Double-group theory on the half-shell and the two-level system. I. Rotation and half-integral spin states

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A geometrical construction by Hamilton is used to simplify the quantum mechanics of half-integral spin. A slide rule is described which can be used to (a) compute products of half-integral or integral spin rotation operators, (b) convert between the Euler-angle and "axis-angle" rotation operator parameters, and (c) calculate the time evolution of a spin-1/2 state for a constant Hamiltonian operator. A type of nomogram is developed which suggests ways to simplify the "double-group" theory of half-integral spin in molecular point symmetry, as well as the "ordinary" group theory for integral spin systems. Cubic and icosahedral symmetry group characters are derived for half-integral spin operators.

I. INTRODUCTION

Among the first things we notice about the physical world are the two kinds of freedom of motion or symmetry associated with translational movement and with rotation. Much of theoretical physics of atoms, molecules, and solids is derived from some obvious and some not so obvious consequences of having some translational or some rotational symmetry.

Of the two kinds, translational symmetry is far more widely understood. The idea of adding translation or velocity vectors in order to make resultant vectors is considered elementary. The concept of Fourier analyzing various quantities in free space or crystalline environments, by taking advantage of translational symmetry, is fundamental to modern physics.

The study of rotations, however, is still reserved almost exclusively for experts in "group theory," a subject that is widely believed to be difficult. Part of the reason for this stems from the difficulty in visualizing and computing various properties of rotations and rotation groups. However, we shall show an approach to this subject which we find simpler and more appealing, and which may help to make it more well known.

To this end we review and develop an early idea of Hamilton uncovered recently by Biedenharn[1] and Louck,[2,3] and we discuss some inventions and techniques that follow from this idea. One of the inventions is a slide rule[4] which can be used to compute products of successive rotations, and which serves as a useful instructional and laboratory tool with a number of applications.

As far as the theory of rotations goes, it seems that it is quite easy to be misled by the appearance of the three-dimensional space in which we live. It becomes fairly easy to accept incomplete and unnecessarily complicated descriptions of rotations and techniques for calculating them. For most physicists the first hint that something is missing comes in the form of the rotational behavior of the electron: a complete rotation (2π or 360°) of an electron state gives (-1) times that state. *Two* complete rotations are needed to return any half-integral wave function back to itself. Indeed, it turns out that the transformations of spinors (spin 1/2) rather than those of vectors (spin 1) provide the most complete yet simple description or rotations in our space. Hamilton's quaternions or hypercomplex numbers are related to Pauli's spinors; roughly speaking they *are* the spinors. (It is certainly a credit to Hamilton that he recognized so much of the significance of his invention so many years before the discovery of quantum spin.)

We will discuss some of the basic theory and a number of physical applications of Hamilton's ideas in this article and in a companion article (II) which follows. We have written the articles so that a reader could, depending upon his interest, start by reading either one; while occasionally referring to the other one for certain details.

This article (I) is concerned with the basic mathematics of rotations, and leads into Hamilton's theory, the slide rule, and its application to rotation and time evolution of the spin-1/2 two-level system. The following article (II) starts out describing the evolution and rotation of another two-level system: photon polarization. Then it leads backward into applications of the slide rule in optics calculations and the theory involved there. Either article is dealing with exactly the same type of mathematics, mainly that of Hamilton, and the two-level quantum mathematics of Feynman, Vernon, and Hellwarth,[5] or the earlier work of Rabbi, Ramsey, and Schwinger.[6]

Most of these articles, with the possible exception of Sec. VII in article I, are written at a level close to that of the *Feynman Lectures Vol. III*.[7] The last section (Sec. VII) of this article deals with the representation theory of half-integral spin in molecular point symmetry. Nevertheless, we hope that even this will be a simplification of previous treatments.[8,9]

II. REVIEW OF ROTATIONS

In order to demonstrate rotations, we need something to rotate. A ball mounted in the gimbal and crank device shown by Fig. 1 would serve this purpose. The device clearly defines the famous Euler rotational coordinates[9] ($\alpha\beta\gamma$). For each setting of the α,β, or γ dials there is a unique rotational position. Note, however, that for each rotational position

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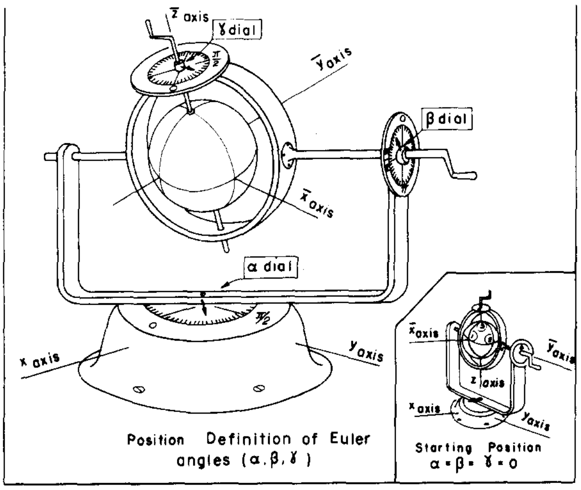


Fig. 1. Euler angles as coordinates. Angles $(\alpha\beta\gamma)$ as read from the dials define the rotational position $(\alpha\beta\gamma)$ of a body.

there are *two* possible settings of the dials: $(\alpha\beta\gamma)$ and $(\alpha - 180°, -\beta, \gamma + 180°)$. It is conventional to eliminate one of these by putting "stops" on the β dial so that $0 \leqslant \beta < 180°$.

