_1 | = \langle \mathbf{r} | R_P^{\text{fixed}}(\gamma, \beta, \alpha). \quad (236)$$

Multiplying both sides of Eq. (236) by $|\ell, m\rangle$ and including the closure relation yield

$$\begin{aligned} \langle \mathbf{r}_1 | \ell, m \rangle &= \langle \mathbf{r} | R_P^{\text{fixed}}(\gamma, \beta, \alpha) | \ell, m \rangle \\ &= \langle \mathbf{r} | \sum_{m'=-\ell}^{+\ell} |\ell, m'\rangle \langle \ell, m' | R_P^{\text{fixed}}(\gamma, \beta, \alpha) | \ell, m \rangle \\ &= \langle \mathbf{r} | \sum_{m'=-\ell}^{+\ell} |\ell, m'\rangle D_{m'm}^{(\ell, P)}(\gamma, \beta, \alpha). \end{aligned} \quad (237)$$

In spherical harmonics notation, we have

$$Y_{\ell,m}(\theta_1, \phi_1) \stackrel{5}{=} \sum_{m'=-\ell}^{+\ell} Y_{\ell,m'}(\theta, \phi) D_{m'm}^{(\ell,P)}(\gamma, \beta, \alpha). \quad (238)$$

The spherical harmonics $Y_{\ell,m}(\theta_1, \phi_1)$, whose arguments are the polar angles of the initial position vector $\mathbf{r}_1$, are expressed in terms of $Y_{\ell,m'}(\theta, \phi)$, whose arguments are the polar angles of the left-hand actively rotated position vector $\mathbf{r}$ (Figure 27C,D).

By extension, introducing the definition of left-handed active rotation of spherical harmonics $R_P^{\text{fixed}}(\gamma, \beta, \alpha)Y_{\ell,m}(\theta, \phi)$ in Eq. (67) yields

$$\begin{aligned} Y'_{\ell,m}(\theta, \phi) &\stackrel{1}{=} R_P^{\text{fixed}}(\gamma, \beta, \alpha)Y_{\ell,m}(\theta, \phi) \stackrel{2}{=} Y_{\ell,m}(\theta_1, \phi_1) \\ &\stackrel{5}{=} \sum_{m'=-\ell}^{+\ell} Y_{\ell,m'}(\theta, \phi) D_{m'm}^{(\ell,P)}(\gamma, \beta, \alpha). \end{aligned} \quad (239)$$

In other words, the operator $R_P^{\text{fixed}}(\gamma, \beta, \alpha)$ in the equality $\stackrel{1}{=}$ expresses either the right-handed rotation of coordinate system keeping spherical harmonics fixed (Eq. (226)) or the left-handed active rotation of spherical harmonics in a single coordinate system (Eq. (239)). The coordinate system is not explicit in the notation $R_P^{\text{fixed}}(\gamma, \beta, \alpha)Y_{\ell,m}(\theta, \phi)$. In contrast with Dirac notation $\langle \mathbf{r} | R_P^{\text{fixed}}(\gamma, \beta, \alpha) | \ell, m \rangle$, the fixed coordinate system is represented by the bra position basis $\langle \mathbf{r} |$.

Equation (239) can be deduced from Eq. (193) about right-handed active rotation of spherical harmonic in a single coordinate system by replacing the Euler angles α, β, γ by $-\gamma, -\beta, -\alpha$, respectively. Indeed, the equality $\stackrel{1}{=}$ in Eq. (193) becomes

$$\begin{aligned} R_A^{\text{fixed}}(\alpha \rightarrow -\gamma, \beta \rightarrow -\beta, \gamma \rightarrow -\alpha)Y_{\ell,m}(\theta, \phi) \\ = R_P^{\text{fixed}}(\gamma, \beta, \alpha)Y_{\ell,m}(\theta, \phi). \end{aligned} \quad (240)$$

That is, the equality $\stackrel{1}{=}$ in Eq. (239). The equality $\stackrel{5}{=}$ in Eq. (193) becomes

$$\begin{aligned} \sum_{m'=-\ell}^{+\ell} Y_{\ell,m'}(\theta, \phi) D_{m'm}^{(\ell,A)}(\alpha \rightarrow -\gamma, \beta \rightarrow -\beta, \gamma \rightarrow -\alpha) \\ = \sum_{m'=-\ell}^{+\ell} Y_{\ell,m'}(\theta, \phi) D_{m'm}^{(\ell,P)}(\gamma, \beta, \alpha). \end{aligned} \quad (241)$$

That is, the equality $\stackrel{5}{=}$ in Eq. (239).

Equation (238) looks like Eq. (191) but they differ by Wigner rotation matrices. Equation (238) describes the left-handed active rotation of spherical harmonics involving Wigner passive rotation matrix, whereas Eq. (191) describes the right-handed active rotation of spherical harmonics in a single coordinate system involving Wigner active rotation matrix.

Similarly, we may express $Y_{\ell,m'}(\theta, \phi)$ in terms of $Y_{\ell,m}(\theta_1, \phi_1)$ as in Eq. (196):

$$Y_{\ell,m}(\theta, \phi) = \sum_{m'=-\ell}^{+\ell} [D_{mm'}^{(\ell,P)}(\gamma, \beta, \alpha)]^* Y_{\ell,m'}(\theta_1, \phi_1). \quad (242)$$

The spherical harmonics are in column matrices. The left-hand actively rotated spherical harmonics in a fixed coordinate system are expressed as a linear combination of spherical harmonics of the same quantum number ℓ before rotation.

In addition to the canonical transformation, we have discussed four other types of rotation in this section. In fact, these four types are related. Knowing one of them allows us to deduce the other three. Figure 28 shows these relations.

9.9 | Example IX.4

Consider the same vector $\mathbf{A}$ used in Example IX.1. Now we left-hand rotate the vector $\mathbf{A}$ about z -axis by Euler angles $\alpha = \frac{\pi}{2}$ and $\beta = \gamma = 0$ (Figure 29B). The Cartesian components (a'_x, a'_y, a'_z) of the rotated vector $\mathbf{A}'$ in the fixed coordinate system are given by the direct product of the Cartesian active rotation matrix with the column component matrix of $\mathbf{A}$. The left-handed active rotation matrix is deduced from that of right-handed active rotation by changing the sign of its rotation angle:

$$\begin{aligned} \begin{pmatrix} a'_x \\ a'_y \\ a'_z \end{pmatrix} &= \begin{pmatrix} \cos \frac{\pi}{2} & \sin \frac{\pi}{2} & 0 \\ -\sin \frac{\pi}{2} & \cos \frac{\pi}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} a_x \\ a_y \\ a_z \end{pmatrix} \\ &= \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} a_x \\ a_y \\ a_z \end{pmatrix} = \begin{pmatrix} a_y \\ -a_x \\ a_z \end{pmatrix}. \end{aligned} \quad (243)$$

As we left-hand rotate vector $\mathbf{A}$, we are studying $R_P^{\text{fixed}}(\gamma, \beta, \alpha) | \Psi \rangle$. The rotation operator is $R_P^{\text{fixed}}(\gamma = 0,$

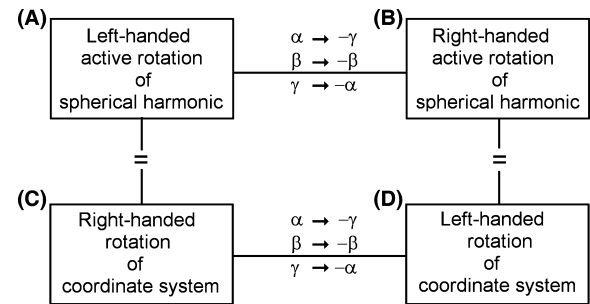


FIGURE 28 Relations between rotations of spherical harmonic and those of coordinate system: (A) left-handed active rotation of spherical harmonic is described by Eq. (239); (B) right-handed active rotation of spherical harmonic is described by Eq. (193); (C) right-handed rotation of coordinate system is described by Eq. (226); (D) left-handed rotation of coordinate system is described by Eq. (209)

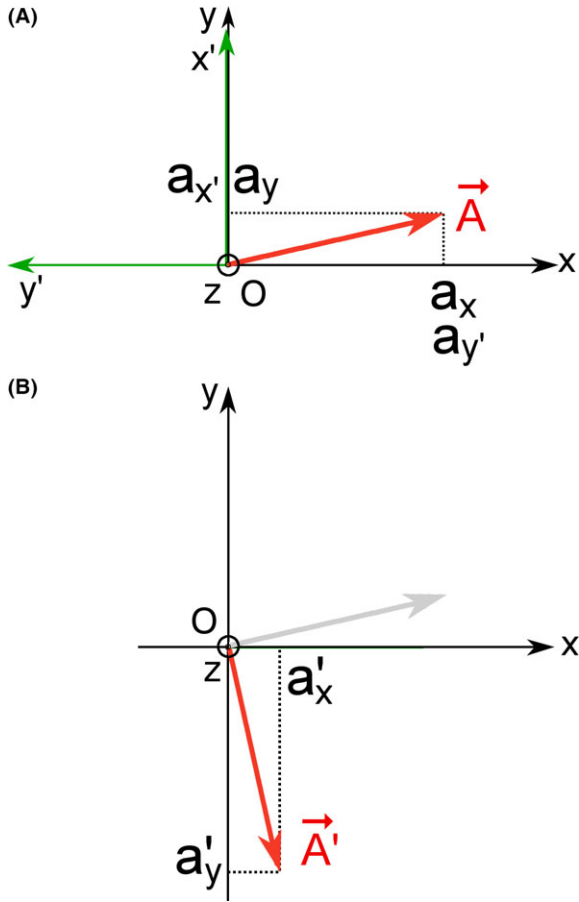


FIGURE 29 (A) Right-handed rotation of coordinate system from (O, x, y, z) to (O, x', y', z) about the z -axis by Euler angles $\alpha=\pi/2$ and $\beta=\gamma=0$ associated with fixed vector $\vec{A}$ is equivalent to (B) left-handed active rotation of vector from $\vec{A}$ to $\vec{A}'$ about the z -axis by Euler angles $\alpha=\pi/2$ and $\beta=\gamma=0$ in a single coordinate system (O, x, y, z)

$\beta = 0, \alpha = \frac{\pi}{2}$). In our case, $\mathbf{D}^{(1,P)}(\gamma, \beta, \alpha)$ defined in Eq. (124) becomes

$$\mathbf{D}^{(1,P)}(\gamma = 0, \beta = 0, \alpha = \frac{\pi}{2}) = \begin{pmatrix} +i & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -i \end{pmatrix}. \quad (244)$$

Numerical application of Eq. (242) is

$$\begin{pmatrix} -\frac{a'_x + ia'_y}{\sqrt{2}} \\ a'_z \\ \frac{a'_x - ia'_y}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} -i & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & +i \end{pmatrix} \begin{pmatrix} -\frac{a_x + ia_y}{\sqrt{2}} \\ a_z \\ \frac{a_x - ia_y}{\sqrt{2}} \end{pmatrix}. \quad (245)$$

It results that

$$a'_x = a_y, a'_y = -a_x, a'_z = a_z, \quad (246)$$

in agreement with the direct Cartesian rotation in Eq. (243). The coordinates of the left-hand actively rotated vector $\vec{A}'$ in the fixed coordinate system are identical to

those in Eq. (234) of Example IX.3 concerning the right-handed rotation of coordinate system keeping the vector $\vec{A}$ fixed. These two examples are equivalent.

9.10 | Rotation of spherical tensor

Any classical tensor can be decomposed into irreducible parts, each of which transforms under a rotation of the coordinate system in the same way as does one of the spherical harmonics. Two definitions of spherical tensor components for rank $r=0$ to 2 in terms of the nine Cartesian tensor components are used^{86,87,119} in the literature. We previously proved¹ that only that provided by Cook and De Lucia¹¹⁹ is used in NMR.

Similarly to Cartesian vectors and tensors, one can define the contravariant and covariant components of a spherical tensor. Again, one need not worry about this terminology, since the angular momentum algebra in most of the literature is based on the covariant components, but without explicit reference to their covariant nature.¹²⁰

Among the four types of rotation (right- and left-handed active rotations of spherical harmonics, and right- and left-handed rotations of coordinate system), we previously show that knowing one of them allows us to deduce the other three types. Therefore, we restrict the presentation of spherical tensor to right-handed active and passive rotations.

A spherical tensor of rank k is defined by a set of $2k + 1$ space functions transforming under coordinate rotations according to

$$R_A^{\text{fixed}}(\alpha, \beta, \gamma) T_{kq}(\mathbf{r}) = \sum_{q'} T_{kq'}(\mathbf{r}) D_{q'q}^{(k,A)}(\alpha, \beta, \gamma), \quad (247)$$

and⁵⁸

$$R_P^{\text{fixed}}(\gamma, \beta, \alpha) T_{kq}(\mathbf{r}''') = \sum_{q'} T_{kq'}(\mathbf{r}''') D_{q'q}^{(k,P)}(\gamma, \beta, \alpha). \quad (248)$$

Note that the same actively rotated position vector $\mathbf{r}$ in the fixed coordinate system appears on both sides of Eq. (247). The same passively rotated position vector $\mathbf{r}'''$ appears on both sides of Eq. (248).

9.10.1 | Right-handed active rotation of spherical tensor in one coordinate system

Now, we provide the transformation rules for Euler angles defined with rotated coordinate systems, α being the first Euler angle. The right-handed active rotation of spherical harmonics of rank $\ell=1$ are already defined in Eqs. (67) and (193). They are gathered below in extended notation:

$$\begin{aligned}
& ((Y''')_{11}(\mathbf{r}) \quad (Y''')_{10}(\mathbf{r}) \quad (Y''')_{1-1}(\mathbf{r})) \\
& \stackrel{1}{=} R_A^{\text{fixed}}(\Omega_1)(Y_{11}(\mathbf{r}) \quad Y_{10}(\mathbf{r}) \quad Y_{1-1}(\mathbf{r})) \\
& \stackrel{2}{=} (Y_{11}(\mathbf{r}_1) \quad Y_{10}(\mathbf{r}_1) \quad Y_{1-1}(\mathbf{r}_1)) \\
& \stackrel{3}{=} (Y_{11}\{\mathbf{P}(\Omega_2)\mathbf{r}\} \quad Y_{10}\{\mathbf{P}(\Omega_2)\mathbf{r}\} \quad Y_{1-1}\{\mathbf{P}(\Omega_2)\mathbf{r}\}) \\
& \stackrel{5}{=} (Y_{11}(\mathbf{r}) \quad Y_{10}(\mathbf{r}) \quad Y_{1-1}(\mathbf{r}))\mathbf{D}^{(1,A)}(\Omega_1), \\
& \text{with } \Omega_1 \equiv (\alpha, \beta, \gamma), \Omega_2 \equiv (\gamma, \beta, \alpha), \text{ and } \mathbf{P} \equiv \mathbf{P}_{\text{rotatedZ3Y2Z1}}.
\end{aligned} \quad (249)$$

The first line in Eq. (249) is a row matrix containing actively rotated spherical harmonics $(Y''')_{1m}$ with components of actively rotated position vector $\mathbf{r}$. The other lines contain initial spherical harmonics Y_{1m} with components of actively rotated position vector $\mathbf{r}$ in equalities ($\stackrel{1}{=}$, $\stackrel{3}{=}$, and $\stackrel{5}{=}$) or components of initial position vector $\mathbf{r}_1$ in equality ($\stackrel{2}{=}$).

The right-handed active rotations of spherical tensor T_{kq} written in compact notations are

$$\begin{aligned}
T'_{kq}(\mathbf{r}) & \stackrel{1}{=} R_A^{\text{fixed}}(\alpha, \beta, \gamma)T_{kq}(\mathbf{r}) \stackrel{2}{=} T_{kq}(\mathbf{r}_1) \\
& \stackrel{5}{=} \sum_{q'} T_{kq'}(\mathbf{r})D_{q'q}^{(k,A)}(\alpha, \beta, \gamma).
\end{aligned} \quad (250)$$

9.10.2 | Canonical transformation

The canonical transformations of spherical harmonics of rank $\ell=1$ are already defined in Eqs. (68) and (221). They are gathered below in extended notation:

$$\begin{aligned}
& ((Y''')_{11}(\mathbf{r}) \quad (Y''')_{10}(\mathbf{r}) \quad (Y''')_{1-1}(\mathbf{r})) \\
& \stackrel{1}{=} R_A^{\text{fixed}}(\Omega_1)(Y_{11}(\mathbf{r}) \quad Y_{10}(\mathbf{r}) \quad Y_{1-1}(\mathbf{r})) \\
& \stackrel{4}{=} (Y_{11}(\mathbf{r}') \quad Y_{10}(\mathbf{r}') \quad Y_{1-1}(\mathbf{r}')) \\
& \stackrel{3}{=} (Y_{11}\{\mathbf{P}(\Omega_2)\mathbf{r}\} \quad Y_{10}\{\mathbf{P}(\Omega_2)\mathbf{r}\} \quad Y_{1-1}\{\mathbf{P}(\Omega_2)\mathbf{r}\}) \\
& \stackrel{5}{=} (Y_{11}(\mathbf{r}) \quad Y_{10}(\mathbf{r}) \quad Y_{1-1}(\mathbf{r}))\mathbf{D}^{(1,A)}(\Omega_1), \\
& \text{with } \Omega_1 \equiv (\alpha, \beta, \gamma), \Omega_2 \equiv (\gamma, \beta, \alpha), \text{ and } \mathbf{P} \equiv \mathbf{P}_{\text{rotatedZ3Y2Z1}}.
\end{aligned} \quad (251)$$

The first line in Eq. (251) is a row matrix containing actively rotated spherical harmonics $(Y''')_{1m}$ with components of rotated position vector $\mathbf{r}$ in the fixed coordinate system. The other lines contain initial spherical harmonics Y_{1m} with components of rotated position vector $\mathbf{r}$ in the fixed coordinate system in equalities ($\stackrel{1}{=}$, $\stackrel{3}{=}$, and $\stackrel{5}{=}$) or the components of the position vector $\mathbf{r}'$ in the body-attached coordinate system in equality ($\stackrel{4}{=}$). The components of position vector $\mathbf{r}'$ in the body-attached coordinate system are identical to those of the position vector $\mathbf{r}_1$ in the fixed coordinate system before rotation.