Now for mathematical purposes we need to define an *operation* $\mathbf{R}(\alpha\beta\gamma)$ which would take the ball from the original position (000) shown in the inset of Fig. 1 to the position $(\alpha\beta\gamma)$. We may do this with just two cranks fixed to the y and z axes of what we shall call the lab frame (xyz). As shown in Fig. 2 these cranks are fitted with suction cups and permitted to slide in or out along their respective axes. In this way the operations of rotation around y or z can be performed one after the other but not simultaneously. Now the order of application of cranks is important.

Starting with $(\alpha = 0, \beta = 0, \gamma = 0)$ in Fig. 1 we see that the γ crank lies along the z axis. Any setting of the γ dial could just as well be done by the z crank and we shall label this operation $\mathbf{R}(00\gamma)$.

After the γ setting is made, we note that the β crank is still lined up with the y axis. Any setting of the β dial could just as well be done by the y crank, and we shall label this operation $\mathbf{R}(0\beta 0)$.

Finally, after all this, we note the axis of the whole machine, i.e., the α axis is still lined up with the z axis. Any setting of the α dial can just as well be done by using the z crank, and we shall label this operation $\mathbf{R}(\alpha 00)$. Now putting these operations together in the right order (in any product AB we assume B acts first, i.e., $AB\psi = A\psi^B = \psi^{AB}$) we have

$$\mathbf{R}(\alpha\beta\gamma) = \mathbf{R}(\alpha 00)\, \mathbf{R}(0\beta 0)\, \mathbf{R}(00\gamma). \tag{2.1}$$

[Some confusion might exist about the difference between $\mathbf{R}(\alpha 00)$ and $\mathbf{R}(00\gamma)$. In fact there is no difference; from Fig. 1 we see that

$$\mathbf{R}(\alpha 00) = \mathbf{R}(00\alpha) = \mathbf{R}(\alpha - \psi 0 \psi) \tag{2.2}$$

for all ψ.]

So we end up with a way to make all rotations using just the two cranks: y once and z twice. The last two z and y rotations by α and β set the polar angles $\Phi = \alpha$ and $\Theta = \beta$ of the body axis, while the first z rotation by γ sets its "twist."

The efficient use of cranks is one of the operational advantages of the Euler angle definition. Crank operators are represented by matrices, and the fewer matrix operations we have to do, the better.

However, the most "popular" definition of rotations is the axis angle or ω definition $\mathbf{R}[\omega] \equiv \mathbf{R}[\phi\theta\omega]$ (note that we use brackets for axis angles), since, more often that not, one has already chosen some symmetry axis in a crystal or molecule at given polar angles $(\phi\theta)$ which is the axis of a rotation by a given angle (ω). Indeed, we may "picture" a rotation operation much more easily by its $\boldsymbol{\omega}$ vector, where $\hat{\omega}$ is the rotation axis and $\omega = \|\boldsymbol{\omega}\|$ is the angle of rotation. [See Fig. 2(b)]

Nevertheless, ω parameters $[\phi\theta\omega]$ serve rather poorly for defining rotational position. (No machine like Fig. 1 exists for ω.) Furthermore, if we have to compute $\mathbf{R}[\phi\theta\omega]$ as it is usually done using just y and z cranks or rotations, then we have roughly twice as much operator multiplication to do as seen in the following:

$$\begin{aligned}\mathbf{R}[\phi\theta\omega] &= (\mathbf{R}(\phi 00)\mathbf{R}(0\theta 0))\, \mathbf{R}(\omega 00)(\mathbf{R}(\phi 00)\mathbf{R}(0\theta 0))^{-1} \\ &= \mathbf{R}(\phi 00)\mathbf{R}(0\theta 0)\mathbf{R}(\omega 00)\mathbf{R}(0 - \theta 0)\mathbf{R}(-\phi 00). \end{aligned} \tag{2.3}$$

[Equation (2.3) is read as follows: To do $\mathbf{R}[\phi\theta\omega]$ first "un"-rotate with $(\mathbf{R}(\phi 00)\mathbf{R}(0\theta 0))^{-1}$ so that the ω axis lines up with the z axis, then rotate ω radians around z with $\mathbf{R}(\omega 00)$, and finally rotate the ω axis back to the $[\phi\theta]$ position using $\mathbf{R}(\phi 00)\mathbf{R}(0\theta 0)$.]