The canonical transformations of spherical tensor T_{kq} written in compact notations^{9,11} are

$$\begin{aligned}
T'_{kq}(\mathbf{r}) & \stackrel{1}{=} R_A^{\text{fixed}}(\alpha, \beta, \gamma)T_{kq}(\mathbf{r}) \stackrel{4}{=} T_{kq}(\mathbf{r}') \\
& \stackrel{5}{=} \sum_{q'} T_{kq'}(\mathbf{r})D_{q'q}^{(k,A)}(\alpha, \beta, \gamma).
\end{aligned} \quad (252)$$

With angle-axis of rotation parameter, Eq. (252) becomes⁵⁵

$$T'_{kq}(\mathbf{r}) \stackrel{1}{=} R_A^{\text{fixed}}(\theta, \mathbf{n})T_{kq}(\mathbf{r}) \stackrel{4}{=} T_{kq}(\mathbf{r}') \stackrel{5}{=} \sum_{q'} T_{kq'}(\mathbf{r})D_{q'q}^{(k,A)}(\theta, \mathbf{n}). \quad (253)$$

9.10.3 | Right-handed rotation of coordinate system

The right-handed passive rotation of spherical harmonics of rank $\ell=1$ are already defined in Eqs. (96) and (226). They are gathered below in extended notation:

$$\begin{aligned}
& ((Y''')_{11}(\mathbf{r}''') \quad (Y''')_{10}(\mathbf{r}''') \quad (Y''')_{1-1}(\mathbf{r}''')) \\
& \stackrel{1}{=} R_P^{\text{fixed}}(\Omega_2)(Y_{11}(\mathbf{r}''') \quad Y_{10}(\mathbf{r}''') \quad Y_{1-1}(\mathbf{r}''')) \\
& \stackrel{2}{=} (Y_{11}(\mathbf{r}) \quad Y_{10}(\mathbf{r}) \quad Y_{1-1}(\mathbf{r})) \\
& \stackrel{3}{=} (Y_{11}\{\mathbf{A}(\Omega_1)\mathbf{r}'''\} \quad Y_{10}\{\mathbf{A}(\Omega_1)\mathbf{r}'''\} \quad Y_{1-1}\{\mathbf{A}(\Omega_1)\mathbf{r}'''\}) \\
& \stackrel{5}{=} (Y_{11}(\mathbf{r}''') \quad Y_{10}(\mathbf{r}''') \quad Y_{1-1}(\mathbf{r}'''))\mathbf{D}^{(1,P)}(\Omega_2), \\
& \text{with } \Omega_1 \equiv (\alpha, \beta, \gamma), \Omega_2 \equiv (\gamma, \beta, \alpha), \text{ and } \mathbf{A} \equiv \mathbf{A}_{\text{rotatedZ1Y2Z3}}.
\end{aligned} \quad (254)$$

The first line in Eq. (254) is a row matrix containing passively rotated spherical harmonics $(Y''')_{1m}$ with components of passively rotated position vector $\mathbf{r}'''$ in the rotated coordinate system. The other lines contain initial spherical harmonics Y_{1m} with components of passively rotated $\mathbf{r}'''$ in equalities ($\stackrel{1}{=}$, $\stackrel{3}{=}$, and $\stackrel{5}{=}$) or components of the position vector $\mathbf{r}$ in the fixed coordinate system in equality ($\stackrel{2}{=}$).

The right-handed passive rotations of spherical tensor T_{kq} written in compact notations^{79,97} are

$$\begin{aligned}
T'''_{kq}(\mathbf{r}''') & \stackrel{1}{=} R_P^{\text{fixed}}(\gamma, \beta, \alpha)T_{kq}(\mathbf{r}''') \stackrel{2}{=} T_{kq}(\mathbf{r}) \\
& \stackrel{5}{=} \sum_{q'} T_{kq'}(\mathbf{r}''')D_{q'q}^{(k,P)}(\gamma, \beta, \alpha).
\end{aligned} \quad (255)$$

Equalities $\stackrel{2}{=}$ and $\stackrel{5}{=}$,

$$T_{kq}(\mathbf{r}) \stackrel{5}{=} \sum_{q'} T_{kq'}(\mathbf{r}''')D_{q'q}^{(k,P)}(\gamma, \beta, \alpha), \quad (256)$$

are used by Landau and Lifshitz,⁶⁵ formula (58.7) of their book, but applied to wave functions.

Equation (256) is also extensively used in NMR for second rank tensors such as the electric-field-gradient tensor $\mathbf{V}$. In Haeberlen's book,¹⁰² the position vector $\mathbf{r}$ refers to the NMR observation coordinate system (OBS), whereas the position vector $\mathbf{r}'''$ refers to the principal-axis coordinate system (PAS). Equation (256) is rewritten as

$$T_{kq}^{(\text{OBS})} \stackrel{5}{=} \sum_{q'} T_{kq'}^{(\text{PAS})} D_{q'q}^{(k,\text{P})}(\gamma, \beta, \alpha). \quad (257)$$

In other words, OBS is the fixed coordinate system in which the static magnetic field $\vec{B}_0$ is along z_{OBS} -axis, whereas PAS is the rotated coordinate system (Figure 30A). Equation (257) is used by Engelhardt and Michel.¹⁰³

In Mehring's books,^{86,121,122} the fixed coordinate system is PAS, whereas the rotated coordinate system is OBS (Figure 30B). As a result, Eq. (257) changes to

$$T_{kq}^{(\text{PAS})} = \sum_{q'} T_{kq'}^{(\text{OBS})} D_{q'q}^{(k,\text{P})}(\gamma, \beta, \alpha). \quad (258)$$

The reverse expression of that in Eq. (258) can be deduced from Eq. (230):

$$\begin{aligned} T_{kq}^{(\text{OBS})} &= \sum_{q'=-k}^{+k} \left[D_{qq'}^{(k,\text{P})}(\gamma, \beta, \alpha) \right]^* T_{kq'}^{(\text{PAS})} \\ &= \sum_{q'=-k}^{+k} T_{kq'}^{(\text{PAS})} \left[D_{qq'}^{(k,\text{P})}(\gamma, \beta, \alpha) \right]^*{}^T \\ &= \sum_{q'=-k}^{+k} T_{kq'}^{(\text{PAS})} D_{q'q}^{(k,\text{A})}(\alpha, \beta, \gamma). \end{aligned} \quad (259)$$

In the expression of Mehring (Eq. (259)) appears the Wigner active rotation matrix despite the fact we are studying passive rotation of spherical tensor. Equation (259) is also used by Spiess.⁹¹

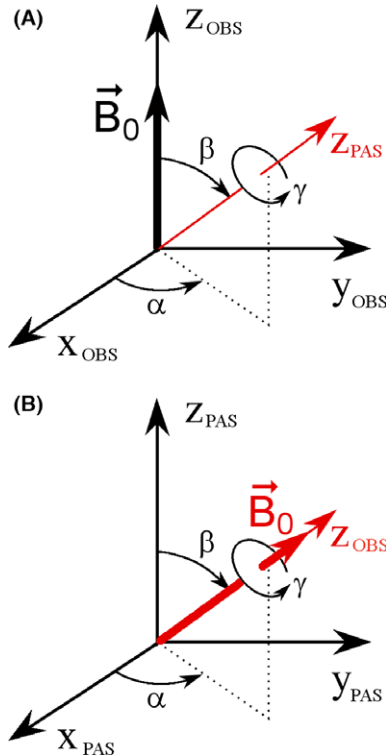


FIGURE 30 Fixed and rotated coordinate systems for (A) Haeberlen and (B) Mehring

10 | ROTATION OF VECTOR OPERATOR

In quantum mechanics, physical observables are represented by Hermitian operators. Operators corresponding to various physical quantities can be classified as scalars, vectors, and tensors. Scalar is a spherical tensor operator of rank-0. Vector operator is a spherical tensor operator of rank-1. Spin operators⁴¹ in NMR are vector operators.

Two approaches for defining an RF pulse propagator related to the convention of sense of rotation appear in NMR literature.¹¹⁰ In the right-handed, mathematically positive convention, a 90° x -pulse rotates a magnetization from the $+z$ direction into the $-y$ direction. In the left-handed convention, a 90° x -pulse rotates a magnetization from the $+z$ direction into the $+y$ direction. These propagators are:

$$P_x(t) = \exp(-i\theta I_x) \quad \text{for right-handed convention,}^{122}$$

$$P_x(t) = \exp(i\theta I_x) \quad \text{for left-handed convention.}^{110} \quad (260)$$

In the tradition of Haeberlen and others, Schmidt-Rohr and Spiess¹¹⁰ adopt the left-handed convention.

When vector operators are sandwiched by a rotation operator and its transpose, it is the operator located at the left-hand side of the vector operator that defines the Euler angles.

Rotations of vector operators and spherical tensor operators are performed about axes of a fixed coordinate system as discussed in Section 5. For simplicity, in this section, we shorten “axes of fixed coordinate system” to “fixed axes”.

In this section, we will see that:

1. in right-handed rotation, vector operator components are in row component matrix and rotation matrix is pre-multiplied by row component matrix;
2. in left-handed rotation, vector operator components are in column component matrix and rotation matrix is post-multiplied by column component matrix.

10.1 | Active rotation of vector operator

In classical system, the three Cartesian components ($v_x = v_1, v_y = v_2, v_z = v_3$) of a vector $\mathbf{v}$ in an orthonormal basis vectors transform like²⁶

$$v_i \longrightarrow \sum_{j=1}^3 [A]_{ij} v_j \quad (261)$$

under right-handed active rotation of vector $\mathbf{v}$, $\mathbf{A}$ being a 3×3 real, orthogonal matrix associated with right-handed active rotation.³ The active rotation matrix $\mathbf{A}$ is post-multiplied by the column component matrix of $\mathbf{v}$. For example, the matrix of right-handed active rotation about z -axis by angle θ is^{3,43}

$$\mathbf{A}_z(\theta) = \begin{pmatrix} \cos \theta & -\sin \theta & 0 \\ \sin \theta & \cos \theta & 0 \\ 0 & 0 & 1 \end{pmatrix}. \quad (262)$$

This definition is not universal. Other definitions are possible.⁴⁹ With orthonormal basis vectors, the contravariant Cartesian components of a vector coincide with the covariant ones.^{1,55} This is not the case for covariant spherical components of a vector expressed in orthonormal basis vectors. Usually, covariant spherical components are used in the literature, because angular momentum coupling theory is designed for use with covariant spherical tensors.⁹⁰

10.1.1 | Left-handed active rotation of vector operator

In quantum systems, the state vector $|\Psi\rangle$ transforms under an active rotation R_A to state vector $|\Psi'\rangle$ as defined in Eq. (5). Experiments that measure the operator V_i involve the matrix element $\langle\Psi_1|V_i|\Psi_2\rangle$. The matrix element of a vector operator $\mathbf{V}$ expressed with the rotated state vectors is related to that of $\mathbf{V}$ expressed with the original state vectors³⁹ as Eq. (8):

$$\langle\Psi_1|V_i|\Psi_2\rangle \xrightarrow{R_A} \langle\Psi'_1|V_i|\Psi'_2\rangle = \langle\Psi_1|(R_A)^\dagger V_i R_A|\Psi_2\rangle. \quad (263)$$

Equation (263) describes an active rotation of the physical system, keeping $\mathbf{V}$ fixed. It is reasonable to demand that the matrix element of a vector operator in quantum mechanics be transformed like a classical vector under an active rotation.²⁶ That is,^{19,43}

$$\langle\Psi'_1|V_i|\Psi'_2\rangle = \langle\Psi_1|(R_A)^\dagger V_i R_A|\Psi_2\rangle = \sum_{j=1}^3 A_{ij} \langle\Psi_1|V_j|\Psi_2\rangle. \quad (264)$$

Equation (264) relates the matrix element of a vector operator in the rotated quantum system to the matrix elements in the original quantum system via the rotation matrix $\mathbf{A}$. This relation has to be valid for any $\langle\Psi_1|$ and $|\Psi_2\rangle$. In short, a vector operator transforms^{19,20,26,43,73,123,124} according to

$$[R_A(\theta)]^\dagger V_i R_A(\theta) = \sum_{j=1}^3 [A(\theta)]_{ij} V_j. \quad (265)$$

In Eq. (265), the three components of the vector operator are gathered in a column matrix. They are also sandwiched by $[R_A(\theta)]^\dagger$ and $R_A(\theta)$. We have shown in Section 3 that this transformation is a left-handed active rotation of “vector” operator in a fixed coordinate system.

Figure 31 from Gerstein and Dybowski¹²⁵ provides a geometrical representation of the result of

$$I'_z = \exp(i\theta I_x) I_z \exp(-i\theta I_x) = I_z \cos \theta + I_y \sin \theta. \quad (266)$$

It shows a left-handed active rotation of spin operator component I_z about x -axis by a positive angle θ . Therefore, the left-handed active rotation of vector operator is symbolized by the operator

$$[R_A(\theta)]^\dagger = \exp(i\theta I_z) \quad (267)$$

at left-hand side of the vector operator in Eq. (265). Sakurai and Napolitano²⁶ discuss a similar example:

$$I'_x = \exp(i\theta I_z) I_x \exp(-i\theta I_z) = I_x \cos \theta - I_y \sin \theta \quad (268)$$

without mentioning the left-handed active rotation of I_x .

Therefore, Table 4 from Gerstein and Dybowski,¹²⁵ Haeberlen,¹⁰² and Zettili³⁹ describes the left-handed active rotations of spin operator $\mathbf{I}$. We deduce that the matrices $\mathbf{A}(\phi)$ in Table 4 and Eq. (265), which are post-multiplied by column component matrix, are left-handed active rotation matrices. They are identical to the right-handed active rotation matrices $\mathbf{A}_x(\theta)$, $\mathbf{A}_y(\theta)$, and $\mathbf{A}_z(\theta)$ derived previously.³

When Euler angles are involved in an active rotation, Eq. (265) can be generalized:

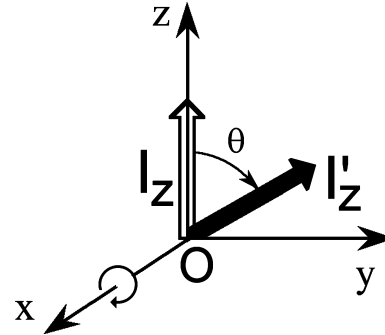


FIGURE 31 Left-handed active rotation of spin operator component I_z about x -axis by a positive angle θ

TABLE 4 Left-handed active rotation of Cartesian spin operator components, the rotation angle ϕ being positive ($\phi > 0$), deduced from Gerstein and Dybowski,¹²⁵ Haeberlen,¹⁰² and Zettili³⁹

$[R_A(\phi)]^\dagger I_i R_A(\phi)$	$\sum_{j=1}^3 [A(\phi)]_{ij} I_j$
$\exp(i\phi I_z) \begin{pmatrix} I_x \\ I_y \\ I_z \end{pmatrix} \exp(-i\phi I_z)$	$\begin{pmatrix} \cos \phi & -\sin \phi & 0 \\ \sin \phi & \cos \phi & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} I_x \\ I_y \\ I_z \end{pmatrix}$
$\exp(i\phi I_y) \begin{pmatrix} I_x \\ I_y \\ I_z \end{pmatrix} \exp(-i\phi I_y)$	$\begin{pmatrix} \cos \phi & 0 & \sin \phi \\ 0 & 1 & 0 \\ -\sin \phi & 0 & \cos \phi \end{pmatrix} \begin{pmatrix} I_x \\ I_y \\ I_z \end{pmatrix}$
$\exp(i\phi I_x) \begin{pmatrix} I_x \\ I_y \\ I_z \end{pmatrix} \exp(-i\phi I_x)$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos \phi & -\sin \phi \\ 0 & \sin \phi & \cos \phi \end{pmatrix} \begin{pmatrix} I_x \\ I_y \\ I_z \end{pmatrix}$

$$\begin{aligned}
& [R_A^{\text{fixed}}(\alpha, \beta, \gamma)]^\dagger \begin{pmatrix} V_x \\ V_y \\ V_z \end{pmatrix} R_A^{\text{fixed}}(\alpha, \beta, \gamma) \\
&= \exp(i\gamma L_z) \exp(i\beta L_y) \exp(i\alpha L_z) \begin{pmatrix} V_x \\ V_y \\ V_z \end{pmatrix} \\
&\quad \exp(-i\alpha L_z) \exp(-i\beta L_y) \exp(-i\gamma L_z) \\
&= \exp(i\gamma L_z) \exp(i\beta L_y) A_z(\alpha) \begin{pmatrix} V_x \\ V_y \\ V_z \end{pmatrix} \exp(-i\beta L_y) \exp(-i\gamma L_z) \\
&= \exp(i\gamma L_z) A_z(\alpha) A_y(\beta) \begin{pmatrix} V_x \\ V_y \\ V_z \end{pmatrix} \exp(-i\gamma L_z) \\
&= A_z(\alpha) A_y(\beta) A_z(\gamma) \begin{pmatrix} V_x \\ V_y \\ V_z \end{pmatrix} \\
&= A_{\text{fixedZ3Y2Z1}}(\alpha, \beta, \gamma) \begin{pmatrix} V_x \\ V_y \\ V_z \end{pmatrix}.
\end{aligned} \tag{269}$$

The order of the three elementary rotation matrices that define $A_{\text{fixedZ3Y2Z1}}(\alpha, \beta, \gamma)$ in Eq. (269) and that of Euler angles in the arguments of $A_{\text{fixedZ3Y2Z1}}(\alpha, \beta, \gamma)$ are due to the fact that rotation operators affect the components of vector operator. This means $A_{\text{fixedZ3Y2Z1}}(\alpha, \beta, \gamma)$ already defined for right-handed active rotation^{1,3} is also the left-handed active rotation matrix for a vector operator whose components are gathered in column matrix. The subscript Z3Y2Z1 of $A_{\text{fixedZ3Y2Z1}}(\alpha, \beta, \gamma)$ is meaningless in left-handed active rotation, because Eq. (269) shows that the first rotation angle is α located at the left-hand side among the three arguments of $A_{\text{fixedZ3Y2Z1}}(\alpha, \beta, \gamma)$. Equation (269) shows that the operator for left-handed active rotation of a vector operator about fixed axes is

$$[R_A^{\text{fixed}}(\alpha, \beta, \gamma)]^\dagger = \exp(i\gamma L_z) \exp(i\beta L_y) \exp(i\alpha L_z). \tag{270}$$

The first, second, and third left-handed active rotation angles for vector operator $\mathbf{V}$ about fixed axes are α , β , and γ , respectively.

Figure 32 provides a geometrical representation of the result of

$$\begin{aligned}
& \exp(i\gamma L_z) \exp(i\beta L_y) \exp(i\alpha L_z) I_x \exp(-i\alpha L_z) \exp(-i\beta L_y) \\
& \quad \exp(-i\gamma L_z), \alpha = \pi/4, \beta = \pi/2, \text{ and } \gamma = 0.
\end{aligned} \tag{271}$$

It describes left-handed active rotations of the spin operator component I_x about fixed axes. The first and second left-

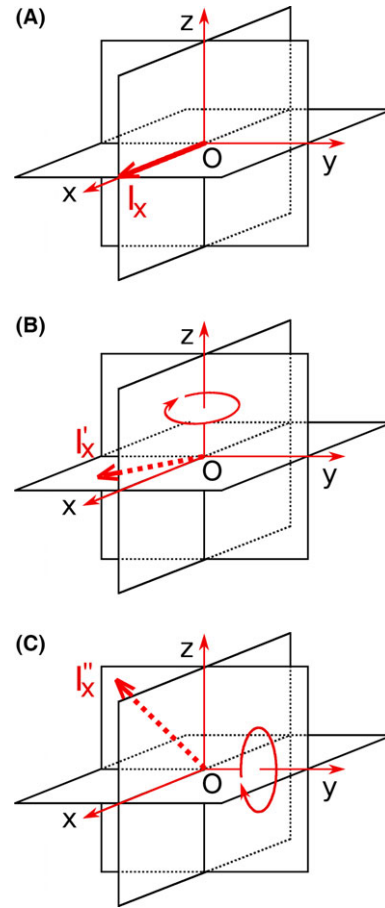


FIGURE 32 Left-handed active rotation of spin operator component I_x about fixed axes: (A) initial configuration; the first (B), and second (C) rotations are about the z -axis by angle $\alpha = \pi/4$ and about the y -axis by angle $\beta = \pi/2$, respectively

handed active rotations are about z -axis by angle $\alpha = \pi/4$ and about y -axis by angle $\beta = \pi/2$, respectively. Figure 32A shows the spin operator component I_x in the fixed coordinate system (O, x, y, z). Figure 32B shows I'_x , the left-handed active rotation of I_x about z -axis by angle $\alpha = \pi/4$. I'_x lies in the $\{x, y\}$ plane. Figure 32C shows I''_x , the left-handed active rotation of I'_x about y -axis by angle $\beta = \pi/2$. I''_x lies in the $\{y, z\}$ plane. The rotated I_x, I''_x , can be calculated using Table 4:

$$\begin{aligned}
I''_x &= \exp(i\frac{\pi}{2} I_y) \exp(i\frac{\pi}{4} I_z) I_x \exp(-i\frac{\pi}{4} I_z) \exp(-i\frac{\pi}{2} I_y) \\
&= \exp(i\frac{\pi}{2} I_y) I'_x \exp(-i\frac{\pi}{2} I_y) \\
&= \exp(i\frac{\pi}{2} I_y) \left[I_x C \frac{\pi}{4} - I_y S \frac{\pi}{4} \right] \exp(-i\frac{\pi}{2} I_y) \\
&= -I_y S \frac{\pi}{4} + I_z C \frac{\pi}{4}.
\end{aligned} \tag{272}$$

For simplicity, we replace cos and sin by C and S. The spin operator component I''_x agrees with that shown in Figure 32C.

We can also determine left-hand actively rotated spin operator component, I''_x , using the rotation matrix $A_{\text{fixedZ3Y2Z1}}(\alpha, \beta, \gamma)$ as in Eq. (269):

$$\begin{aligned} \begin{pmatrix} e^{i\frac{\pi}{2}I_y} e^{i\frac{\pi}{4}I_z} I_x e^{-i\frac{\pi}{4}I_z} e^{-i\frac{\pi}{2}I_y} \\ e^{i\frac{\pi}{2}I_y} e^{i\frac{\pi}{4}I_z} I_y e^{-i\frac{\pi}{4}I_z} e^{-i\frac{\pi}{2}I_y} \\ e^{i\frac{\pi}{2}I_y} e^{i\frac{\pi}{4}I_z} I_z e^{-i\frac{\pi}{4}I_z} e^{-i\frac{\pi}{2}I_y} \end{pmatrix} &= A_{\text{fixedZ3Y2Z1}}\left(\frac{\pi}{4}, \frac{\pi}{2}, 0\right) \begin{pmatrix} I_x \\ I_y \\ I_z \end{pmatrix} \\ &= \begin{pmatrix} 0 & -S\frac{\pi}{4} & C\frac{\pi}{4} \\ 0 & C\frac{\pi}{4} & S\frac{\pi}{4} \\ -1 & 0 & 0 \end{pmatrix} \begin{pmatrix} I_x \\ I_y \\ I_z \end{pmatrix}. \end{aligned} \quad (273)$$

We deduce that

$$I''_x = e^{i\frac{\pi}{2}I_y} e^{i\frac{\pi}{4}I_z} I_x e^{-i\frac{\pi}{4}I_z} e^{-i\frac{\pi}{2}I_y} = -I_y S\frac{\pi}{4} + I_z C\frac{\pi}{4}. \quad (274)$$

Equation (274) is identical to Eq. (272). We have at our disposal two methods for determining the left-hand rotated vector operator $\mathbf{V}'$. They are provided by

$$\begin{aligned} \begin{pmatrix} V'_x \\ V'_y \\ V'_z \end{pmatrix} &= [R_A^{\text{fixed}}(\alpha, \beta, \gamma)]^\dagger \begin{pmatrix} V_x \\ V_y \\ V_z \end{pmatrix} R_A^{\text{fixed}}(\alpha, \beta, \gamma) \\ &= A_{\text{fixedZ3Y2Z1}}(\alpha, \beta, \gamma) \begin{pmatrix} V_x \\ V_y \\ V_z \end{pmatrix}. \end{aligned} \quad (275)$$

The transformation $[R_A^{\text{fixed}}(\alpha, \beta, \gamma)]^\dagger (V_x \ V_y \ V_z)^T R_A^{\text{fixed}}(\alpha, \beta, \gamma)$ describes the left-handed active rotation about fixed axes for a vector operator $\mathbf{V}$ expressed with Cartesian components. $A_{\text{fixedZ3Y2Z1}}(\alpha, \beta, \gamma)$ is the corresponding left-handed active rotation matrix. The first rotation angle is α . Covariant spherical components (V_{+1} , V_0 , V_{-1}) and Cartesian components (V_x , V_y , V_z) are related:

$$V_{+1} = -\frac{1}{\sqrt{2}}(V_x + iV_y), \quad V_0 = V_z, \quad V_{-1} = \frac{1}{\sqrt{2}}(V_x - iV_y). \quad (276)$$

In contrast, Wigner¹⁰⁰ uses the contravariant spherical components. Table 4 allows us to determine the transformation law for covariant spherical components of vector operator.¹⁰²

$$\begin{aligned} \exp(i\phi L_x) \begin{pmatrix} V_{+1} \\ V_0 \\ V_{-1} \end{pmatrix} \exp(-i\phi L_x) \\ = \begin{pmatrix} C^2\frac{\phi}{2} & \frac{iS\phi}{\sqrt{2}} & -S^2\frac{\phi}{2} \\ \frac{iS\phi}{\sqrt{2}} & C\phi & \frac{iS\phi}{\sqrt{2}} \\ -S^2\frac{\phi}{2} & \frac{iS\phi}{\sqrt{2}} & C^2\frac{\phi}{2} \end{pmatrix} \begin{pmatrix} V_{+1} \\ V_0 \\ V_{-1} \end{pmatrix} \end{aligned}$$

$$= [\mathbf{D}^{(1,A)}(-\frac{\pi}{2}, \phi, \frac{\pi}{2})]^* \begin{pmatrix} V_{+1} \\ V_0 \\ V_{-1} \end{pmatrix}, \quad (277)$$

$$\begin{aligned} \exp(i\phi L_y) \begin{pmatrix} V_{+1} \\ V_0 \\ V_{-1} \end{pmatrix} \exp(-i\phi L_y) &= \begin{pmatrix} C^2\frac{\phi}{2} & \frac{-S\phi}{\sqrt{2}} & S^2\frac{\phi}{2} \\ \frac{S\phi}{\sqrt{2}} & C\phi & \frac{-S\phi}{\sqrt{2}} \\ S^2\frac{\phi}{2} & \frac{S\phi}{\sqrt{2}} & C^2\frac{\phi}{2} \end{pmatrix} \begin{pmatrix} V_{+1} \\ V_0 \\ V_{-1} \end{pmatrix} \\ &= \mathbf{D}^{(1,A)}(0, \phi, 0) \begin{pmatrix} V_{+1} \\ V_0 \\ V_{-1} \end{pmatrix}, \end{aligned}$$

$$\begin{aligned} \exp(i\phi L_z) \begin{pmatrix} V_{+1} \\ V_0 \\ V_{-1} \end{pmatrix} \exp(-i\phi L_z) &= \begin{pmatrix} e^{i\phi} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & e^{-i\phi} \end{pmatrix} \begin{pmatrix} V_{+1} \\ V_0 \\ V_{-1} \end{pmatrix} \\ &= [\mathbf{D}^{(1,A)}(0, 0, \phi)]^* \begin{pmatrix} V_{+1} \\ V_0 \\ V_{-1} \end{pmatrix}. \end{aligned}$$

The 3X3 Wigner active rotation matrix $\mathbf{D}^{(1,A)}(\alpha, \beta, \gamma)$ defined in Eq. (116) is for right-handed active rotation. Equation (277) can be generalized to Euler angles:^{26,73}

$$\begin{aligned} [R_A^{\text{fixed}}(\alpha, \beta, \gamma)]^\dagger \begin{pmatrix} V_{+1} \\ V_0 \\ V_{-1} \end{pmatrix} R_A^{\text{fixed}}(\alpha, \beta, \gamma) \\ = \exp(i\gamma L_z) \exp(i\beta L_y) \exp(i\alpha L_z) \begin{pmatrix} V_{+1} \\ V_0 \\ V_{-1} \end{pmatrix} \\ \exp(-i\alpha L_z) \exp(-i\beta L_y) \exp(-i\gamma L_z) \\ = \exp(i\gamma L_z) \exp(i\beta L_y) \begin{pmatrix} e^{i\alpha} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & e^{-i\alpha} \end{pmatrix} \begin{pmatrix} V_{+1} \\ V_0 \\ V_{-1} \end{pmatrix} \\ \exp(-i\beta L_y) \exp(-i\gamma L_z) \end{aligned} \quad (278)$$

$$\begin{aligned} = \exp(i\gamma L_z) \begin{pmatrix} e^{i\alpha} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & e^{-i\alpha} \end{pmatrix} \begin{pmatrix} C^2\frac{\beta}{2} & \frac{-S\beta}{\sqrt{2}} & S^2\frac{\beta}{2} \\ \frac{S\beta}{\sqrt{2}} & C\beta & \frac{-S\beta}{\sqrt{2}} \\ S^2\frac{\beta}{2} & \frac{S\beta}{\sqrt{2}} & C^2\frac{\beta}{2} \end{pmatrix} \begin{pmatrix} V_{+1} \\ V_0 \\ V_{-1} \end{pmatrix} \\ \exp(-i\gamma L_z) \\ = \begin{pmatrix} e^{i\alpha} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & e^{-i\alpha} \end{pmatrix} \begin{pmatrix} C^2\frac{\beta}{2} & \frac{-S\beta}{\sqrt{2}} & S^2\frac{\beta}{2} \\ \frac{S\beta}{\sqrt{2}} & C\beta & \frac{-S\beta}{\sqrt{2}} \\ S^2\frac{\beta}{2} & \frac{S\beta}{\sqrt{2}} & C^2\frac{\beta}{2} \end{pmatrix} \begin{pmatrix} e^{i\gamma} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & e^{-i\gamma} \end{pmatrix} \begin{pmatrix} V_{+1} \\ V_0 \\ V_{-1} \end{pmatrix} \end{aligned}$$

$$= [\mathbf{D}^{(1,A)}(\alpha, \beta, \gamma)]^* \begin{pmatrix} V_{+1} \\ V_0 \\ V_{-1} \end{pmatrix}$$

The order of the three elementary Wigner rotation matrices that define $[\mathbf{D}^{(1,A)}(\alpha, \beta, \gamma)]^*$ in Eq. (278) and that of Euler angles in the arguments of $[\mathbf{D}^{(1,A)}(\alpha, \beta, \gamma)]^*$ are due to the fact that rotation operators affect covariant spherical components of vector operator. The first rotation angle is α located at the left-hand side among the three arguments of $[\mathbf{D}^{(1,A)}(\alpha, \beta, \gamma)]^*$. When covariant spherical components are used for left-handed active rotation of vector operator as in Eq. (278), the complex conjugate $[\mathbf{D}^{(1,A)}(\alpha, \beta, \gamma)]^*$ of the Wigner active rotation matrix is post-multiplied by the column matrix of these components. In contrast, when Cartesian components are used as in Eq. (269), the active rotation matrix $\mathbf{A}_{\text{fixedZ3Y2Z1}}(\alpha, \beta, \gamma)$ is post-multiplied by the column matrix of these components.

Consider the same example about the rotation defined in Eq. (271) but with covariant spherical components of spin operator. The covariant spherical spin operator components I_{+1} , I_0 , and I_{-1} are defined similarly as those of vector operator in Eq. (276). We apply Eq. (278):

$$\begin{pmatrix} e^{i\frac{\pi}{2}I_y} e^{i\frac{\pi}{4}I_z} I_{+1} e^{-i\frac{\pi}{4}I_z} e^{-i\frac{\pi}{2}I_y} \\ e^{i\frac{\pi}{2}I_y} e^{i\frac{\pi}{4}I_z} I_z e^{-i\frac{\pi}{4}I_z} e^{-i\frac{\pi}{2}I_y} \\ e^{i\frac{\pi}{2}I_y} e^{i\frac{\pi}{4}I_z} I_{-1} e^{-i\frac{\pi}{4}I_z} e^{-i\frac{\pi}{2}I_y} \end{pmatrix} = [\mathbf{D}^{(1,A)}(\frac{\pi}{4}, \frac{\pi}{2}, 0)]^* \begin{pmatrix} I_{+1} \\ I_z \\ I_{-1} \end{pmatrix} \\ = \begin{pmatrix} \frac{e^{i\frac{\pi}{4}}}{2} & \frac{-e^{i\frac{\pi}{4}}}{\sqrt{2}} & \frac{e^{i\frac{\pi}{4}}}{2} \\ \frac{1}{\sqrt{2}} & 0 & \frac{-1}{\sqrt{2}} \\ \frac{e^{-i\frac{\pi}{4}}}{2} & \frac{e^{-i\frac{\pi}{4}}}{\sqrt{2}} & \frac{e^{-i\frac{\pi}{4}}}{2} \end{pmatrix} \begin{pmatrix} I_{+1} \\ I_z \\ I_{-1} \end{pmatrix}. \quad (279)$$

We deduce that

$$I_z'' = e^{i\frac{\pi}{2}I_y} e^{i\frac{\pi}{4}I_z} I_z e^{-i\frac{\pi}{4}I_z} e^{-i\frac{\pi}{2}I_y} = -I_x, \\ I_x'' + iI_y'' = e^{i\frac{\pi}{2}I_y} e^{i\frac{\pi}{4}I_z} (I_x + iI_y) e^{-i\frac{\pi}{4}I_z} e^{-i\frac{\pi}{2}I_y} \\ = -I_y S \frac{\pi}{4} + I_z C \frac{\pi}{4} + i(I_y C \frac{\pi}{4} + I_z S \frac{\pi}{4}). \quad (280)$$

The relations of Eq. (280) agree with those in Eq. (273). In other words, we have at our disposal a third method for determining the left-hand rotated vector operator using the complex conjugate of Wigner active rotation matrix. The transformation $[\mathbf{R}_A^{\text{fixed}}(\alpha, \beta, \gamma)]^\dagger (V_{+1} \ V_0 \ V_{-1})^T \mathbf{R}_A^{\text{fixed}}(\alpha, \beta, \gamma)$ describes the left-handed active rotation about fixed axes for a vector operator $\mathbf{V}$ expressed with covariant spherical components. The superscript T means transposition. As the Wigner active rotation matrix $\mathbf{D}^{(1,A)}(\alpha, \beta, \gamma)$ is

derived for right-handed rotation, it is its complex conjugate that is involved in left-handed active rotation.⁷³

10.1.2 | Right-handed active rotation of vector operator

We do not develop this case in details but leave it to the reader as an exercise. First, change the sign of rotation angle θ in Eq. (265):^{34,37,43,47,56,71,93,123,126}

$$R_A(\theta) V_i [R_A(\theta)]^\dagger = \sum_{j=1}^3 V_j [A(\theta)]_{ji}. \quad (281)$$

The three Cartesian components of vector operator are gathered in a row matrix. They are also sandwiched by $R_A(\theta)$ and $[R_A(\theta)]^\dagger$. The unconventional summation facilitates comparison with formulas for spherical tensors. We have shown in Section 3 that this transformation is a right-handed active rotation of “vector” operator in a fixed coordinate system. Figure 33 shows a right-handed active rotation of spin operator component I_z about x -axis by a positive angle θ .¹²⁷

$$I_z' = \exp(-i\theta I_x) I_z \exp(i\theta I_x) = I_z \cos \theta - I_y \sin \theta. \quad (282)$$

Therefore, the right-handed active rotation of vector operator is symbolized by the operator

$$R_A(\theta) = \exp(-i\theta I_x), \quad (283)$$

at left-hand side of the vector operator in Eq. (281). Then, deduce Table 5 from Table 4 by changing the sign of the rotation angle ϕ . The active rotation matrix $A(\theta)$ has two meanings in rotation of vector operator: It is a left-handed rotation matrix when it is post-multiplied by a column component matrix. It is a right-handed rotation matrix when it is pre-multiplied by a row component matrix. When Euler angles are involved in an active rotation, Eq. (281) can be generalized:

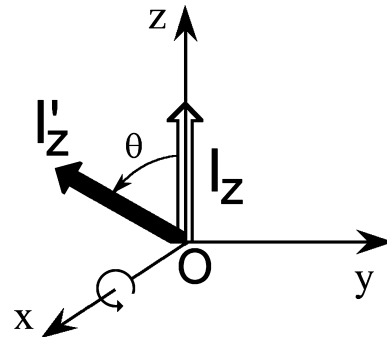


FIGURE 33 Right-handed active rotation of spin operator component I_z about x -axis by a positive angle θ

TABLE 5 Right-handed active rotation of Cartesian spin operator components, the rotation angle ϕ being positive ($\phi > 0$), deduced from Mehring and Weberuss,^{86,121,122} Günther and co-workers,¹⁴⁶ Duer,¹⁴⁷ Kimmich,⁷ Slichter,¹⁴⁴ Schmidt-Rohr and Spiess,¹¹⁰ and Siemens and co-workers⁶⁶

$R_A(\phi)I_i[R_A(\phi)]^\dagger$	$\sum_{j=1}^3 I_j[A(\phi)]_{ji}$
$\exp(-i\phi I_z)(I_x \ I_y \ I_z)$ $\exp(i\phi I_z)$	$(I_x \ I_y \ I_z) \begin{pmatrix} \cos \phi & -\sin \phi & 0 \\ \sin \phi & \cos \phi & 0 \\ 0 & 0 & 1 \end{pmatrix}$
$\exp(-i\phi I_y)(I_x \ I_y \ I_z)$ $\exp(i\phi I_y)$	$(I_x \ I_y \ I_z) \begin{pmatrix} \cos \phi & 0 & \sin \phi \\ 0 & 1 & 0 \\ -\sin \phi & 0 & \cos \phi \end{pmatrix}$
$\exp(-i\phi I_x)(I_x \ I_y \ I_z)$ $\exp(i\phi I_x)$	$(I_x \ I_y \ I_z) \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos \phi & -\sin \phi \\ 0 & \sin \phi & \cos \phi \end{pmatrix}$

$$\begin{aligned} R_A^{\text{fixed}}(\alpha, \beta, \gamma)(V_x \ V_y \ V_z)[R_A^{\text{fixed}}(\alpha, \beta, \gamma)]^\dagger \\ = (V_x \ V_y \ V_z)A_z(\alpha)A_y(\beta)A_z(\gamma) \\ = (V_x \ V_y \ V_z)A_{\text{fixedZ3Y2Z1}}(\alpha, \beta, \gamma). \end{aligned} \quad (284)$$

$A_{\text{fixedZ3Y2Z1}}(\alpha, \beta, \gamma)$ in Eq. (284) is identical to that defined in Eq. (269). Therefore, it also has two meanings: It is a left-handed active rotation matrix when it is post-multiplied by a column component matrix as in Eq. (269). It is a right-handed active rotation matrix when it is pre-multiplied by a row component matrix as in Eq. (284). The latter shows that the first rotation angle is γ located at the right-hand side among the three arguments of $A_{\text{fixedZ3Y2Z1}}(\alpha, \beta, \gamma)$. Equation (284) shows that the operator for right-handed active rotation of a vector operator about fixed axes is

$$R_A^{\text{fixed}}(\alpha, \beta, \gamma) = \exp(-i\alpha L_z) \exp(-i\beta L_y) \exp(-i\gamma L_x). \quad (285)$$

Similar to the active rotations of space function and spherical harmonics about fixed axes, the first, second, and third right-handed active rotation angles for vector operator $\mathbf{V}$ about fixed axes are γ , β , and α , respectively. The operators for right-handed (Eq. (285)) and left-handed (Eq. (270)) active rotations of a vector operator about fixed axes are Hermitian conjugated.