However, we will discuss in Sec. IV a slide rule makes it possible to convert back and forth between the Euler $(\alpha\beta\alpha)$ and the axis angle $[\phi\theta\omega]$ systems of parameters very easily. Therefore, we will be able to enjoy the advantages of either system.

III. REVIEW OF ROTATION REPRESENTATION

The representation of a rotation by ω_c around a crank axis $\hat{\omega}_c$ may be computed from the equation (see Appendix A)

$$\mathbf{R}[\omega_c] = e^{\omega_c \mathbf{J}_c / i} \tag{3.1}$$

using the representation of the angular momentum operator $\mathbf{J}_c$. (We set $\hbar = 1$.) We shall be interested in the spin-1/2 representations

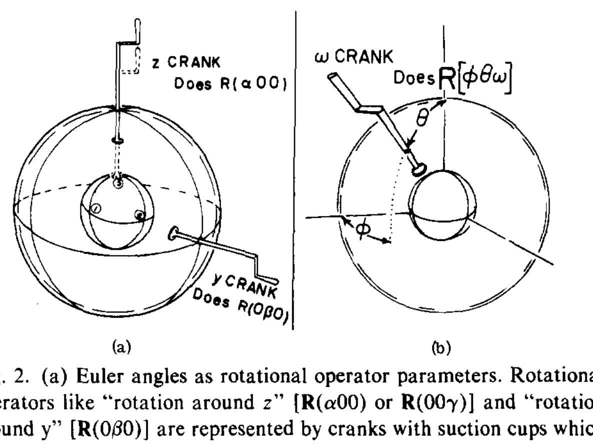


Fig. 2. (a) Euler angles as rotational operator parameters. Rotational operators like "rotation around z" $[\mathbf{R}(\alpha 00)$ or $\mathbf{R}(00\gamma)]$ and "rotation around y" $[\mathbf{R}(0\beta 0)]$ are represented by cranks with suction cups which can be stuck to the body during rotation. The operator $\mathbf{R}(\alpha\beta\gamma)$ which converts the starting position (000) in Fig. 1 (see inset) to the $(\alpha\beta\gamma)$ position is thought of as an ordered product $\mathbf{R}(\alpha 00)\mathbf{R}(0\gamma 0)\mathbf{R}(00\gamma) = \mathbf{R}(\alpha\beta\gamma)$, i.e., as successive applications of the crank operations, as explained in the text. (b) Axis angles as rotational operator parameters. A *single* crank turn of the (000) body by ω around the $[\phi\theta]$ axis could rotate it to any given rotational position $(\alpha\beta\gamma)$, i.e., $\mathbf{R}(\alpha\beta\gamma) = \mathbf{R}[\phi\theta\omega]$.

$$\langle \mathbf{R}(\alpha 00)\rangle = e^{\alpha\langle \mathbf{J}_z\rangle/i} = e^{\alpha\langle \sigma_z\rangle/2i}$$

$$= \exp\left[\alpha\begin{pmatrix}1/2 & 0\\ 0 & 1/2\end{pmatrix}\Big/ i\right] = \begin{pmatrix}e^{-\alpha i/2} & 0\\ 0 & e^{\alpha i/2}\end{pmatrix}, \qquad (3.2)$$

$$\langle \mathbf{R}(0\beta 0)\rangle = e^{\beta\langle \mathbf{J}_y\rangle/i} = e^{\beta\langle \sigma_y\rangle/2i}$$

$$= \exp\left[\beta\begin{pmatrix}0 & -i/2\\ i/2 & 0\end{pmatrix}\Big/ i\right] = \begin{pmatrix}\cos(\beta/2) & -\sin(\beta/2)\\ \sin(\beta/2) & \cos(\beta/2)\end{pmatrix},$$

which are derived using the Pauli spinors $\sigma_c = 2\mathbf{J}_c$ in Appendix B. Combining Eq. (2.4) using Eqs. (2.1) and (2.2) we have the Euler spin-1/2 rotation matrices.

$$\langle \mathbf{R}(\alpha\beta\gamma)\rangle = \langle \mathbf{R}(\alpha 00)\mathbf{R}(0\beta 0)\mathbf{R}(00\gamma)\rangle$$

$$\begin{pmatrix}e^{-i(\alpha+\gamma)/2}\cos(\beta/2) & -e^{i(\gamma-\alpha)/2}\sin(\beta/2)\\ e^{i(\alpha-\gamma)/2}\sin(\beta/2) & e^{i(\alpha+\gamma)/2}\cos(\beta/2)\end{pmatrix}. \qquad (3.3)$$