Table 5 allows us to determine the transformation law¹²⁶ for covariant spherical components of vector operator defined in Eq. (276):^{43,128}

$$\begin{aligned} R_A^{\text{fixed}}(\alpha, \beta, \gamma)(V_{+1} \ V_0 \ V_{-1})[R_A^{\text{fixed}}(\alpha, \beta, \gamma)]^\dagger \\ = (V_{+1} \ V_0 \ V_{-1})\mathbf{D}^{(1,A)}(\alpha, \beta, \gamma). \end{aligned} \quad (286)$$

The first rotation angle is γ located at the right-hand side among the three arguments of $\mathbf{D}^{(1,A)}(\alpha, \beta, \gamma)$. Figure 34 provides a geometrical representation of the result of

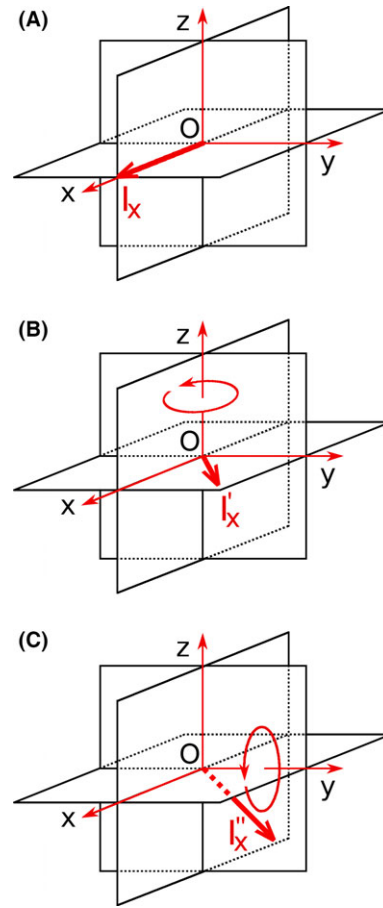


FIGURE 34 Right-handed active rotation of spin operator component I_x about fixed axes: (A) initial configuration; the first (B), and second (C) rotations are about the z -axis by angle $\gamma = \pi/4$ and about the y -axis by angle $\beta = \pi/2$, respectively

$$\begin{aligned} \exp(-i\alpha L_z) \exp(-i\beta L_y) \exp(-i\gamma L_x) I_x \exp(i\gamma L_x) \\ \exp(i\beta L_y) \exp(i\alpha L_z), \alpha = 0, \beta = \pi/2, \text{ and } \gamma = \pi/4. \end{aligned} \quad (287)$$

It describes right-handed active rotations of the spin operator component I_x about fixed axes. The first and second right-handed active rotations are about z -axis by angle $\gamma = \pi/4$ and about y -axis by angle $\beta = \pi/2$, respectively. I''_x lies in the $\{y, z\}$ plane. We have at our disposal three methods for determining the right-hand rotated vector operator:

$$I''_x = I_y S \frac{\pi}{4} - I_z C \frac{\pi}{4}. \quad (288)$$

1. rotation operator in Table 5;
2. rotation matrix $A_{\text{fixedZ3Y2Z1}}(\alpha, \beta, \gamma)$ as in Eq. (284);
3. Wigner rotation matrix $\mathbf{D}^{(1,A)}(\alpha, \beta, \gamma)$ as in Eq. (286).

The spin operator component I''_x agrees with that shown in Figure 34C. These results are examples of general expressions

$$\begin{aligned}
 \begin{pmatrix} V'_x & V'_y & V'_z \end{pmatrix} &= R_A^{\text{fixed}}(\alpha, \beta, \gamma) \begin{pmatrix} V_x & V_y & V_z \end{pmatrix} [R_A^{\text{fixed}}(\alpha, \beta, \gamma)]^\dagger \\
 &= \begin{pmatrix} V_x & V_y & V_z \end{pmatrix} A_{\text{fixedZ3Y2Z1}}(\alpha, \beta, \gamma),
 \end{aligned} \tag{289}$$

and

$$\begin{aligned}
 \begin{pmatrix} V'_{+1} & V'_0 & V'_{-1} \end{pmatrix} &= R_A^{\text{fixed}}(\alpha, \beta, \gamma) \begin{pmatrix} V_{+1} & V_0 & V_{-1} \end{pmatrix} \\
 &\quad [R_A^{\text{fixed}}(\alpha, \beta, \gamma)]^\dagger \\
 &= \begin{pmatrix} V_{+1} & V_0 & V_{-1} \end{pmatrix} \mathbf{D}^{(1,A)}(\alpha, \beta, \gamma).
 \end{aligned} \tag{290}$$

The transformation $R_A^{\text{fixed}}(\alpha, \beta, \gamma) \begin{pmatrix} V_x & V_y & V_z \end{pmatrix} [R_A^{\text{fixed}}(\alpha, \beta, \gamma)]^\dagger$ describes the right-handed active rotation about fixed axes for a vector operator $\mathbf{V}$ expressed with Cartesian components. $A_{\text{fixedZ3Y2Z1}}(\alpha, \beta, \gamma)$ is the corresponding right-handed active rotation matrix. The first rotation angle is γ .

When covariant spherical components are used for right-handed active rotation of vector operator as in Eq. (286), Wigner active rotation matrix $\mathbf{D}^{(1,A)}(\alpha, \beta, \gamma)$ is pre-multiplied by the row matrix of these components.⁷¹ When Cartesian components are used as in Eq. (284), $A_{\text{fixedZ3Y2Z1}}(\alpha, \beta, \gamma)$ is also pre-multiplied by the row matrix of these components.

The transformation $R_A^{\text{fixed}}(\alpha, \beta, \gamma) \begin{pmatrix} V_{+1} & V_0 & V_{-1} \end{pmatrix} [R_A^{\text{fixed}}(\alpha, \beta, \gamma)]^\dagger$ describes the right-handed active rotation about fixed axes for a vector operator $\mathbf{V}$ expressed with covariant spherical components. Furthermore, the Wigner active rotation matrix $\mathbf{D}^{(1,A)}(\alpha, \beta, \gamma)$ is that derived with right-handed active rotation.

When Cartesian components are used, the same rotation matrix $A_{\text{fixedZ3Y2Z1}}(\alpha, \beta, \gamma)$ is either a left-handed active rotation matrix in left-handed active rotation of vector operator or a right-handed active rotation matrix in right-handed active rotation of vector operator. In contrast, when covariant spherical components are used, Wigner active rotation matrix is involved in right-handed active rotation of vector operator and its complex conjugate is involved in left-handed active rotation of vector operator. As the orders of Euler angles in the arguments of $A_{\text{fixedZ3Y2Z1}}(\alpha, \beta, \gamma)$, $[\mathbf{D}^{(1,A)}(\alpha, \beta, \gamma)]^*$, and $\mathbf{D}^{(1,A)}(\alpha, \beta, \gamma)$ are identical, the first rotation angles are α for left-handed and γ for right-handed active rotations of vector operator.

The left-hand members of Eqs. (269) and (284) show that we can deduce expressions of the right-handed active rotation of vector operator from those of left-handed case by replacing the Euler angles α, β, γ in left-handed active rotation by $-\gamma, -\beta, -\alpha$, respectively. Indeed, the replacement in the term on the final right-hand side of Eq. (269) gives

$$\begin{aligned}
 A_{\text{fixedZ3Y2Z1}}(\alpha \rightarrow -\gamma, \beta \rightarrow -\beta, \gamma \rightarrow -\alpha) \begin{pmatrix} V_x \\ V_y \\ V_z \end{pmatrix} \\
 = \mathbf{P}_{\text{fixedZ1Y2Z3}}(\gamma, \beta, \alpha) \begin{pmatrix} V_x \\ V_y \\ V_z \end{pmatrix}
 \end{aligned}$$

$$\begin{aligned}
 &= \begin{pmatrix} V_x & V_y & V_z \end{pmatrix} [\mathbf{P}_{\text{fixedZ1Y2Z3}}(\gamma, \beta, \alpha)]^T \\
 &= \begin{pmatrix} V_x & V_y & V_z \end{pmatrix} A_{\text{fixedZ3Y2Z1}}(\alpha, \beta, \gamma),
 \end{aligned} \tag{291}$$

the term on the final right-hand side of Eq. (284). Similarly, the replacement in the term on the final right-hand side of Eq. (278) gives

$$\begin{aligned}
 &[\mathbf{D}^{(1,A)}(\alpha \rightarrow -\gamma, \beta \rightarrow -\beta, \gamma \rightarrow -\alpha)]^* \begin{pmatrix} V_{+1} \\ V_0 \\ V_{-1} \end{pmatrix} \\
 &= [\mathbf{D}^{(1,P)}(\gamma, \beta, \alpha)]^* \begin{pmatrix} V_{+1} \\ V_0 \\ V_{-1} \end{pmatrix} \\
 &= \begin{pmatrix} V_{+1} & V_0 & V_{-1} \end{pmatrix} [\mathbf{D}^{(1,P)}(\gamma, \beta, \alpha)]^{*T} \\
 &= \begin{pmatrix} V_{+1} & V_0 & V_{-1} \end{pmatrix} \mathbf{D}^{(1,A)}(\alpha, \beta, \gamma),
 \end{aligned} \tag{292}$$

the term on the final right-hand side of Eq. (286).

10.2 | Rotation of coordinate system

In classical system, the three Cartesian components ($v_x = v_1, v_y = v_2, v_z = v_3$) of a vector $\mathbf{v}$ in an orthonormal basis vectors transform like

$$v_i \longrightarrow \sum_{j=1}^3 [\mathbf{P}]_{ij} v_j \tag{293}$$

under a right-handed passive rotation of vector $\mathbf{v}$ or under a right-handed rotation of coordinate system keeping vector $\mathbf{v}$ fixed, $\mathbf{P}$ being a 3X3 real, orthogonal matrix associated with a right-handed passive rotation.³ $\mathbf{P}$ is post-multiplied by the column component matrix of $\mathbf{v}$. For example, the matrix of right-handed passive rotation about z -axis by angle θ is

$$\mathbf{P}_z(\theta) = \begin{pmatrix} \cos \theta & \sin \theta & 0 \\ -\sin \theta & \cos \theta & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{294}$$

We will show that left-handed rotation of coordinate system about fixed axes keeping the vector operator fixed is equivalent to right-handed active rotation of vector operator about fixed axes. Similarly, right-handed rotation of coordinate system about fixed axes keeping the vector operator fixed is equivalent to left-handed active rotation of vector operator about fixed axes.

10.2.1 | Left-handed rotation of coordinate system

In quantum system, the state vector $|\Psi\rangle$ remains unchanged under a passive rotation R_P as defined in Eq. (10). The matrix element of a passively rotated vector operator component V'_i is related to that of the original vector operator component V_i as in Eq. (12):

$$\langle\Psi_1|V_i|\Psi_2\rangle \xrightarrow{R_P} \langle\Psi_1|V'_i|\Psi_2\rangle = \langle\Psi_1|(R_P)^\dagger V_i R_P|\Psi_2\rangle. \quad (295)$$

Equation (295) describes the rotation of the vector operator from $\mathbf{V}$ to $\mathbf{V}'$, keeping the physical system fixed. It is reasonable to demand that the matrix element of a vector operator component in quantum mechanics be transformed like a classical vector under a passive rotation:⁸⁰

$$\langle\Psi_1|V'_i|\Psi_2\rangle = \langle\Psi_1|(R_P)^\dagger V_i R_P|\Psi_2\rangle = \sum_{j=1}^3 P_{ij} \langle\Psi_1|V_j|\Psi_2\rangle. \quad (296)$$

Equation (296) relates the matrix element of a passively rotated vector operator component V'_i to those of the original vector operator components V_i . This relation has to be valid for any $\langle\Psi_1|$ and $|\Psi_2\rangle$. In short, a vector operator in passive rotation transforms according to⁸⁰

$$[R_P(\theta)]^\dagger V_i R_P(\theta) = \sum_{j=1}^3 [P(\theta)]_{ij} V_j. \quad (297)$$

As $R_P(\theta) = [R_A(\theta)]^\dagger$, we improve Eq. (297):

$$[R_P(\theta)]^\dagger V_i R_P(\theta) = R_A(\theta) V_i [R_A(\theta)]^\dagger = \sum_{j=1}^3 [P(\theta)]_{ij} V_j. \quad (298)$$

The three components of vector operator are gathered in a column matrix. They are also sandwiched by $[R_P(\theta)]^\dagger$ and $R_P(\theta)$.

Figure 35 represents the spin operator component I_z and a left-handed rotation of the coordinate system about x -axis by a positive angle θ , from (O, x, y, z) to (O, x', y', z') . This is also called a left-handed passive rotation of spin operator component I_z about x -axis by angle θ . That is, I_z remains fixed but the coordinate system is left-hand rotated. In practice, the expression of I_z in the left-hand rotated coordinate system (O, x', y', z') can be determined as a right-handed active rotation of I_z about x -axis by angle θ (Eq. (282)):

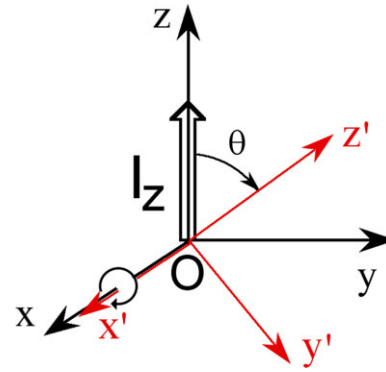


FIGURE 35 Left-handed rotation of coordinate system from (O, x, y, z) to (O, x', y', z') about x -axis by a positive angle θ , the spin operator component I_z remains fixed

$$\exp(-i\theta I_x) I_z \exp(i\theta I_x) = I_z \cos \theta - I_y \sin \theta. \quad (299)$$

Therefore, Table 6, which is deduced from Table 4 by changing the sign of rotation angle ϕ , describes left-handed passive rotations of spin operator $\mathbf{I}$. We deduce that the rotation matrices $\mathbf{P}(\phi)$ in Table 6 and Eq. (298), which are post-multiplied by column component matrix, are left-handed passive rotation matrices. They are identical to the right-handed passive rotation matrices $\mathbf{P}_x(\phi)$, $\mathbf{P}_y(\phi)$, and $\mathbf{P}_z(\phi)$ derived previously.³

In Section 5 about rotation of space function and Section 9 about rotation of spherical harmonics, the coordinate system is represented by bra position basis at the left-hand side of the rotation operators and the space function is represented by the ket state at the right-hand side of the rotation operator. The generalization of Eq. (298) to Euler angles in passive rotation is less obvious than that in active rotation because coordinate system is not explicit in Eq. (298). Fortunately, we can rely on Eq. (296) to introduce the coordinate system fictitiously as

TABLE 6 Left-handed passive rotation of Cartesian spin operator components deduced from Table 4, the rotation angle ϕ being positive ($\phi > 0$)

$[R_P(\phi)]^\dagger I_i R_P(\phi)$	$\sum_{j=1}^3 [P(\phi)]_{ij} I_j$
$\exp(-i\phi I_z) \begin{pmatrix} I_x \\ I_y \\ I_z \end{pmatrix} \exp(i\phi I_z)$	$\begin{pmatrix} \cos \phi & \sin \phi & 0 \\ -\sin \phi & \cos \phi & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} I_x \\ I_y \\ I_z \end{pmatrix}$
$\exp(-i\phi I_y) \begin{pmatrix} I_x \\ I_y \\ I_z \end{pmatrix} \exp(i\phi I_y)$	$\begin{pmatrix} \cos \phi & 0 & -\sin \phi \\ 0 & 1 & 0 \\ \sin \phi & 0 & \cos \phi \end{pmatrix} \begin{pmatrix} I_x \\ I_y \\ I_z \end{pmatrix}$
$\exp(-i\phi I_x) \begin{pmatrix} I_x \\ I_y \\ I_z \end{pmatrix} \exp(i\phi I_x)$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos \phi & \sin \phi \\ 0 & -\sin \phi & \cos \phi \end{pmatrix} \begin{pmatrix} I_x \\ I_y \\ I_z \end{pmatrix}$

$$\langle [R_P(\theta)]^\dagger V_i R_P(\theta) \rangle = (\langle [R_P(\theta)]^\dagger V_i(R_P(\theta)) \rangle). \quad (300)$$

We deduce that left-handed rotation of coordinate system is the transformation:

$$\langle [R_P(\theta)]^\dagger. \quad (301)$$

When Euler angles are involved, the left-handed rotation of coordinate system about fixed axes, keeping the vector operator fixed, is expressed by the operator $[R_P^{\text{fixed}}(\gamma, \beta, \alpha)]^\dagger$:

$$\begin{aligned} \langle [R_P^{\text{fixed}}(\gamma, \beta, \alpha)]^\dagger &= \langle [\exp(i\gamma L_z) \exp(i\beta L_y) \exp(i\alpha L_z)]^\dagger \\ &= \langle [\exp(-i\alpha L_z) \exp(-i\beta L_y) \exp(-i\gamma L_z)]. \end{aligned} \quad (302)$$

The first, second, and third left-handed rotations of coordinate system about fixed axes are about z -axis by angle α , about y -axis by angle β , and about z -axis by angle γ , respectively.

When Euler angles are involved in a rotation of coordinate system, Eq. (298) can be generalized as⁸⁰

$$\begin{aligned} [R_P^{\text{fixed}}(\gamma, \beta, \alpha)]^\dagger &\begin{pmatrix} V_x \\ V_y \\ V_z \end{pmatrix} R_P^{\text{fixed}}(\gamma, \beta, \alpha) \\ &= \exp(-i\alpha L_z) \exp(-i\beta L_y) \exp(-i\gamma L_z) \begin{pmatrix} V_x \\ V_y \\ V_z \end{pmatrix} \\ &\quad \exp(i\gamma L_z) \exp(i\beta L_y) \exp(i\alpha L_z) \\ &= \exp(-i\alpha L_z) \exp(-i\beta L_y) P_z(\gamma) \begin{pmatrix} V_x \\ V_y \\ V_z \end{pmatrix} \exp(i\beta L_y) \exp(i\alpha L_z) \\ &= \exp(-i\alpha L_z) P_z(\gamma) P_y(\beta) \begin{pmatrix} V_x \\ V_y \\ V_z \end{pmatrix} \exp(i\alpha L_z) \\ &= P_z(\gamma) P_y(\beta) P_z(\alpha) \begin{pmatrix} V_x \\ V_y \\ V_z \end{pmatrix} \\ &= P_{\text{fixedZ1Y2Z3}}(\gamma, \beta, \alpha) \begin{pmatrix} V_x \\ V_y \\ V_z \end{pmatrix}. \end{aligned} \quad (303)$$

The order of the three elementary rotation matrices that define $P_{\text{fixedZ1Y2Z3}}(\gamma, \beta, \alpha)$ in Eq. (303) and that of Euler angles in the arguments of $P_{\text{fixedZ1Y2Z3}}(\gamma, \beta, \alpha)$ are due to the fact that rotation operators affect the components of vector operator. This means $P_{\text{fixedZ1Y2Z3}}(\gamma, \beta, \alpha)$ already defined for right-handed passive rotation^{1,3} is also the left-handed passive rotation matrix for a vector operator whose components are gathered in column matrix. The

subscript Z1Y2Z3 of $P_{\text{fixedZ1Y2Z3}}(\gamma, \beta, \alpha)$ is meaningless in left-handed rotation of coordinate system because Eq. (302) shows that the first rotation angle is α located at the right-hand side among the three arguments of $P_{\text{fixedZ1Y2Z3}}(\gamma, \beta, \alpha)$.

We may replace $[R_P^{\text{fixed}}(\gamma, \beta, \alpha)]^\dagger$ by its equivalent operator $R_A^{\text{fixed}}(\alpha, \beta, \gamma)$:

$$\begin{aligned} \langle [R_P^{\text{fixed}}(\gamma, \beta, \alpha)]^\dagger &\begin{pmatrix} V_x \\ V_y \\ V_z \end{pmatrix} R_P^{\text{fixed}}(\gamma, \beta, \alpha) \\ &\equiv \langle R_A^{\text{fixed}}(\alpha, \beta, \gamma) \begin{pmatrix} V_x \\ V_y \\ V_z \end{pmatrix} [R_A^{\text{fixed}}(\alpha, \beta, \gamma)]^\dagger. \end{aligned} \quad (304)$$

That is, the first, second, and third right-handed active rotations of V_i in fixed coordinate system are about z -axis by angle γ , about y -axis by angle β , and about z -axis by angle α , respectively. It is worth noting that in Eq. (304) the vector operator components are in column matrix, whereas in Eq. (284) they are in row matrix.

As the two operators $[R_P^{\text{fixed}}(\gamma, \beta, \alpha)]^\dagger$ and $R_A^{\text{fixed}}(\alpha, \beta, \gamma)$ are equivalent, the left-hand member of Eq. (304) shows that the first rotation angle is α in left-handed rotations of coordinate system (see also Eq. (302)), whereas the right-hand member of Eq. (304) shows that it is γ in right-handed active rotations of vector operator.

Figure 36 provides a geometrical representation of the result of

$$\begin{aligned} [R_P^{\text{fixed}}(\gamma, \beta, \alpha)]^\dagger I_x R_P^{\text{fixed}}(\gamma, \beta, \alpha) \\ &\equiv R_A^{\text{fixed}}(\alpha, \beta, \gamma) I_x [R_A^{\text{fixed}}(\alpha, \beta, \gamma)]^\dagger \\ &= \exp(-i\alpha L_z) \exp(-i\beta L_y) \exp(-i\gamma L_z) I_x \exp(i\gamma L_z) \\ &\quad \exp(i\beta L_y) \exp(i\alpha L_z), \end{aligned} \quad (305)$$

$\alpha = \pi/4$, $\beta = \pi/2$, and $\gamma = 0$.

It describes left-handed rotations of coordinate system about fixed axes. The first and second left-handed rotations of coordinate system are about z -axis by angle $\alpha = \pi/4$ and about y -axis by angle $\beta = \pi/2$, respectively. It also describes right-handed active rotations of I_x about fixed axes. As $\gamma = 0$, the first and second right-handed active rotations of I_x are about y -axis by angle $\beta = \pi/2$ and about z -axis by angle $\alpha = \pi/4$, respectively.

Figure 36A shows the spin operator component I_x in the fixed coordinate system (O, x, y, z) . Figure 36B shows I_x in two coordinate systems (O, x, y, z) and (O, x'', y'', z'') . The latter is left-handed rotation of (O, x, y, z) about z -axis by angle $\alpha = \pi/4$. Figure 36C shows I_x in two coordinate systems (O, x, y, z) and (O, x''', y''', z''') . The latter is left-handed rotation of

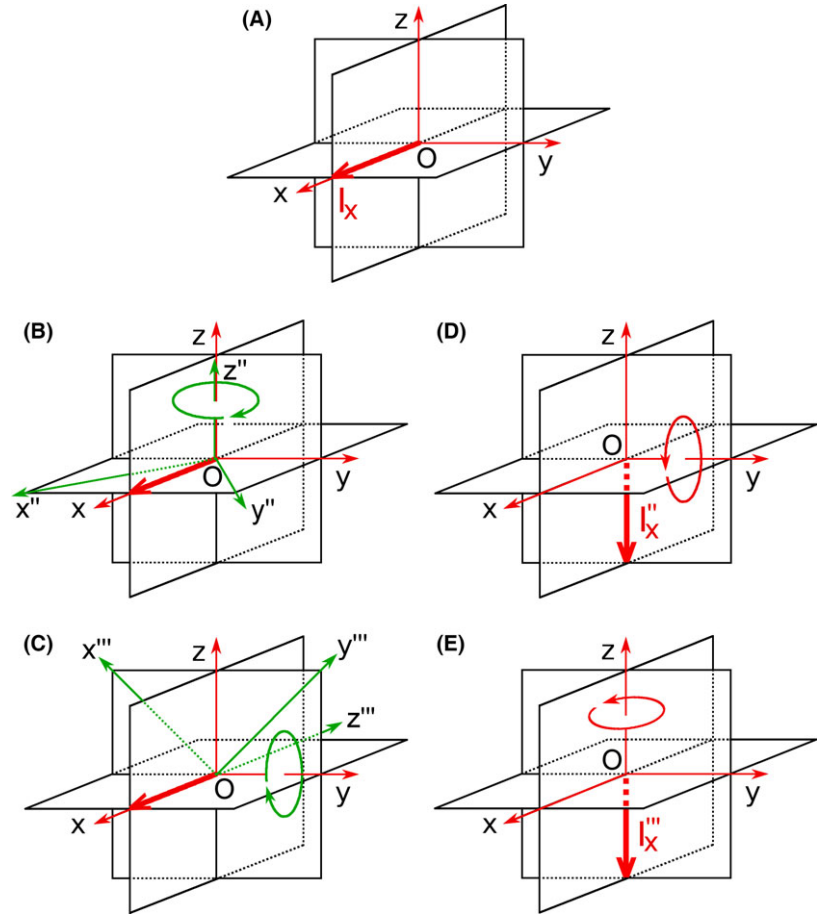


FIGURE 36 Equivalence between (A, B, C) left-handed rotations of coordinate system about fixed axes with spin operator component I_x fixed and (A, D, E) right-handed active rotations of I_x about fixed axes. (A) Initial configuration. The first (B) and second (C) left-handed rotations of the coordinate system are about z -axis by angle $\alpha = \pi/4$ and about y -axis by angle $\beta = \pi/2$, respectively. The first (D) and second (E) right-handed active rotations of I_x are about y -axis by angle $\beta = \pi/2$ and about z -axis by angle $\alpha = \pi/4$, respectively

(O, x'', y'', z'') about y -axis by angle $\beta = \pi/2$. I_x lies in the negative direction of z'' -axis. Figure 36D shows I''_x , the right-handed active rotation of I_x about y -axis by angle $\beta = \pi/2$. I''_x lies in the negative direction of z -axis. Figure 36E shows I'''_x , the right-handed active rotation of I''_x about z -axis by angle $\alpha = \pi/4$. I'''_x remains in the negative direction of z -axis. In left-handed rotation of coordinate system, I_x lies in the negative direction of z''' -axis of the rotated coordinate system (O, x''', y''', z''') , whereas in right-handed active rotation, the rotated component I'''_x lies in the negative direction of z -axis of the fixed coordinate system (O, x, y, z) .

We can determine the expression of I_x in (O, x''', y''', z''') or equivalently that of I'''_x in (O, x, y, z) using Table 6:

$$\begin{aligned} I'''_x &= \exp(-i\frac{\pi}{4}I_z) \exp(-i\frac{\pi}{2}I_y) I_x \exp(i\frac{\pi}{2}I_y) \exp(i\frac{\pi}{4}I_z) \\ &= \exp(-i\frac{\pi}{4}I_z) I''_x \exp(i\frac{\pi}{4}I_z) \\ &= \exp(-i\frac{\pi}{4}I_z) (-I_z) \exp(i\frac{\pi}{4}I_z) = -I_z. \end{aligned} \quad (306)$$

The spin operator component I'''_x agrees with that shown in Figure 36E.

We can also determine the expression of I_x in (O, x''', y''', z''') or equivalently that of I'''_x in (O, x, y, z) using the rotation matrix $P_{\text{fixedZ1Y2Z3}}(\gamma, \beta, \alpha)$ as in Eq. (303):

$$\begin{aligned} \begin{pmatrix} e^{-i\frac{\pi}{4}I_z} e^{-i\frac{\pi}{2}I_y} I_x e^{i\frac{\pi}{2}I_y} e^{i\frac{\pi}{4}I_z} \\ e^{-i\frac{\pi}{4}I_z} e^{-i\frac{\pi}{2}I_y} I_y e^{i\frac{\pi}{2}I_y} e^{i\frac{\pi}{4}I_z} \\ e^{-i\frac{\pi}{4}I_z} e^{-i\frac{\pi}{2}I_y} I_z e^{i\frac{\pi}{2}I_y} e^{i\frac{\pi}{4}I_z} \end{pmatrix} &= P_{\text{fixedZ1Y2Z3}}(0, \frac{\pi}{2}, \frac{\pi}{4}) \begin{pmatrix} I_x \\ I_y \\ I_z \end{pmatrix} \\ &= \begin{pmatrix} 0 & 0 & -1 \\ -S\frac{\pi}{4} & C\frac{\pi}{4} & 0 \\ C\frac{\pi}{4} & S\frac{\pi}{4} & 0 \end{pmatrix} \begin{pmatrix} I_x \\ I_y \\ I_z \end{pmatrix}. \end{aligned} \quad (307)$$

We deduce that

$$I'''_x = e^{-i\frac{\pi}{4}I_z} e^{-i\frac{\pi}{2}I_y} I_x e^{i\frac{\pi}{2}I_y} e^{i\frac{\pi}{4}I_z} = -I_z. \quad (308)$$

Equation (308) is identical to Eq. (306). These two results verify the relation

$$\begin{pmatrix} V'_x \\ V'_y \\ V'_z \end{pmatrix} = [R_{\text{P}}^{\text{fixed}}(\gamma, \beta, \alpha)]^\dagger \begin{pmatrix} V_x \\ V_y \\ V_z \end{pmatrix} R_{\text{P}}^{\text{fixed}}(\gamma, \beta, \alpha)$$

$$\begin{aligned}
&\equiv R_A^{\text{fixed}}(\alpha, \beta, \gamma) \begin{pmatrix} V_x \\ V_y \\ V_z \end{pmatrix} [R_A^{\text{fixed}}(\alpha, \beta, \gamma)]^\dagger \\
&= P_{\text{fixedZ1Y2Z3}}(\gamma, \beta, \alpha) \begin{pmatrix} V_x \\ V_y \\ V_z \end{pmatrix}. \quad (309)
\end{aligned}$$

The transformation $[R_P^{\text{fixed}}(\gamma, \beta, \alpha)]^\dagger (V_x \ V_y \ V_z)^T R_P^{\text{fixed}}(\gamma, \beta, \alpha)$ describes the left-handed rotation of coordinate system about fixed axes for a vector operator $\mathbf{V}$ expressed with Cartesian components. $P_{\text{fixedZ1Y2Z3}}(\gamma, \beta, \alpha)$ is the corresponding left-handed passive rotation matrix. The first left-handed rotation angle of the coordinate system is α .

Table 6 allows us to determine the transformation law for covariant spherical components of vector operator defined in Eq. (276):

$$\begin{aligned}
&\exp(-i\phi L_x) \begin{pmatrix} V_{+1} \\ V_0 \\ V_{-1} \end{pmatrix} \exp(i\phi L_x) \\
&= \begin{pmatrix} C^2 \frac{\phi}{2} & \frac{-iS\phi}{\sqrt{2}} & -S^2 \frac{\phi}{2} \\ \frac{-iS\phi}{\sqrt{2}} & C\phi & \frac{-iS\phi}{\sqrt{2}} \\ -S^2 \frac{\phi}{2} & \frac{-iS\phi}{\sqrt{2}} & C^2 \frac{\phi}{2} \end{pmatrix} \begin{pmatrix} V_{+1} \\ V_0 \\ V_{-1} \end{pmatrix} \\
&= [\mathbf{D}^{(1,P)}(\frac{\pi}{2}, \phi, -\frac{\pi}{2})]^* \begin{pmatrix} V_{+1} \\ V_0 \\ V_{-1} \end{pmatrix}, \quad (310)
\end{aligned}$$

$$\begin{aligned}
&\exp(-i\phi L_y) \begin{pmatrix} V_{+1} \\ V_0 \\ V_{-1} \end{pmatrix} \exp(i\phi L_y) = \begin{pmatrix} C^2 \frac{\phi}{2} & \frac{S\phi}{\sqrt{2}} & S^2 \frac{\phi}{2} \\ \frac{-S\phi}{\sqrt{2}} & C\phi & \frac{S\phi}{\sqrt{2}} \\ S^2 \frac{\phi}{2} & \frac{-S\phi}{\sqrt{2}} & C^2 \frac{\phi}{2} \end{pmatrix} \begin{pmatrix} V_{+1} \\ V_0 \\ V_{-1} \end{pmatrix} \\
&= \mathbf{D}^{(1,P)}(0, \phi, 0) \begin{pmatrix} V_{+1} \\ V_0 \\ V_{-1} \end{pmatrix},
\end{aligned}$$

$$\begin{aligned}
&\exp(-i\phi L_z) \begin{pmatrix} V_{+1} \\ V_0 \\ V_{-1} \end{pmatrix} \exp(i\phi L_z) = \begin{pmatrix} e^{-i\phi} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & e^{i\phi} \end{pmatrix} \begin{pmatrix} V_{+1} \\ V_0 \\ V_{-1} \end{pmatrix} \\
&= [\mathbf{D}^{(1,P)}(0, 0, \phi)]^* \begin{pmatrix} V_{+1} \\ V_0 \\ V_{-1} \end{pmatrix}.
\end{aligned}$$

The 3X3 Wigner passive rotation matrices in Eq. (310) are those of Eq. (277), in which we have changed the sign of angle ϕ .

Equation (310) can be generalized to Euler angles:⁸⁰

$$\begin{aligned}
&[R_P^{\text{fixed}}(\gamma, \beta, \alpha)]^\dagger \begin{pmatrix} V_{+1} \\ V_0 \\ V_{-1} \end{pmatrix} R_P^{\text{fixed}}(\gamma, \beta, \alpha) \\
&\equiv R_A^{\text{fixed}}(\alpha, \beta, \gamma) \begin{pmatrix} V_{+1} \\ V_0 \\ V_{-1} \end{pmatrix} [R_A^{\text{fixed}}(\alpha, \beta, \gamma)]^\dagger \\
&= \exp(-i\alpha L_z) \exp(-i\beta L_y) \exp(-i\gamma L_z) \begin{pmatrix} V_{+1} \\ V_0 \\ V_{-1} \end{pmatrix} \\
&\quad \exp(i\gamma L_z) \exp(i\beta L_y) \exp(i\alpha L_z) \\
&= \exp(-i\alpha L_z) \exp(-i\beta L_y) \begin{pmatrix} e^{-i\gamma} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & e^{i\gamma} \end{pmatrix} \begin{pmatrix} V_{+1} \\ V_0 \\ V_{-1} \end{pmatrix} \\
&\quad \exp(i\beta L_y) \exp(i\alpha L_z) \quad (311) \\
&= \exp(-i\alpha L_z) \begin{pmatrix} e^{-i\gamma} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & e^{i\gamma} \end{pmatrix} \begin{pmatrix} C^2 \frac{\beta}{2} & \frac{S\beta}{\sqrt{2}} & S^2 \frac{\beta}{2} \\ \frac{-S\beta}{\sqrt{2}} & C\beta & \frac{S\beta}{\sqrt{2}} \\ S^2 \frac{\beta}{2} & \frac{-S\beta}{\sqrt{2}} & C^2 \frac{\beta}{2} \end{pmatrix} \\
&\quad \times \begin{pmatrix} V_{+1} \\ V_0 \\ V_{-1} \end{pmatrix} \exp(i\alpha L_z) \\
&= \begin{pmatrix} e^{-i\gamma} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & e^{i\gamma} \end{pmatrix} \begin{pmatrix} C^2 \frac{\beta}{2} & \frac{S\beta}{\sqrt{2}} & S^2 \frac{\beta}{2} \\ \frac{-S\beta}{\sqrt{2}} & C\beta & \frac{S\beta}{\sqrt{2}} \\ S^2 \frac{\beta}{2} & \frac{-S\beta}{\sqrt{2}} & C^2 \frac{\beta}{2} \end{pmatrix} \\
&\quad \times \begin{pmatrix} e^{-i\alpha} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & e^{i\alpha} \end{pmatrix} \begin{pmatrix} V_{+1} \\ V_0 \\ V_{-1} \end{pmatrix} \\
&= [\mathbf{D}^{(1,P)}(\gamma, \beta, \alpha)]^* \begin{pmatrix} V_{+1} \\ V_0 \\ V_{-1} \end{pmatrix}.
\end{aligned}$$

The order of the three elementary Wigner rotation matrices that define $[\mathbf{D}^{(1,P)}(\gamma, \beta, \alpha)]^*$ in Eq. (311) and that of Euler angles in the arguments of $[\mathbf{D}^{(1,P)}(\gamma, \beta, \alpha)]^*$ are due to the fact that rotation operators affect the covariant spherical components of vector operator. The first left-handed rotation angle of the coordinate system is α located at the right-hand side among the three arguments of $[\mathbf{D}^{(1,P)}(\gamma, \beta, \alpha)]^*$.

When covariant spherical components are used for left-handed rotation of coordinate system as in Eq. (311), the complex conjugate $[\mathbf{D}^{(1,P)}(\gamma, \beta, \alpha)]^*$ of the Wigner passive rotation matrix is post-multiplied by the column matrix of these components.⁸⁰ In contrast, when Cartesian

components are used as in Eq. (303), the passive rotation matrix $\mathbf{P}_{\text{fixedZ1Y2Z3}}(\gamma, \beta, \alpha)$ is post-multiplied by the column matrix of these components.⁸⁰

Consider the same example about the rotation defined in Eq. (305) but with covariant spherical spin operator components. We apply Eq. (311):

$$\begin{aligned} e^{-i\frac{\pi}{4}I_z} e^{-i\frac{\pi}{4}I_y} \begin{pmatrix} I_{+1} \\ I_z \\ I_{-1} \end{pmatrix} e^{i\frac{\pi}{4}I_y} e^{i\frac{\pi}{4}I_z} &= [\mathbf{D}^{(1,P)}(0, \frac{\pi}{2}, \frac{\pi}{4})]^* \begin{pmatrix} I_{+1} \\ I_z \\ I_{-1} \end{pmatrix} \\ &= \begin{pmatrix} \frac{e^{-i\frac{\pi}{4}}}{2} & \frac{1}{\sqrt{2}} & \frac{e^{i\frac{\pi}{4}}}{2} \\ \frac{-e^{-i\frac{\pi}{4}}}{\sqrt{2}} & 0 & \frac{e^{i\frac{\pi}{4}}}{\sqrt{2}} \\ \frac{e^{-i\frac{\pi}{4}}}{2} & \frac{-1}{\sqrt{2}} & \frac{e^{i\frac{\pi}{4}}}{2} \end{pmatrix} \begin{pmatrix} I_{+1} \\ I_z \\ I_{-1} \end{pmatrix}. \end{aligned} \quad (312)$$

We deduce that

$$\begin{aligned} I_z''' &= e^{-i\frac{\pi}{4}I_z} e^{-i\frac{\pi}{4}I_y} I_z e^{i\frac{\pi}{4}I_y} e^{i\frac{\pi}{4}I_z} = I_x C \frac{\pi}{4} + I_y S \frac{\pi}{4}, \\ I_x''' + iI_y''' &= e^{-i\frac{\pi}{4}I_z} e^{-i\frac{\pi}{4}I_y} (I_x + iI_y) e^{i\frac{\pi}{4}I_y} e^{i\frac{\pi}{4}I_z} \\ &= -I_z + i \left(-I_x S \frac{\pi}{4} + I_y C \frac{\pi}{4} \right). \end{aligned} \quad (313)$$

The relations of Eq. (313) agree with those in Eq. (307). We have at our disposal three methods for determining the expression of vector operator in a left-hand rotated coordinate system: (1) rotation operator as in Eq. (306); (2) rotation matrix as in Eq. (307); (3) the complex conjugate of Wigner rotation matrix as in Eq. (312).