Similarly by carrying out the multiplications in Eq. (2.3) we have the axis-angle rotation matrices for spin 1/2.

$$\langle \mathbf{R}[\phi\theta\omega]\rangle = \begin{pmatrix}\cos(\omega/2) - i\sin(\omega/2)\cos\theta & -i\cos\phi\sin\theta\sin(\omega/2) - \sin\phi\sin\theta\sin(\omega/2)\\ -i\cos\phi\sin\theta\sin(\omega/2) + \sin\phi\sin(\omega/2)\sin\theta & \cos(\omega/2) + i\sin(\omega/2)\cos\theta\end{pmatrix}. \qquad (3.4)$$

We may expand the preceding matrix in terms of Pauli spinors as follows:

$$\langle \mathbf{R}[\phi\theta\omega]\rangle = \cos(\omega/2)\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}$$
$$-i\cos\phi\sin\theta\sin(\omega/2)\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$$
$$-i\sin\phi\sin\theta\sin(\omega/2)\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}$$
$$-i\cos\theta\sin(\omega/2)\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}, \qquad (3.5)$$

$$\mathbf{R}[\phi\theta\omega] = \cos(\omega/2)\,\mathbf{1} - i\cos\phi\sin\theta\sin(\omega/2)\,\sigma_x - i\sin\phi\sin\theta\sin\omega/2)\,\sigma_y - i\cos\theta\sin(\omega/2)\,\sigma_z.$$

We note that the coefficients of $-i\sigma_c$ is the cth Cartesian component of the vector $[\sin(\omega/2)]\hat{\omega}$.

$$\mathbf{R}[\phi\theta\omega] = \cos(\omega/2)\,\mathbf{1} - i\sin(\omega/2)\,(\hat{\omega}_x\,\sigma_x + \hat{\omega}_y\,\sigma_y + \hat{\omega}_z\,\sigma_z) \qquad (3.6)$$
$$= \cos(\omega/2)\,\mathbf{1} - i\sin(\omega/2)\,\hat{\omega}\cdot\sigma$$

This leads to a multiplication rule for a product of two rotation operators.

$$\mathbf{R}[\phi'\theta'\omega']\mathbf{R}[\phi\theta\omega] = (\cos(\omega/2)\,\mathbf{1} - i\sin(\omega'/2)\,\hat{\omega}\cdot\sigma) \times (\cos(\omega/2)\,\mathbf{1} - i\sin(\omega/2)\,\omega\cdot\sigma) \qquad (3.7)$$
$$= \cos(\omega'/2)\cos(\omega/2)\,\mathbf{1} - i\,[\cos(\omega'/2)\sin(\omega/2)\,\hat{\omega} + \cos(\omega/2)\sin(\omega'/2)\,\hat{\omega}']\cdot\sigma - \sin(\omega'/2)\sin(\omega/2)\,(\hat{\omega}'\cdot\sigma)(\hat{\omega}\cdot\sigma).$$

Finally using Pauli's identity

$$(\hat{\omega}'\cdot\sigma)\,(\hat{\omega}\cdot\sigma) = \hat{\omega}'\cdot\omega\,\mathbf{1} + i(\hat{\omega}'\times\hat{\omega})\cdot\sigma, \qquad (3.8)$$

we have the following expression for the product:

$$\mathbf{R}[\phi'\theta'\omega']\,\mathbf{R}\,[\phi\theta\omega] = [\cos(\omega'/2)\cos(\omega/2) - \sin(\omega'/2)\sin(\omega/2)\,\hat{\omega}'\cdot\hat{\omega}] - i\,[\cos(\omega'/2)\sin(\omega/2)\,\hat{\omega} + \cos(\omega/2)\sin(\omega'2)\,\hat{\omega}' + \sin(\omega'/2)\sin(\omega/2)\,\hat{\omega}'\times\omega]\cdot\sigma. \qquad (3.9)$$

This is the well-known Cayley-Klein formula for rotational products.[10]

If we compare the preceding formula with a generalized "cosine law" for a spherical triangle defined by unit vectors $\hat{v}$ (1), $\hat{v}$ (2), and $\hat{v}$ (3), as shown in Fig. 3 we will be able to derive Hamilton's multiplication rule. To derive the cosine law we express the vector $\hat{v}(2)$ and $\hat{v}(3)$ in terms of $\hat{v}(1)$. First we have

$$\hat{v}(2) = \cos(12)\,\hat{v}(1) + \sin(12)\,\hat{v}(1)\times\hat{\omega}(12), \qquad (3.10a)$$

$$\hat{v}(3) = \cos(23)\,\hat{v}(2) + \sin(23)\,\hat{v}(2)\times\hat{\omega}(23), \qquad (3.10b)$$

where the cross product definition is

$$\hat{v}(1)\times\hat{v}(2) \equiv \sin(12)\,\hat{\omega}(12),$$
$$\hat{v}(2)\times\hat{v}(3) \equiv \sin(23)\,\hat{\omega}(23),$$

and (ij) is the unit circle arc length or angle between $\hat{v}(i)$ and $\hat{v}(j)$. Then, substituting (3.10a) into (3.10b) gives the following

$$\hat{v}(3) = \cos(23)\cos(12)\,\hat{v}(1) + [\cos(23)\sin(12)\,\hat{\omega} + \sin(23)\cos(12)\,\hat{\omega}']\times\hat{v}(1) + \sin(23)\sin(12)\,\hat{\omega}'\times[\hat{\omega}\times\hat{v}(1)]. \qquad (3.11)$$

Finally using the vector identities

$$\hat{\omega}'\times(\hat{\omega}\times\hat{v}(1)) \equiv (\hat{\omega}'\cdot\hat{v}(1))\hat{\omega} - (\hat{\omega}'\cdot\hat{\omega})\,\hat{v}(1),$$
$$(\hat{\omega}'\times\hat{\omega})\times\hat{v}(1) \equiv (\hat{\omega}'\cdot\hat{v}(1))\hat{\omega} - (\omega\cdot\hat{v}(1))\hat{\omega}' = (\hat{\omega}'\cdot\hat{v}(1))\hat{\omega},$$

we derive $\hat{v}(3)$ in terms of $\hat{v}(1)$, $\hat{\omega}$, and $\hat{\omega}'$

$$\hat{v}(3) = [\cos(23)\cos(12) - \sin(23)\sin(12)\,\hat{\omega}'\cdot\hat{\omega}]\hat{v}(1) + [\cos(23)\sin(12)\hat{\omega} + \cos(12)\sin(23)\,\hat{\omega}' + \sin(23)\sin(12)\,\hat{\omega}'\times\hat{\omega}]\times\hat{v}(1). \qquad (3.12)$$

We can see that the expressions within parentheses or brackets in the preceding Eq. (3.12) are identical in form to those in Eq. (3.9). By comparing the form of Eq. (3.10) to that of (3.6) we see that each great circle arc in Fig. 3 represents one of the rotations in the product equation.

$$\mathbf{R}[\phi''\theta''\omega''] = \mathbf{R}[\phi'\theta'\omega']\cdot\mathbf{R}\,[\phi\theta\omega]. \qquad (3.13)$$

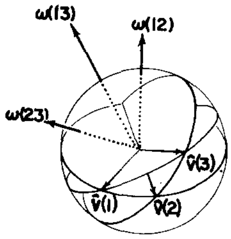
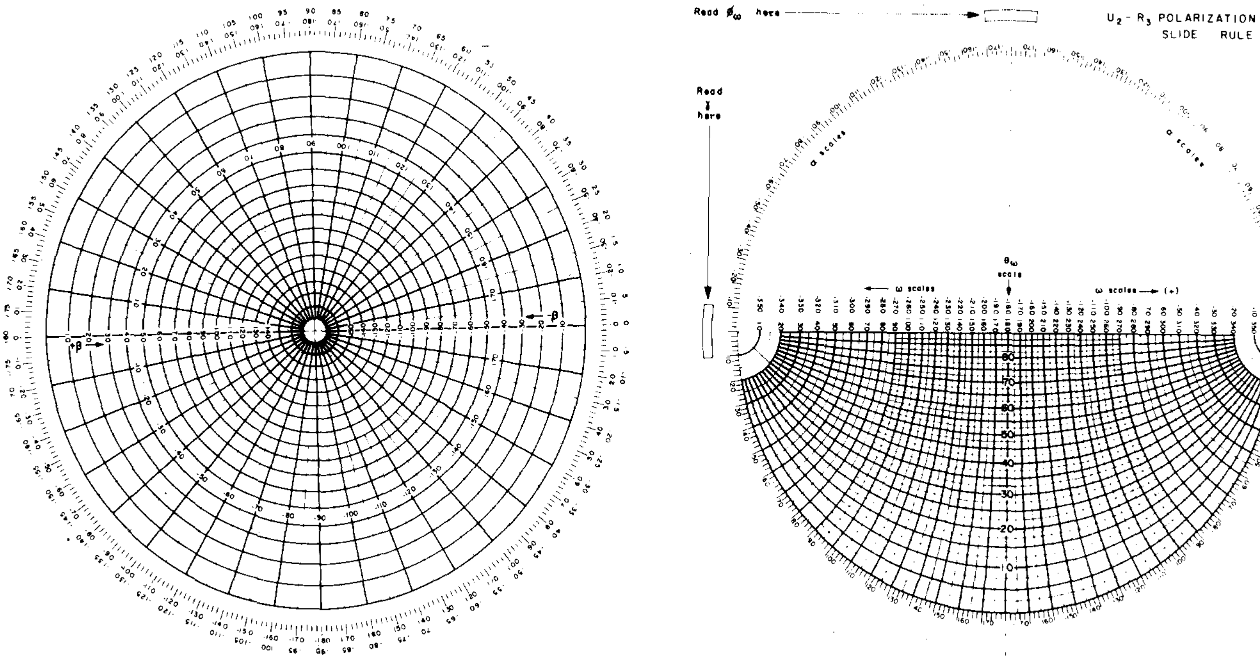


Fig. 3. Great circle arcs and their polar axes.