The transformation $[R_P^{\text{fixed}}(\gamma, \beta, \alpha)]^\dagger (V_{+1} \ V_0 \ V_{-1})^T R_P^{\text{fixed}}(\gamma, \beta, \alpha)$ is a shorthand notation for “left-handed rotations of coordinate system about fixed axes by Euler angles, the vector operator remaining fixed”. Its equivalent expression $R_A^{\text{fixed}}(\alpha, \beta, \gamma) (V_{+1} \ V_0 \ V_{-1})^T [R_A^{\text{fixed}}(\alpha, \beta, \gamma)]^\dagger$ allows us to visualize $(V'_{+1} \ V'_0 \ V'_{-1})^T$ via a right-handed active rotation of vector operator about fixed axes. As the Wigner passive rotation matrix $\mathbf{D}^{(1,P)}(\gamma, \beta, \alpha)$ is derived for right-handed rotation of coordinate system, its complex conjugate is involved in the left-handed rotation of coordinate system.⁸⁰

10.2.2 | Right-handed rotation of coordinate system

We do not develop this case in details but let it to reader as exercises. First, change the sign of the rotation angle θ in Eq. (297):

$$R_P(\theta) V_i [R_P(\theta)]^\dagger = [R_A(\theta)]^\dagger V_i R_A(\theta) = \sum_{j=1}^3 V_j [\mathbf{P}(\theta)]_{ji}. \quad (314)$$

Figure 37 shows a right-handed passive rotation of I_z about x -axis by angle θ from (O, x, y, z) to (O, x', y', z') .

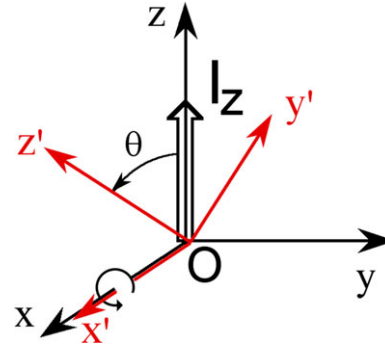


FIGURE 37 Right-handed rotation of coordinate system about x -axis by a positive angle θ from (O, x, y, z) to (O, x', y', z') , the spin operator component I_z remains fixed

In practice, the expression of I_z in the right-handed rotated coordinate system (O, x', y', z') can be determined as a left-handed active rotation of I_z about x -axis by angle θ in (O, x, y, z) (see Eq. (266)):

$$\exp(i\theta I_x) I_z \exp(-i\theta I_x) = I_z \cos \theta + I_y \sin \theta. \quad (315)$$

Then, deduce Table 7 from Table 5 by changing the sign of the rotation angle ϕ . This table describes right-handed passive rotations of spin operator $\mathbf{I}$ by left-handed active rotations of the spin operator $\mathbf{I}$. The passive rotation matrix $\mathbf{P}(\theta)$ has two meanings: It is a left-handed rotation matrix when it is post-multiplied by a column component matrix as in Table 6. It is a right-handed rotation matrix when it is pre-multiplied by a row component matrix as in Table 7.

Introducing the coordinate system fictitiously yields the right-handed rotations of coordinate system about fixed axes, keeping the vector operator fixed, which is expressed by the operator $R_P^{\text{fixed}}(\gamma, \beta, \alpha)$:

TABLE 7 Right-handed passive rotation of Cartesian spin operator components deduced from Table 5, the rotation angle ϕ being positive ($\phi > 0$)

$R_P(\phi) I_i [R_P(\phi)]^\dagger$	$\sum_{j=1}^3 I_j [\mathbf{P}(\phi)]_{ji}$
$\exp(i\phi I_z) \begin{pmatrix} I_x & I_y & I_z \end{pmatrix} \exp(-i\phi I_z)$	$\begin{pmatrix} I_x & I_y & I_z \end{pmatrix} \begin{pmatrix} \cos \phi & \sin \phi & 0 \\ -\sin \phi & \cos \phi & 0 \\ 0 & 0 & 1 \end{pmatrix}$
$\exp(i\phi I_y) \begin{pmatrix} I_x & I_y & I_z \end{pmatrix} \exp(-i\phi I_y)$	$\begin{pmatrix} I_x & I_y & I_z \end{pmatrix} \begin{pmatrix} \cos \phi & 0 & -\sin \phi \\ 0 & 1 & 0 \\ \sin \phi & 0 & \cos \phi \end{pmatrix}$
$\exp(i\phi I_x) \begin{pmatrix} I_x & I_y & I_z \end{pmatrix} \exp(-i\phi I_x)$	$\begin{pmatrix} I_x & I_y & I_z \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos \phi & \sin \phi \\ 0 & -\sin \phi & \cos \phi \end{pmatrix}$

$$\langle |R_P^{\text{fixed}}(\gamma, \beta, \alpha) = \langle | \exp(i\gamma L_z) \exp(i\beta L_y) \exp(i\alpha L_z). \quad (316)$$

The first, second, and third right-handed rotations of coordinate systems about fixed axes are about z -axis by angle γ , about y -axis by angle β , and about z -axis by angle α , respectively.

Equation (314) can be generalized to Euler angles as

$$\begin{aligned} R_P^{\text{fixed}}(\gamma, \beta, \alpha) \begin{pmatrix} V_x & V_y & V_z \end{pmatrix} [R_P^{\text{fixed}}(\gamma, \beta, \alpha)]^\dagger \\ = \begin{pmatrix} V_x & V_y & V_z \end{pmatrix} P_z(\gamma) P_y(\beta) P_z(\alpha) \\ = \begin{pmatrix} V_x & V_y & V_z \end{pmatrix} P_{\text{fixedZ1Y2Z3}}(\gamma, \beta, \alpha). \end{aligned} \quad (317)$$

The passive rotation matrix $P_{\text{fixedZ1Y2Z3}}(\gamma, \beta, \alpha)$ in Eq. (317) is identical to that defined in Eq. (303). It also has two meanings: It is a right-handed rotation matrix when it is pre-multiplied by a row component matrix as in Eq. (317). It is a left-handed rotation matrix when it is post-multiplied by a column component matrix as in Eq. (303).

Table 7 allows us to determine the transformation law for covariant spherical components of vector operator defined in Eq. (276):^{129–131}

$$\begin{aligned} R_P^{\text{fixed}}(\gamma, \beta, \alpha) \begin{pmatrix} V_{+1} & V_0 & V_{-1} \end{pmatrix} [R_P^{\text{fixed}}(\gamma, \beta, \alpha)]^\dagger \\ = [R_A^{\text{fixed}}(\alpha, \beta, \gamma)]^\dagger \begin{pmatrix} V_{+1} & V_0 & V_{-1} \end{pmatrix} R_A^{\text{fixed}}(\alpha, \beta, \gamma) \\ = \begin{pmatrix} V_{+1} & V_0 & V_{-1} \end{pmatrix} \mathbf{D}^{(1,P)}(\gamma, \beta, \alpha). \end{aligned} \quad (318)$$

The first right-handed rotation angle of the coordinate system is γ (see Eq. (316)) located at the left-hand side among the three arguments of $\mathbf{D}^{(1,P)}(\gamma, \beta, \alpha)$.

When covariant spherical components are used for right-handed rotation of coordinate system as in Eq. (318), the Wigner passive rotation matrix $\mathbf{D}^{(1,P)}(\gamma, \beta, \alpha)$ is pre-multiplied by the row matrix of these components. When Cartesian components are used as in Eq. (317), the passive rotation matrix $P_{\text{fixedZ1Y2Z3}}(\gamma, \beta, \alpha)$ is pre-multiplied by the row matrix of these components.

We may replace $R_P^{\text{fixed}}(\gamma, \beta, \alpha)$ by its equivalent operator $[R_A^{\text{fixed}}(\alpha, \beta, \gamma)]^\dagger$:

$$\begin{aligned} \langle |R_P^{\text{fixed}}(\gamma, \beta, \alpha) \begin{pmatrix} V_x & V_y & V_z \end{pmatrix} [R_P^{\text{fixed}}(\gamma, \beta, \alpha)]^\dagger \\ \equiv \langle | [R_A^{\text{fixed}}(\alpha, \beta, \gamma)]^\dagger \begin{pmatrix} V_x & V_y & V_z \end{pmatrix} R_A^{\text{fixed}}(\alpha, \beta, \gamma). \end{aligned} \quad (319)$$

That is, the first, second, and third left-handed active rotations of V_i in fixed coordinate system are about z -axis by angle α , about y -axis by angle β , and about z -axis by angle γ , respectively.

Figure 38 provides a geometrical representation of the result of

$$\begin{aligned} R_P^{\text{fixed}}(\gamma, \beta, \alpha) I_x [R_P^{\text{fixed}}(\gamma, \beta, \alpha)]^\dagger \\ = \exp(i\gamma L_z) \exp(i\beta L_y) \exp(i\alpha L_z) I_x \exp(-i\alpha L_z) \\ \exp(-i\beta L_y) \exp(-i\gamma L_z), \\ \alpha = \pi/4, \beta = \pi/2, \text{ and } \gamma = 0. \end{aligned} \quad (320)$$

Figure 38(A–C) describe right-handed rotations of coordinate system about fixed axes. The first and second right-handed rotations of coordinate system are about y -axis by angle $\beta = \pi/2$ and about z -axis by angle $\alpha = \pi/4$, respectively. Figure 38(A,D,E) describe left-handed active rotations of I_x about fixed axes. The first and second left-handed active rotations of I_x are about z -axis by angle $\alpha = \pi/4$ and about y -axis by angle $\beta = \pi/2$, respectively. In right-handed rotation of coordinate system, I_x lies in $\{y'', z''\}$ plane of the rotated coordinate system (O, x'', y'', z''), whereas in left-handed active rotation of the spin operator component, the rotated component I''_x lies in $\{y, z\}$ plane of the fixed coordinate system (O, x, y, z).

We have three ways to determine the expression of I_x in (O, x'', y'', z'') or equivalently that of I''_x in (O, x, y, z),

$$\begin{aligned} I''_x &= \exp(i\frac{\pi}{2} I_y) \exp(i\frac{\pi}{4} I_z) I_x \exp(-i\frac{\pi}{4} I_z) \exp(-i\frac{\pi}{2} I_y) \\ &= -I_y S\frac{\pi}{4} + I_z C\frac{\pi}{4}, \end{aligned} \quad (321)$$

1. using rotation matrices in Table 7;
2. using the rotation matrix $P_{\text{fixedZ1Y2Z3}}(\gamma, \beta, \alpha)$ as in Eq. (317);
3. using Wigner passive rotation matrix $\mathbf{D}^{(1,P)}(\gamma, \beta, \alpha)$ as in Eq. (318).

The expression of the spin operator component I''_x agrees with that shown in Figure 38E. These results are examples of general expressions

$$\begin{aligned} \begin{pmatrix} V'_x & V'_y & V'_z \end{pmatrix} &= R_P^{\text{fixed}}(\gamma, \beta, \alpha) \begin{pmatrix} V_x & V_y & V_z \end{pmatrix} [R_P^{\text{fixed}}(\gamma, \beta, \alpha)]^\dagger \\ &= [R_A^{\text{fixed}}(\alpha, \beta, \gamma)]^\dagger \begin{pmatrix} V_x & V_y & V_z \end{pmatrix} R_A^{\text{fixed}}(\alpha, \beta, \gamma) \\ &= \begin{pmatrix} V_x & V_y & V_z \end{pmatrix} P_{\text{fixedZ1Y2Z3}}(\gamma, \beta, \alpha), \end{aligned} \quad (322)$$

and

$$\begin{aligned} \begin{pmatrix} V'_{+1} & V'_0 & V'_{-1} \end{pmatrix} &= R_P^{\text{fixed}}(\gamma, \beta, \alpha) \begin{pmatrix} V_{+1} & V_0 & V_{-1} \end{pmatrix} \\ &\quad [R_P^{\text{fixed}}(\gamma, \beta, \alpha)]^\dagger \\ &= [R_A^{\text{fixed}}(\alpha, \beta, \gamma)]^\dagger \begin{pmatrix} V_{+1} & V_0 & V_{-1} \end{pmatrix} R_A^{\text{fixed}}(\alpha, \beta, \gamma) \\ &= \begin{pmatrix} V_{+1} & V_0 & V_{-1} \end{pmatrix} \mathbf{D}^{(1,P)}(\gamma, \beta, \alpha). \end{aligned} \quad (323)$$

The transformation $R_P^{\text{fixed}}(\gamma, \beta, \alpha) \begin{pmatrix} V_x & V_y & V_z \end{pmatrix} [R_P^{\text{fixed}}(\gamma, \beta, \alpha)]^\dagger$ describes the right-handed rotation of coordinate system about fixed axes for a fixed vector operator $\mathbf{V}$ with Cartesian components. $P_{\text{fixedZ1Y2Z3}}(\gamma, \beta, \alpha)$ is the corresponding right-handed passive rotation matrix. The first right-handed rotation angle of the coordinate system is γ .

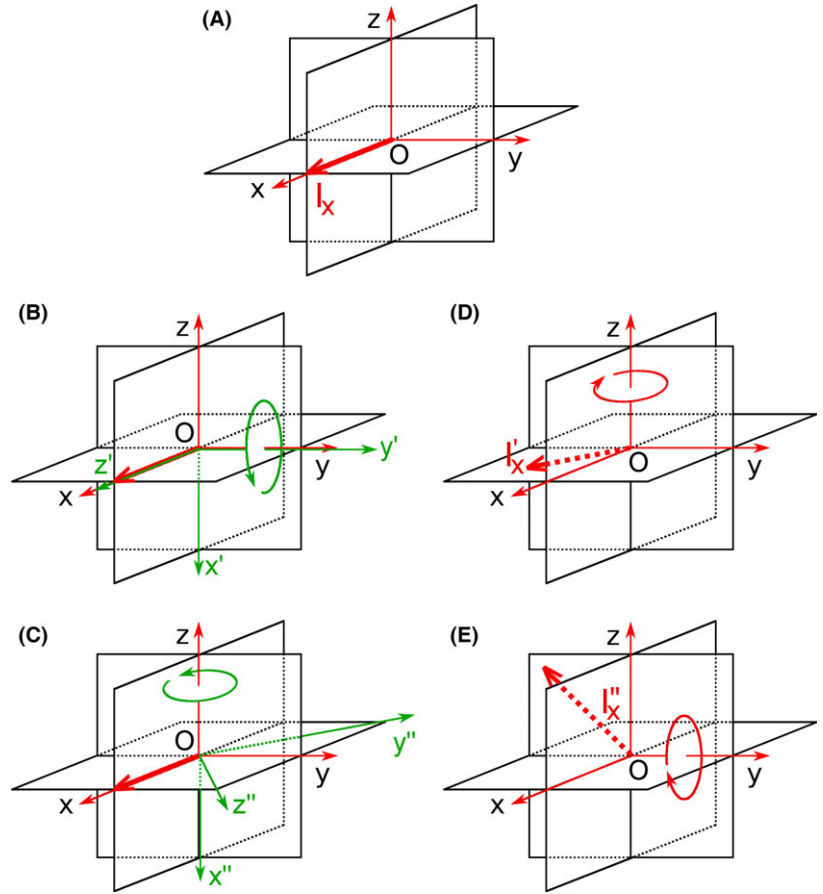


FIGURE 38 Equivalence between (A, B, C) right-handed rotations of coordinate system about fixed axes with spin operator component I_x fixed and (A, D, E) left-handed active rotations of I_x about fixed axes. (A) Initial configuration. The first (B) and second (C) right-handed rotations of the coordinate system are about y -axis by angle $\beta=\pi/2$ and about z -axis by angle $\alpha=\pi/4$, respectively. The first (D) and second (E) left-handed rotations of I_x are about z -axis by angle $\alpha=\pi/4$ and about y -axis by angle $\beta=\pi/2$, respectively

The transformation $R_p^{\text{fixed}}(\gamma, \beta, \alpha)(V_{+1} \ V_0 \ V_{-1})[R_p^{\text{fixed}}(\gamma, \beta, \alpha)]^\dagger$ is a shorthand notation for “right-handed rotations of coordinate system about fixed axes by Euler angles, the vector operator remaining fixed”. Its equivalent expression $[R_A^{\text{fixed}}(\alpha, \beta, \gamma)]^\dagger(V_{+1} \ V_0 \ V_{-1})R_A^{\text{fixed}}(\alpha, \beta, \gamma)$ allows us to visualize $(V'_{+1} \ V'_0 \ V'_{-1})$ in fixed coordinate system via a left-handed active rotation of vector operator about fixed axes.

When Cartesian components are used, the same rotation matrix $P_{\text{fixedZ1Y2Z3}}(\gamma, \beta, \alpha)$ is either a left-handed passive rotation matrix in a left-handed rotation of coordinate system or a right-handed passive rotation matrix in a right-handed rotation of coordinate system. In contrast, when covariant spherical components are used, the Wigner passive rotation matrix is involved in a right-handed rotation of coordinate system and its complex conjugate is involved in the left-handed rotation of coordinate system. As the orders of the Euler angles in the arguments of $P_{\text{fixedZ1Y2Z3}}(\gamma, \beta, \alpha)$, $[\mathbf{D}^{(1,P)}(\gamma, \beta, \alpha)]^*$, and $\mathbf{D}^{(1,P)}(\gamma, \beta, \alpha)$ are identical, the first rotation angles are α for left-handed and γ for right-handed rotations of coordinate system.

The left-hand members of Eqs. (303) and (317) show that we can deduce expressions of the right-handed of coordinate system from those of left-handed case by replacing the Euler angles α, β, γ in left-handed rotation of coordinate system by $-\gamma, -\beta, -\alpha$, respectively. Indeed, the replacement in the right-hand member of Eq. (303) gives

$$\begin{aligned} P_{\text{fixedZ1Y2Z3}}(\gamma \rightarrow -\alpha, \beta \rightarrow -\beta, \alpha \rightarrow -\gamma) \begin{pmatrix} V_x \\ V_y \\ V_z \end{pmatrix} \\ = A_{\text{fixedZ3Y2Z1}}(\alpha, \beta, \gamma) \begin{pmatrix} V_x \\ V_y \\ V_z \end{pmatrix} = \\ = (V_x \ V_y \ V_z) [A_{\text{fixedZ3Y2Z1}}(\alpha, \beta, \gamma)]^T \\ = (V_x \ V_y \ V_z) P_{\text{fixedZ1Y2Z3}}(\gamma, \beta, \alpha), \end{aligned} \quad (324)$$

the right-hand member of Eq. (317). Similarly, the replacement in the right-hand member of Eq. (311) gives

$$\begin{aligned} [\mathbf{D}^{(1,P)}(\gamma \rightarrow -\alpha, \beta \rightarrow -\beta, \alpha \rightarrow -\gamma)]^* \begin{pmatrix} V_{+1} \\ V_0 \\ V_{-1} \end{pmatrix} \\ = [\mathbf{D}^{(1,A)}(\alpha, \beta, \gamma)]^* \begin{pmatrix} V_{+1} \\ V_0 \\ V_{-1} \end{pmatrix} \\ = (V_{+1} \ V_0 \ V_{-1}) [\mathbf{D}^{(1,A)}(\alpha, \beta, \gamma)]^{*T} \\ = (V_{+1} \ V_0 \ V_{-1}) \mathbf{D}^{(1,P)}(\gamma, \beta, \alpha), \end{aligned} \quad (325)$$

the right-hand member of Eq. (318).