(a) (b)

Fig. 4. Rotational slide rule (copyright William G. Harter 1976). (a) Upper scale; (b) lower scale.

Arc (12) represents the first rotation $\mathbf{R}[\phi\theta\omega]$ around $\hat{\omega}$, arc (23) represents the second rotation $\mathbf{R}[\phi'\theta'\omega']$ around $\hat{\omega}$, and arc (13) represents their product $\mathbf{R}[\phi''\theta''\omega'']$. One interesting thing is that the arcs are each *one-half* of their corresponding angle of rotation.

$$(12) = \omega/2, \quad (23) = \omega'/2, \quad (13) = \omega''/2. \quad (3.14)$$

This 1/2 comes more or less directly from the $\langle\langle \mathbf{J}_z \rangle\rangle = 1/2$ value of angular momentum. Indeed, the "spherical vector addition" of Hamilton must give the correct multiplication rules for rotations of electron waves of half-integral spin states since the fundamental spin-1/2 algebra was used to derive it.

IV. HAMILTON'S RULES AND THE ROTATIONAL SLIDE RULE

Hamilton's rules, as derived in the preceding section, are the following: To find the product of two rotations $\mathbf{R}[\boldsymbol{\omega}]$ and $\mathbf{R}[\boldsymbol{\omega}']$, (a) construct the great circle arcs perpendicular to $\boldsymbol{\omega}$ and $\boldsymbol{\omega}'$, respectively, on the unit sphere, (b) draw arrows or "vectors" along each arc of length $\omega/2$ and $\omega'/2$, respectively, and pointed in the directions of rotation so that the head of the arrow of the first rotation touches the tail of the arrow of the second one, and (c) find the great circle arc between the tail of the first arrow and the head of the second. The resulting vector-sum arrow defines the desired product rotation.

Figure 4 shows the slide rule that permits one to carry out the spherical vector addition accurately. The upper scale should be printed on a transparent plastic and fastened so its center stays precisely over the center of the lower scale. A small bolt through the centers, or better, a guiding rim is needed so that the upper scale may turn smoothly over the bottom one. (Both scales should be put on transparent plastic if the device is to be used with an overhead projector for instruction.)

To compute a product of two rotations $\mathbf{R}[\phi\theta\omega]$ and $\mathbf{R}[\phi'\theta'\omega']$ we first draw the arcs of the respective rotations onto the upper scale. An arc is drawn by setting the desired ϕ in the "ϕ window" (see top of lower scale) and tracing the desired (θ,ω) arc using the θ and ω scales of the lower scale. (One may use a fine overhead projector pencil or a Leroy acetate pen. Either one erases easily from Plexiglas.) It is necessary to first find the intersection of the $[\phi\theta]$ arc with the $[\phi'\theta']$ arc. Then we count back ω degrees along the $[\phi\theta]$ arc to mark the tail of the first vector, and we count forward ω' degrees along the $[\phi'\theta']$ arc to mark the head of the second vector. The "ω scale" is used for each counting. Finally the slide rule is turned until the head and the tail points lie along a θ line. (Interpolation may be necessary.) Then the desired answer ϕ'' in the product $\mathbf{R}[\phi''\theta''\omega''] = \mathbf{R}[\phi'\theta'\omega']$ $\mathbf{R}[\phi\theta\omega]$ is read in the ϕ window, while θ'' and ω'' are shown by their respective scales.

The upper slide rule scale is a stereographic projection of the "northern" hemisphere of a globe while the lower scale is the same projection of half the "western" hemisphere. The structure of rotations as described by Hamilton makes it possible for us to do all products on just half of a sphere. A rotation for which ω is less than 180° corresponds to an arc of less than 90°. Any rotation with ω between 180° and 360° can be replaced by a rotation that goes the other way by angle $-(360° - \omega)$ and has an arc of $-(180° - \omega/2)$ which again is less than 90°. Whenever we do this trick while operating on electron wave functions, we need to multiply the result by (-1).

$$\mathbf{R}(\cdots\omega\cdots) = \begin{cases} \mathbf{R}(\omega - 2\pi\cdots) \text{ for integral spin} \\ -\mathbf{R}(\omega - 2\pi\cdots) \text{ for half-integral spin.} \end{cases} \quad (4.1)$$