10.3 | Discussion

Given a vector operator in a coordinate system, a left-handed rotation of the coordinate system described by $[R_P^{\text{fixed}}(\gamma, \beta, \alpha)]^\dagger (V_x \ V_y \ V_z)^T R_P^{\text{fixed}}(\gamma, \beta, \alpha)$ or by its equivalent expression $R_A^{\text{fixed}}(\alpha, \beta, \gamma) (V_x \ V_y \ V_z)^T [R_A^{\text{fixed}}(\alpha, \beta, \gamma)]^\dagger$, followed by a left-handed active rotation of the vector operator described by $[R_A^{\text{fixed}}(\alpha, \beta, \gamma)]^\dagger (V_x \ V_y \ V_z)^T R_A^{\text{fixed}}(\alpha, \beta, \gamma)$, yield the same vector operator in the same coordinate system. We can show this using either vector operators:

$$\begin{aligned} & [R_A^{\text{fixed}}(\alpha, \beta, \gamma)]^\dagger [R_P^{\text{fixed}}(\gamma, \beta, \alpha)]^\dagger \begin{pmatrix} V_x \\ V_y \\ V_z \end{pmatrix} \\ & R_P^{\text{fixed}}(\gamma, \beta, \alpha) R_A^{\text{fixed}}(\alpha, \beta, \gamma) \\ & = [R_A^{\text{fixed}}(\alpha, \beta, \gamma)]^\dagger R_A^{\text{fixed}}(\alpha, \beta, \gamma) \begin{pmatrix} V_x \\ V_y \\ V_z \end{pmatrix} \\ & [R_A^{\text{fixed}}(\alpha, \beta, \gamma)]^\dagger R_A^{\text{fixed}}(\alpha, \beta, \gamma) = \begin{pmatrix} V_x \\ V_y \\ V_z \end{pmatrix}, \end{aligned} \quad (326)$$

or Cartesian rotation matrices:

$$\begin{aligned} & [R_A^{\text{fixed}}(\alpha, \beta, \gamma)]^\dagger [R_P^{\text{fixed}}(\gamma, \beta, \alpha)]^\dagger \begin{pmatrix} V_x \\ V_y \\ V_z \end{pmatrix} \\ & R_P^{\text{fixed}}(\gamma, \beta, \alpha) R_A^{\text{fixed}}(\alpha, \beta, \gamma) \\ & = A_{\text{fixedZ3Y2Z1}}(\alpha, \beta, \gamma) P_{\text{fixedZ1Y2Z3}}(\gamma, \beta, \alpha) \begin{pmatrix} V_x \\ V_y \\ V_z \end{pmatrix} \\ & = A_z(\alpha) A_y(\beta) A_z(\gamma) P_z(\gamma) P_y(\beta) P_z(\alpha) \begin{pmatrix} V_x \\ V_y \\ V_z \end{pmatrix} = \begin{pmatrix} V_x \\ V_y \\ V_z \end{pmatrix}, \end{aligned} \quad (327)$$

or Wigner rotation matrices:

$$\begin{aligned} & [R_A^{\text{fixed}}(\alpha, \beta, \gamma)]^\dagger [R_P^{\text{fixed}}(\gamma, \beta, \alpha)]^\dagger \begin{pmatrix} V_{+1} \\ V_0 \\ V_{-1} \end{pmatrix} \\ & R_P^{\text{fixed}}(\gamma, \beta, \alpha) R_A^{\text{fixed}}(\alpha, \beta, \gamma) \\ & = [\mathbf{D}^{(1,A)}(\alpha, \beta, \gamma) \mathbf{D}^{(1,P)}(\gamma, \beta, \alpha)]^* \begin{pmatrix} V_{+1} \\ V_0 \\ V_{-1} \end{pmatrix} \\ & = \begin{pmatrix} V_{+1} \\ V_0 \\ V_{-1} \end{pmatrix}. \end{aligned} \quad (328)$$

Given a vector operator in a coordinate system, a right-handed rotation of the coordinate system described by

$R_P^{\text{fixed}}(\gamma, \beta, \alpha) (V_x \ V_y \ V_z) [R_P^{\text{fixed}}(\gamma, \beta, \alpha)]^\dagger$ or by its equivalent expression $[R_A^{\text{fixed}}(\alpha, \beta, \gamma)]^\dagger (V_x \ V_y \ V_z) R_A^{\text{fixed}}(\alpha, \beta, \gamma)$, followed by a right-handed active rotation of the vector operator described by $R_A^{\text{fixed}}(\alpha, \beta, \gamma) (V_x \ V_y \ V_z) [R_A^{\text{fixed}}(\alpha, \beta, \gamma)]^\dagger$, yield the same vector operator in the same coordinate system. We can show this using either vector operators:

$$\begin{aligned} & R_A^{\text{fixed}}(\alpha, \beta, \gamma) R_P^{\text{fixed}}(\gamma, \beta, \alpha) (V_x \ V_y \ V_z) \\ & [R_P^{\text{fixed}}(\gamma, \beta, \alpha)]^\dagger [R_A^{\text{fixed}}(\alpha, \beta, \gamma)]^\dagger \\ & = R_A^{\text{fixed}}(\alpha, \beta, \gamma) [R_A^{\text{fixed}}(\alpha, \beta, \gamma)]^\dagger (V_x \ V_y \ V_z) \\ & R_A^{\text{fixed}}(\alpha, \beta, \gamma) [R_A^{\text{fixed}}(\alpha, \beta, \gamma)]^\dagger = (V_x \ V_y \ V_z), \end{aligned} \quad (329)$$

or Cartesian rotation matrices:

$$\begin{aligned} & R_A^{\text{fixed}}(\alpha, \beta, \gamma) R_P^{\text{fixed}}(\gamma, \beta, \alpha) (V_x \ V_y \ V_z) \\ & [R_P^{\text{fixed}}(\gamma, \beta, \alpha)]^\dagger [R_A^{\text{fixed}}(\alpha, \beta, \gamma)]^\dagger \\ & = (V_x \ V_y \ V_z) P_{\text{fixedZ1Y2Z3}}(\gamma, \beta, \alpha) A_{\text{fixedZ3Y2Z1}}(\alpha, \beta, \gamma) \\ & = (V_x \ V_y \ V_z) P_z(\gamma) P_y(\beta) P_z(\alpha) A_z(\alpha) A_y(\beta) A_z(\gamma) \\ & = (V_x \ V_y \ V_z), \end{aligned} \quad (330)$$

or Wigner rotation matrices:

$$\begin{aligned} & [R_A^{\text{fixed}}(\alpha, \beta, \gamma)]^\dagger [R_P^{\text{fixed}}(\gamma, \beta, \alpha)]^\dagger (V_{+1} \ V_0 \ V_{-1}) R_P^{\text{fixed}}(\gamma, \beta, \alpha) R_A^{\text{fixed}}(\alpha, \beta, \gamma) \\ & = (V_{+1} \ V_0 \ V_{-1}) \mathbf{D}^{(1,P)}(\gamma, \beta, \alpha) \mathbf{D}^{(1,A)}(\alpha, \beta, \gamma) \\ & = (V_{+1} \ V_0 \ V_{-1}). \end{aligned} \quad (331)$$

Throughout the article, we show that left- and right-handed rotations of coordinate system are equivalent to right- and left-handed active rotations of position vector, space function, and spherical harmonics, respectively. This obviously remains true for vector operator. We have derived left- and right-handed rotations of coordinate system independently of right- and left-handed active rotations of vector operator. In fact these rotations are related.

Equation (269), which describes the left-handed active rotation of vector operator with Cartesian components, should be equivalent to Eq. (317), which describes the right-handed rotation of coordinate system. Indeed, replacing $[R_A^{\text{fixed}}(\alpha, \beta, \gamma)]^\dagger$ and $R_A^{\text{fixed}}(\alpha, \beta, \gamma)$ in the term on the initial left-hand side of Eq. (269) by $R_P^{\text{fixed}}(\gamma, \beta, \alpha)$ and $[R_P^{\text{fixed}}(\gamma, \beta, \alpha)]^\dagger$ yield the term on the initial left-hand side of Eq. (317). The term on the final right-hand side of Eq. (269) can be written as the transposed expression:

$$\begin{aligned} \mathbf{A}_{\text{fixedZ3Y2Z1}}(\alpha, \beta, \gamma) \begin{pmatrix} V_x \\ V_y \\ V_z \end{pmatrix} &= \begin{pmatrix} V_x & V_y & V_z \end{pmatrix} \\ &\quad [\mathbf{A}_{\text{fixedZ3Y2Z1}}(\alpha, \beta, \gamma)]^T \\ &= \begin{pmatrix} V_x & V_y & V_z \end{pmatrix} \mathbf{P}_{\text{fixedZ1Y2Z3}}(\gamma, \beta, \alpha), \end{aligned} \quad (332)$$

which is the term on the final right-hand side of Eq. (317). Similarly for spherical components of vector operator, Eq. (278) is equivalent to Eq. (318). Indeed, the term on the final right-hand member of Eq. (278) can be written as the transposed expression:

$$\begin{aligned} [\mathbf{D}^{(1,A)}(\alpha, \beta, \gamma)]^* \begin{pmatrix} V_{+1} \\ V_0 \\ V_{-1} \end{pmatrix} &= \begin{pmatrix} V_{+1} & V_0 & V_{-1} \end{pmatrix} [\mathbf{D}^{(1,A)}(\alpha, \beta, \gamma)]^{*T} \\ &= \begin{pmatrix} V_{+1} & V_0 & V_{-1} \end{pmatrix} \mathbf{D}^{(1,P)}(\gamma, \beta, \alpha), \end{aligned} \quad (333)$$

which is the term on the final right-hand side of Eq. (318).

Equation (284), which describes the right-handed active rotation of vector operator with Cartesian components, should be equivalent to Eq. (303), which describe the left-handed rotation of coordinate system. Similarly for spherical components of vector operator, Eq. (286) is equivalent to Eq. (311).

We have discussed four types of rotation in this section (left- and right-handed active rotations of vector operator, and left- and right-handed rotations of coordinate system). In fact, they are related. Knowing one of them allows us to deduce the other three. The relations between these four types of rotation of vector operator are similar to those between the four types of rotation of spherical harmonics shown in Figure 28.

11 | ROTATION OF SPHERICAL TENSOR OPERATOR

In quantum mechanics, operators representing various physical quantities are classified as scalars, vectors, and tensors according to their behaviors under rotations. The analog of spherical tensor in classical mechanics is the spherical tensor operator in quantum mechanics.¹³² Spherical tensor operators are widely used in NMR.^{133–142} The spherical vector operator discussed in Section 10 is readily generalized to spherical tensor operator of arbitrary rank. We restrict the definitions to right-hand active rotation of spherical tensor operator and right-hand rotation of coordinate system. Left-hand rotations can be deduced easily as shown in Section 10.

11.1 | Spherical tensor operator

In general, a tensor operator can be constructed from tensor operators of lower ranks using the relationship^{41,122,132}

$$\begin{aligned} T_{kq} &= \sqrt{2k+1} \sum_{q_1, q_2} (-1)^{-k_1+k_2-m} \begin{pmatrix} k_1 & k_2 & k \\ q_1 & q_2 & -q \end{pmatrix} T_{k_1 q_1} T_{k_2 q_2} \\ &= \sum_{q_1, q_2} \langle k_1 q_1 k_2 q_2 | kq \rangle T_{k_1 q_1} T_{k_2 q_2} \end{aligned} \quad (334)$$

where $\begin{pmatrix} k_1 & k_2 & k \\ q_1 & q_2 & -q \end{pmatrix}$ is the Wigner $3j$ symbol and $\langle k_1 q_1 k_2 q_2 | kq \rangle$ the Clebsch-Gordon coefficient. Compatible with the symmetry properties of the elements of the Wigner $3j$ symbol, the set of q_1 and q_2 values is restricted by the selection rule $q_1 + q_2 = q$. Furthermore, k_1 , k_2 , and k are linked via $k = |k_1 - k_2|, |k_1 - k_2| + 1, \dots, k_1 + k_2$.

A spin I , which has $2I + 1$ energy levels, is described by spherical tensor operators up to rank $k=2I$.

The $k=1$ spherical tensor operators in terms of Cartesian spin operators are^{38,77,132}

$$\begin{aligned} T_{10} &= I_z, \\ T_{1+1} &= -\frac{1}{\sqrt{2}} I_+ = -\frac{1}{\sqrt{2}} (I_x + iI_y), \\ T_{1-1} &= \frac{1}{\sqrt{2}} I_- = \frac{1}{\sqrt{2}} (I_x - iI_y). \end{aligned} \quad (335)$$

The $k=2$ and $q=0$ spherical tensor operator is^{1,38,91,94,96,122,132,133,143}

$$\begin{aligned} T_{20} &= \sum_{q_1, q_2} \langle 1q_1 1q_2 | 20 \rangle T_{1q_1} T_{1q_2} \\ &= \sqrt{\frac{1}{6}} T_{1+1} T_{1-1} + \sqrt{\frac{1}{6}} T_{1-1} T_{1+1} + \sqrt{\frac{2}{3}} T_{10} T_{10} \\ &= \sqrt{\frac{1}{6}} (3I_z^2 - I(I+1)). \end{aligned} \quad (336)$$

The $k=2$ and $q=1$ spherical tensor operator is^{1,38,91,94,96,122,132,133,143}

$$\begin{aligned} T_{2+1} &= \sum_{q_1, q_2} \langle 1q_1 1q_2 | 2+1 \rangle T_{1q_1} T_{1q_2} \\ &= \sqrt{\frac{1}{2}} T_{1+1} T_{10} + \sqrt{\frac{1}{2}} T_{10} T_{1+1} \\ &= -\frac{1}{2} (I_+ I_z + I_z I_+) \\ &= -\frac{1}{2} (2I_+ I_z + I_z I_+ - I_+ I_z) \\ &= -\frac{1}{2} I_+ (2I_z + 1). \end{aligned} \quad (337)$$

The $k=2$ and $q=-1$ spherical tensor operator is^{1,38,91,94,96,122,132,133,143}

$$\begin{aligned}
T_{2-1} &= \sum_{q_1, q_2} \langle 1q_1 1q_2 | 2-1 \rangle T_{1q_1} T_{1q_2} \\
&= \sqrt{\frac{1}{2}} T_{1-1} T_{10} + \sqrt{\frac{1}{2}} T_{10} T_{1-1} \\
&= \frac{1}{2} (I_- I_z + I_z I_-) \\
&= \frac{1}{2} (2I_- I_z + I_z I_- - I_- I_z) \\
&= \frac{1}{2} I_- (2I_z - 1).
\end{aligned} \tag{338}$$

The $k=2$ and $q=2$ spherical tensor operator is^{1,38,91,94,96,122,132,133,143}

$$T_{2+2} = \sum_{q_1, q_2} \langle 1q_1 1q_2 | 2+2 \rangle T_{1q_1} T_{1q_2} = T_{1+1} T_{1+1} = \frac{1}{2} (I_+)^2. \tag{339}$$

The $k=2$ and $q=-2$ spherical tensor operator is^{1,38,91,94,96,122,132,133,143}

$$T_{2-2} = \sum_{q_1, q_2} \langle 1q_1 1q_2 | 2-2 \rangle T_{1q_1} T_{1q_2} = T_{1-1} T_{1-1} = \frac{1}{2} (I_-)^2. \tag{340}$$

The most important property of irreducible tensor operators is given by the Wigner-Eckart theorem.³⁴ Irreducible spherical tensor operators of rank k and order q may be defined via the Wigner-Eckart theorem.¹³⁴

Irreducible spherical tensor operators of rank k and order q can be defined either by commutation relations of T_{kq} with the angular momentum operators $J_{\pm}$ and J_z or by their transformation properties under rotation. These two definitions are entirely equivalent.^{22,29,36,57,68,70,128} The commutation relations^{7,22,34,39,63,71,122,144} correspond to the definition of spherical tensor operator given by Racah:¹⁴⁵

$$\begin{aligned}
[J_{\pm}, T_{kq}] &= T_{kq\pm 1} \sqrt{(k \mp q)(k \pm q + 1)} \\
&= T_{kq\pm 1} \sqrt{k(k+1) - q(q \pm 1)}, \\
[J_z, T_{kq}] &= q T_{kq}.
\end{aligned} \tag{341}$$

Below, we discuss their transformation properties under active and passive rotations.

11.2 | Active rotation

We gather four typical definitions about active rotation of irreducible spherical tensor operators available in the literature. Messiah³⁴ provides the following definition of irreducible tensor operator in Appendix C of his book: The $2k+1$ operators $T_q^{(k)}$ ($q = -k, \dots, +k$) are by definition the standard components of an irreducible tensor operator of order k , $T^{(k)}$, if they transform *under rotation* according to the formula

$$\begin{aligned}
R(\alpha, \beta, \gamma) T_q^{(k)} [R(\alpha, \beta, \gamma)]^{-1} &= \sum_{q'} T_{q'}^{(k)} D_{q'q}^{(k)}(\alpha, \beta, \gamma), \\
R(\alpha, \beta, \gamma) &= R_A^{\text{fixed}}(\alpha, \beta, \gamma).
\end{aligned} \tag{342}$$

This is the generalization of our right-handed active rotation of vector operator (Eq. (286)).

Sakurai and Napolitano²⁶ provide the following definition of spherical tensor operator in Chapter 3 of their book: A spherical tensor operator of rank k with $2k+1$ components transform *under rotations* as

$$[D(\alpha, \beta, \gamma)]^{\dagger} T_q^{(k)} D(\alpha, \beta, \gamma) = \sum_{q'=-k}^k [D_{qq'}^{(k)}(\alpha, \beta, \gamma)]^* T_{q'}^{(k)}, \tag{343}$$

or equivalently

$$\begin{aligned}
D(\alpha, \beta, \gamma) T_q^{(k)} [D(\alpha, \beta, \gamma)]^{\dagger} &= \sum_{q'=-k}^k T_{q'}^{(k)} D_{q'q}^{(k)}(\alpha, \beta, \gamma), \\
D(\alpha, \beta, \gamma) &= R_A^{\text{fixed}}(\alpha, \beta, \gamma).
\end{aligned} \tag{344}$$

Equation (343) is the generalization of our left-handed active rotation of vector operator (Eq.(278)).

Varshalovich et al.⁵⁵ provide the following definition of irreducible tensor operators in Chapter 3 of their book: *Under rotations of the coordinate system* described by Euler angles, the components of irreducible tensors undergo linear transformations. The coefficients of such transformation are the Wigner active rotation matrix.

$$\begin{aligned}
T_{JM'}(X') &= D(\alpha, \beta, \gamma) T_{JM'}(X) [D(\alpha, \beta, \gamma)]^{-1} \\
&= \sum_{M=-J}^J T_{JM}(X) D_{MM'}^{(J)}(\alpha, \beta, \gamma), \\
D(\alpha, \beta, \gamma) &= R_A^{\text{fixed}}(\alpha, \beta, \gamma).
\end{aligned} \tag{345}$$

In contrast to most definitions of spherical tensor operators, the coordinates X and X' are provided in Eq. (345).