So anytime there appears an arc vector that extends over the edge of the slide rule, we simply replace it by one of length $(360° - \omega)$ going the other way. [Remember the

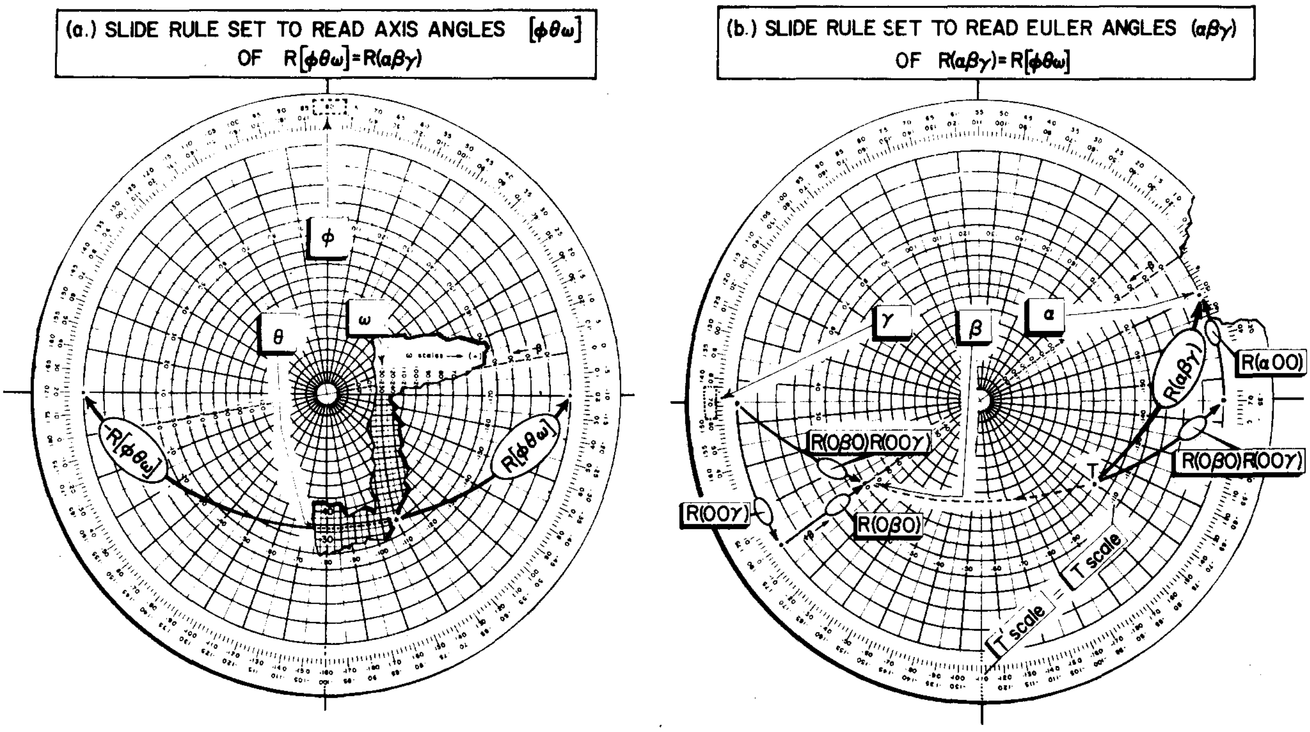


Fig. 5. (Euler angle [axis angle] conversion on the slide rule. (a) Axis angles are (approximately) $[\partial\theta\omega] = [80° \ 34° \ 129°]$; (b) Euler angles are $(\alpha\beta\gamma) = (50° \ 60° \ 70°)$.

factor of (-1) for all half-integral spin problems, but forget it for the others.]

Using Fig. 5 we can understand how the slide rule may be used to convert back and forth between Euler angles $(\alpha\beta\gamma)$ and axis angles $[\phi\theta\omega]$ in the equation

$$\mathbf{R}(\alpha\beta\gamma) = \mathbf{R}[\phi\theta\omega] \equiv \mathbf{R}[\omega]. \qquad (4.2)$$

Figure 5(b) shows a given rotation $\mathbf{R}[\omega]$ reduced by two vector sums into the product $\mathbf{R}(\alpha 00)$ $\mathbf{R}(0\beta 0)$ $\mathbf{R}(00\gamma) = \mathbf{R}(\alpha\beta\gamma)$ given by Eq. (2.1). The scales of the slide rule have been designed so that these products can be done without drawing arrows. To obtain the position shown in Fig. 5(b) one must move the upper scale so that the angle between the meridian passing through the tail of $\mathbf{R}[\omega]$ and the $+\beta$ scale is bisected by the center (θ) line of the lower scale. The "tail scales" or T scales indicated in Fig. 5(b) make this easy. We simply read the angle of $\mathbf{R}[\omega]$'s tail using the T scale, find this number on the T' scale, and set it over the center line below, as shown in Fig. 5(b).