If contravariant spherical tensor components $T^{(k)q}$ are used, they transform according to⁹⁰

$$D(R) T^{(k)q} [D(R)]^{\dagger} = \sum_{q'=-k}^k T^{(k)q'} [D_{q'q}^{(k)}(R)]^*. \tag{346}$$

Most definitions (Messiah,³⁴ Baym,⁵² Rose,³⁶ Brink and Satchler,⁹ Varshalovich et al.⁵⁵) provide the following relation:

$$\begin{aligned}
R_A^{\text{fixed}}(\alpha, \beta, \gamma) T_{Ik}(\mathbf{r}) [R_A^{\text{fixed}}(\alpha, \beta, \gamma)]^{-1} \\
= \sum_{k'} T_{Ik'}(\mathbf{r}) D_{k'k}^{(I,A)}(\alpha, \beta, \gamma).
\end{aligned} \tag{347}$$

We need more details to distinguish one and two coordinate systems. In one coordinate system, we have

$$(T''')_{lk}(\mathbf{r}) \stackrel{1}{=} R_A^{\text{fixed}}(\alpha, \beta, \gamma) T_{lk}(\mathbf{r}) [R_A^{\text{fixed}}(\alpha, \beta, \gamma)]^{-1} \\ \stackrel{2}{=} T_{lk}(\mathbf{r}_1) \stackrel{5}{=} \sum_{k'} T_{lk'}(\mathbf{r}) D_{k'k}^{(I,A)}(\alpha, \beta, \gamma). \quad (348)$$

In two coordinate systems or canonical transformation, we have

$$(T''')_{lk}(\mathbf{r}) \stackrel{1}{=} R_A^{\text{fixed}}(\alpha, \beta, \gamma) T_{lk}(\mathbf{r}) [R_A^{\text{fixed}}(\alpha, \beta, \gamma)]^{-1} \\ \stackrel{4}{=} T_{lk}(\mathbf{r}') \stackrel{5}{=} \sum_{k'} T_{lk'}(\mathbf{r}) D_{k'k}^{(I,A)}(\alpha, \beta, \gamma). \quad (349)$$

The only differences between one and two coordinate systems are the equalities $\stackrel{2}{=}$ and $\stackrel{4}{=}$. In one coordinate system, $T_{lk}(\mathbf{r}_1)$ is the spherical tensor operator component before the active rotation. In two coordinate systems, $T_{lk}(\mathbf{r}')$ is the spherical tensor operator component in its body-attached coordinate system after the active rotation. Without the equalities $\stackrel{2}{=}$ and $\stackrel{4}{=}$, the definitions for one and two coordinate systems become identical (Eq. (347)).

11.3 | Passive rotation

Edmonds' third edition (1974) book,⁷⁰ Dawson,⁸⁰ and Silver⁵⁸ in Chapter 5 of his book provide the following definition of spherical (irreducible) tensor operators: A spherical (irreducible) tensor operator $T(k)$ is a set of $2k + 1$ operators $T(kq)$ ($q = -k, -k + 1, \dots, k - 1, k$) which transform under rotations of coordinate system like the components of the spherical tensor namely as

$$D(\gamma, \beta, \alpha) T(kq) [D(\gamma, \beta, \alpha)]^{-1} = \sum_{q'=-k}^{+k} T(kq') D_{q'q}^{(k)}(\gamma, \beta, \alpha), \quad (350)$$

$$D(\gamma, \beta, \alpha) = \exp \frac{i\gamma}{\hbar} L_z \exp \frac{i\beta}{\hbar} L_y \exp \frac{i\alpha}{\hbar} L_z \\ = R_P^{\text{fixed}}(\gamma, \beta, \alpha).$$

Equation (350) is a generalization definition of our right-handed passive rotation of vector operator defined in Eq. (318) and is the main definition found in the literature.

Blum⁹⁷ in Page 120 of his book provides the following definition: Operators which transform under rotations according to the following relation,

$$T(J'J)_{KQ} = \sum_{q=-K}^{+K} T(J'J)_{Kq} D_{qQ}^{(K)}(\gamma, \beta, \alpha), \quad (351)$$

are called spherical (irreducible) tensor operators of rank K and components Q . Equation (351) expresses the operators $T(J'J)_{KQ}$ defined in the XYZ coordinate system, in terms of the operators $T(J'J)_{Kq}$ defined in the xyz coordinate system. The convention for the $\mathbf{D}^{(K)}(\gamma, \beta, \alpha)$ matrices

adopted by Blum is that of Landau and Lifschitz.⁶⁵ The relation between the notation of Blum and that of Zare³⁸ is

$$D_{qQ}^{(K)}(\gamma, \beta, \alpha) = [D_{Qq}^{(K)}(\alpha, \beta, \gamma)]_{\text{ZARE}}^*. \quad (352)$$

That is, we can use Zare's equations by interchanging q and Q , α and γ , and taking the complex conjugate. The xyz coordinate system (a rotated coordinate system) corresponds to our (O, x'', y'', z'') , whereas the XYZ coordinate system (a fixed coordinate system) corresponds to our (O, x, y, z) . Our coordinate systems are defined in Figure 11.

We add more relations for right-handed passive rotation for spherical tensor component operators, which corresponds to right-handed rotation of the coordinate system or left-handed active rotation of spherical tensor component operators:

$$(T''')_{lk}(\mathbf{r}''') \quad (353)$$

$$\stackrel{1}{=} R_P^{\text{fixed}}(\gamma, \beta, \alpha) T_{lk}(\mathbf{r}''') [R_P^{\text{fixed}}(\gamma, \beta, \alpha)]^\dagger \quad (354)$$

$$\stackrel{2}{=} T_{lk}(\mathbf{r}) \quad (355)$$

$$\stackrel{5}{=} \sum_{k'} T_{lk'}(\mathbf{r}''') D_{k'k}^{(I,P)}(\gamma, \beta, \alpha), \quad (356)$$

$\mathbf{r}'''$ is in the final or rotated coordinate system and $\mathbf{r}$ is in the initial or fixed coordinate system.

For passive rotation, most definitions provide the following relation:¹³¹

$$D(\gamma, \beta, \alpha) T_{lk}(\mathbf{r}''') [D(\gamma, \beta, \alpha)]^{-1} = \sum_{k'} T_{lk'}(\mathbf{r}''') D_{k'k}^{(I,P)}(\gamma, \beta, \alpha), \quad (357)$$

relating Eqs. (354) and (356). In contrast, Blum's definition in Eq. (351) relates Eqs. (355) and (356).

11.4 | Application

We study the off-resonance excitation of an isolated spin $I = 1$ system by an x -pulse during a duration t_p using Wigner rotation matrices. An isolated spin $I = 1$ system is considered here because we want to use $\mathbf{D}^{(1,A)}$ and $\mathbf{D}^{(1,P)}$. In fact, the results are identical to those of an isolated spin $I = 1/2$ system not submitted to any internal interaction. In other words, the quadrupole interaction is neglected during the excitation of the spin $I = 1$ system by the x -pulse. The effective magnetic field that excites the spin system is along the x' -axis in the tilted coordinate system. There are two coordinate systems as shown Figure 39: the rotating

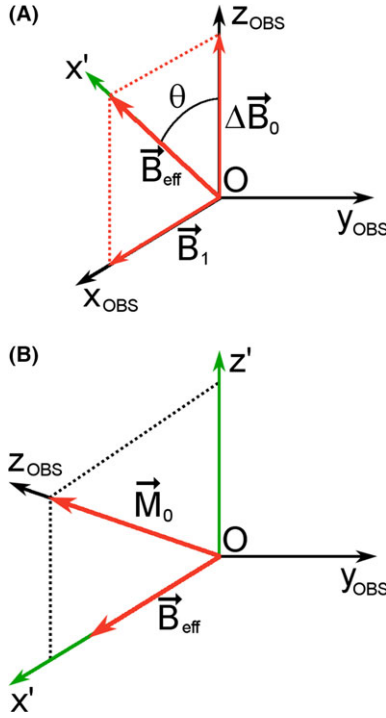


FIGURE 39 X-pulse irradiation of a spin system off-resonance by $\Delta\mathbf{B}_0$ in NMR rotating coordinate system ($O, x_{\text{OBS}}, y_{\text{OBS}}, z_{\text{OBS}}$) (A) and in tilted coordinate system ($O, x', y_{\text{OBS}}, z'$) (B). The magnetization vector $\mathbf{M}_0$ is along z_{OBS} -axis

coordinate system ($O, x_{\text{OBS}}, y_{\text{OBS}}, z_{\text{OBS}}$) and the tilted coordinate system ($O, x', y_{\text{OBS}}, z'$).

11.4.1 | Initial state

The nuclear magnetization vector is along the z_{OBS} -axis of the rotating coordinate system.

$$T_{1k}(\mathbf{r}_1) = I_0 \begin{pmatrix} 0 & 1 & 0 \end{pmatrix}. \quad (358)$$

The position vector before excitation $\mathbf{r}_1$ is in the rotating coordinate system.

11.4.2 | Passage from rotating coordinate system to tilted coordinate system

Figure 39A shows that the passage from the rotating coordinate system to the tilted coordinate system is a passive rotation about y_{OBS} -axis of angle $\beta = -(\frac{\pi}{2} - \theta)$. Equalities $\stackrel{2}{=}$ in Eq. (355) and $\stackrel{5}{=}$ in Eq. (356) allow us to write

$$\sum_{k'} T_{1k'}(\mathbf{r}'_1) \left[\mathbf{D}^{(1,P)} \left(0, -\left\{ \frac{\pi}{2} - \theta \right\}, 0 \right) \right]_{k'k} = T_{1k}(\mathbf{r}_1). \quad (359)$$

The position vector before excitation $\mathbf{r}'_1$ is in the tilted coordinate system. Conversely,

$$T_{1k}(\mathbf{r}'_1) = \sum_{k'} T_{1k'}(\mathbf{r}_1) \left[\mathbf{D}^{(1,P)} \left(0, -\left\{ \frac{\pi}{2} - \theta \right\}, 0 \right) \right]_{k'k}^{-1}. \quad (360)$$

11.4.3 | Nutation of the magnetization vector about $\mathbf{B}_{\text{eff}}$

In the tilted coordinate system, the rotation of the magnetization vector is about x' -axis (Figure 39B). As Wigner rotation matrices are defined for rotation about the y_{OBS} -axis, we must first rotate our spin system and the NMR spectrometer about the z' -axis by angle $\gamma = \frac{\pi}{2}$. Then we apply the irradiation to rotate the magnetization vector about $\mathbf{B}_{\text{eff}}$ along y_{OBS} -axis by angle $\beta = -\omega_e t_p = -\gamma_0 t_p \sqrt{\mathbf{B}_1^2 + (\Delta\mathbf{B}_0)^2}$. Finally, we rotate the spin system and the spectrometer about the z' -axis by angle $\alpha = -\frac{\pi}{2}$. Equalities $\stackrel{2}{=}$ and $\stackrel{5}{=}$ in Eq. (348) allow us to write

$$\sum_{m'} T_{1m'}(\mathbf{r}') \left[\mathbf{D}^{(1,A)} \left(-\frac{\pi}{2}, -\omega_e t_p, \frac{\pi}{2} \right) \right]_{m'm} = T_{1m}(\mathbf{r}'_1). \quad (361)$$

The position vector after excitation $\mathbf{r}'$ is in the tilted coordinate system. Conversely

$$T_{1m}(\mathbf{r}') = \sum_{m'} T_{1m'}(\mathbf{r}'_1) \left[\mathbf{D}^{(1,A)} \left(-\frac{\pi}{2}, -\omega_e t_p, \frac{\pi}{2} \right) \right]_{m'm}^{-1}. \quad (362)$$

11.4.4 | Passage from the tilted coordinate system to the rotating coordinate system

As NMR signal is detected in the rotating coordinate system, we return back to the rotating coordinate system from the tilted coordinate system. This is a passive rotation of angle $\beta = \frac{\pi}{2} - \theta$ about y_{OBS} -axis.

$$\sum_{n'} T_{1n'}(\mathbf{r}) \left[\mathbf{D}^{(1,P)} \left(0, \frac{\pi}{2} - \theta, 0 \right) \right]_{n'n} = T_{1n}(\mathbf{r}'). \quad (363)$$

The position vector after excitation $\mathbf{r}$ is in the rotating coordinate system. Conversely,

$$T_{1n}(\mathbf{r}) = \sum_{n'} T_{1n'}(\mathbf{r}') \left[\mathbf{D}^{(1,P)} \left(0, \frac{\pi}{2} - \theta, 0 \right) \right]_{n'n}^{-1}. \quad (364)$$

Putting Eqs. (364), (362), (360), and (358) together yields

$$T_{1n}(\mathbf{r}) = I_0(0 \ 1 \ 0) \sum_{n'} \sum_{m'} \sum_{k'} \left[\mathbf{D}^{(1,P)} \left(0, -\left\{ \frac{\pi}{2} - \theta \right\}, 0 \right) \right]_{k'm'}^{-1} \quad (365)$$

$$\times \left[\mathbf{D}^{(1,A)} \left(-\frac{\pi}{2}, -\omega_e t_p, \frac{\pi}{2} \right) \right]_{m'n'}^{-1} \left[\mathbf{D}^{(1,P)} \left(0, \frac{\pi}{2} - \theta, 0 \right) \right]_{n'n}^{-1}.$$

In matrix form, Eq. (365) becomes

$$(T_{11} \ T_{10} \ T_{1-1}) = I_0(0 \ 1 \ 0) \left[\mathbf{D}^{(1,P)} \left(0, -\left\{ \frac{\pi}{2} - \theta \right\}, 0 \right) \right]^{-1} \quad (366)$$

$$\times \left[\mathbf{D}^{(1,A)} \left(-\frac{\pi}{2}, -\omega_e t_p, \frac{\pi}{2} \right) \right]^{-1} \left[\mathbf{D}^{(1,P)} \left(0, \frac{\pi}{2} - \theta, 0 \right) \right]^{-1}.$$

These Wigner rotation matrices are

$$\left[\mathbf{D}^{(1,P)} \left(0, -\left\{ \frac{\pi}{2} - \theta \right\}, 0 \right) \right]^{-1} = \mathbf{D}^{(1,A)} \left(0, -\left\{ \frac{\pi}{2} - \theta \right\}, 0 \right) \quad (367)$$

$$= \begin{pmatrix} \frac{1}{2}(1 + S\theta) & \frac{1}{\sqrt{2}}C\theta & \frac{1}{2}(1 - S\theta) \\ -\frac{1}{\sqrt{2}}C\theta & S\theta & \frac{1}{\sqrt{2}}C\theta \\ \frac{1}{2}(1 - S\theta) & -\frac{1}{\sqrt{2}}C\theta & \frac{1}{2}(1 + S\theta) \end{pmatrix}.$$

Short notations with C=cos and S=sin are used.

$$\begin{aligned} \left[\mathbf{D}^{(1,A)} \left(-\frac{\pi}{2}, -\omega_e t_p, \frac{\pi}{2} \right) \right]^{-1} &= \mathbf{D}^{(1,P)} \left(\frac{\pi}{2}, -\omega_e t_p, -\frac{\pi}{2} \right) \\ &= \begin{pmatrix} \frac{1}{2}(1 + C\omega_e t_p) & -\frac{1}{\sqrt{2}}S\omega_e t_p e^{i\frac{\pi}{2}} & \frac{1}{2}(1 - C\omega_e t_p) e^{i\pi} \\ \frac{1}{\sqrt{2}}S\omega_e t_p e^{-i\frac{\pi}{2}} & C\omega_e t_p & -\frac{1}{\sqrt{2}}S\omega_e t_p e^{i\frac{\pi}{2}} \\ \frac{1}{2}(1 - C\omega_e t_p) e^{-i\pi} & \frac{1}{\sqrt{2}}S\omega_e t_p e^{-i\frac{\pi}{2}} & \frac{1}{2}(1 + C\omega_e t_p) \end{pmatrix} \\ &= \begin{pmatrix} \frac{1}{2}(1 + C\omega_e t_p) & -\frac{i}{\sqrt{2}}S\omega_e t_p & -\frac{1}{2}(1 - C\omega_e t_p) \\ -\frac{i}{\sqrt{2}}S\omega_e t_p & C\omega_e t_p & -\frac{i}{\sqrt{2}}S\omega_e t_p \\ -\frac{1}{2}(1 - C\omega_e t_p) & -\frac{i}{\sqrt{2}}S\omega_e t_p & \frac{1}{2}(1 + C\omega_e t_p) \end{pmatrix}. \end{aligned} \quad (368)$$

Finally,

$$\left[\mathbf{D} \left(0, \frac{\pi}{2} - \theta, 0 \right) \right]^{-1} = \begin{pmatrix} \frac{1}{2}(1 + S\theta) & -\frac{1}{\sqrt{2}}C\theta & \frac{1}{2}(1 + S\theta) \\ \frac{1}{\sqrt{2}}C\theta & S\theta & -\frac{1}{\sqrt{2}}C\theta \\ \frac{1}{2}(1 - S\theta) & \frac{1}{\sqrt{2}}C\theta & \frac{1}{2}(1 + S\theta) \end{pmatrix}. \quad (369)$$

Including these Wigner rotation matrices into Eq. (366) yields

$$\begin{aligned} (T_{11} \ T_{10} \ T_{1-1}) &= I_0 \begin{pmatrix} -\frac{1}{\sqrt{2}}C\theta & S\theta & \frac{1}{\sqrt{2}}C\theta \end{pmatrix} \\ &\times \left[\mathbf{D}^{(1,A)} \left(-\frac{\pi}{2}, -\omega_e t_p, \frac{\pi}{2} \right) \right]^{-1} \quad (370) \\ &\times \left[\mathbf{D}^{(1,P)} \left(0, \frac{\pi}{2} - \theta, 0 \right) \right]^{-1} \end{aligned}$$

$$\begin{aligned} &= I_0 \begin{pmatrix} -\frac{1}{\sqrt{2}}C\theta - \frac{i}{\sqrt{2}}S\theta S\omega_e t_p & S\theta C\omega_e t_p & \frac{1}{\sqrt{2}}C\theta - \frac{i}{\sqrt{2}}S\theta S\omega_e t_p \end{pmatrix} \\ &\times \left[\mathbf{D}^{(1,P)} \left(0, \frac{\pi}{2} - \theta, 0 \right) \right]^{-1} \\ &= I_0 \begin{pmatrix} \frac{1}{\sqrt{2}}C\theta S\theta (C\omega_e t_p - 1) - \frac{i}{\sqrt{2}}S\theta S\omega_e t_p & C^2\theta + S^2\theta C\omega_e t_p \\ -\frac{1}{\sqrt{2}}C\theta S\theta (C\omega_e t_p - 1) - \frac{i}{\sqrt{2}}S\theta S\omega_e t_p \end{pmatrix}. \end{aligned}$$

The three Cartesian components are

$$\begin{aligned} I_x &= \frac{T_{1-1} - T_{11}}{\sqrt{2}} = I_0 \cos \theta \sin \theta (1 - \cos \omega_e t_p), \quad (371) \\ I_y &= -\frac{T_{1-1} + T_{11}}{i\sqrt{2}} = I_0 \sin \theta \sin \omega_e t_p, \\ I_z &= T_{10} = I_0 (\cos^2 \theta + \sin^2 \theta \cos \omega_e t_p). \end{aligned}$$

We do not comment on the spin operator components in Eq. (371). They have been discussed in detail elsewhere.³ Cartesian rotation matrices and Wigner rotation matrices allow us to determine the same results.

12 | CONCLUSION

Throughout the article, we have explored the equivalence between the active rotation of a physical quantity in one direction and the rotation of the coordinate system in the opposite direction in a progressive way. We use both the left- and right-handed rotation conventions whereas the right-handed rotation convention is mainly used in the literature. Then we extend this rule to Euler angles. The article presents redundant mathematical demonstrations between active and passive rotations, but they clarify the meanings of some important expressions not well developed in the literature. Now we have at our disposal the mathematical tools for describing the dynamics of spin with the density matrix operator.

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How to cite this article: Man PP. Wigner active and passive rotation matrices applied to NMR tensor. *Concepts Magn Reson Part A*. 2017;45A:e21385. <https://doi.org/10.1002/cmr.a.21385>.