So the procedure for converting an $\mathbf{R}[\phi\theta\omega]$ to an equal $\mathbf{R}(\alpha\beta\gamma)$ is simple. After setting the ϕ in the ϕ window and locating the tail using the θ and ω scales (if $\mathbf{R}[\phi\theta\omega]$ has just been given by a previous calculation the ϕ position will be all set up. We only have to locate by subtraction (ω (head) $-\omega$ (tail) where the tail would be if the head is moved to the edge of the slide rule), we bisect the tail angle using the T scales and read off the answers α,β, and γ. γ is in the γ window, α is pointed out by the $\mathbf{R}[\omega]$ vector head, and β is on the $+\beta$ scale "across from" the tail. (Follow a circle or a θ line to $+\beta$.)

The inverse calculation: converting $\mathbf{R}(\alpha\beta\gamma)$ to $\mathbf{R}[\phi\theta\omega]$, is just as easy. After setting γ in the γ window, we locate the tail of $\mathbf{R}[\phi\theta\omega]$ using the $+\beta$ and T scales, and the head of $\mathbf{R}[\phi\theta\omega]$ on the edge using the α scale. (It helps to put a dot at each end point with the marking pen.) Then we rotate the slide rule until the head is over an $\alpha = 0$ position so we read off ω and θ from the tail point and ϕ in the ϕ window.

When doing the conversions for spin 1/2 we may need to include a (-1) phase. The (-1) will be necessary for all $\mathbf{R}[\omega]$ vectors that cross the lower scale center line, i.e., the θ-scale line. Note that for each α and tail point you can choose one vector that does cross the center line and one that does not. Both are right but the former has the (-1).

If a tail falls near the $-\beta$ axis one may find it to be more convenient and accurate to bisect with respect to it. As we mentioned in Sec. II $+\beta$ and $-\beta$ rotations are related by

$$\begin{aligned}\mathbf{R}(\alpha - \beta\gamma) &= \mathbf{R}(\alpha + 180° \ \beta \ \gamma - 180°) \\ &= \mathbf{R}(\alpha - 180° \beta \ \gamma + 180°). \qquad (4.3)\end{aligned}$$

A number of other interesting problems can be solved on the slide rule or abstractly using Hamilton's theory. For example, suppose we want to find which rotations $\mathbf{T}$ will transform one given rotation $\mathbf{R}$ into rotation $\mathbf{R}'$ given by

$$\mathbf{R}' = \mathbf{T}\mathbf{R}\mathbf{T}^{-1}. \qquad (4.4)$$

The great circles belonging to $\mathbf{R}$ and $\mathbf{R}'$ must intersect in two antipodal points on the sphere as shown in Fig. 6 and one of these points must show up on the slide rule. Obviously one of the possible solutions to Eq. (4.4) is a rotation $\mathbf{T}$ around an axis through the two antipodal points which takes the $\mathbf{R}$ great circle into that of $\mathbf{R}'$. The great circle corresponding to this particular $\mathbf{T}$ rotation intersects the $\mathbf{R}$ and $\mathbf{R}'$ circles at points 90° from either antipodal point, as shown in Fig. 6. We may measure the 90° arcs on the slide rule using the ω scales, however, we must measure 180° of ω since the ω scale is half-angle. Two such measurements are sufficient to construct the arc between two 90° points on $\mathbf{R}$ and $\mathbf{R}'$ circles. The Hamilton arc vector corresponding to the rotation $\mathbf{T}$ is exactly half of the arc between the 90° points as seen in Fig. 6.

We note that if $\mathbf{R} = \mathbf{R}[\phi\theta\omega]$, then $\mathbf{R}' = \mathbf{R}[\phi'\theta'\omega']$ must be a rotation by the same angle $\omega = \omega'$. Indeed, this is a necessary and sufficient condition for $\mathbf{R}$ and $\mathbf{R}'$ to be in the same *class* of the rotation group R_3.

Furthermore, since the subgroup C_R of all rotations $\mathbf{R}''$ $= \mathrm{R}[\phi\theta\omega'']$, having the same axis as $\mathbf{R}$, will commute with $\mathbf{R}$, i.e.,

$$\mathbf{R}[\phi\theta\omega] = \mathbf{R}[\phi\theta\omega'']\,\mathbf{R}[\phi\theta\omega]\,\mathbf{R}^{-1}\,[\phi\theta\omega''],$$

we then see that all rotations $\mathbf{T}'' = \mathbf{TR}''$ will satisfy Eq. (4.4) as well as $\mathbf{T}$. [The set of all rotations $\mathbf{TR}''$ is called the (**T**) *left coset* of C_R.]

The problem of finding **T** is equivalent to another: find the rotation transformation that transforms one orthogonal coordinate system to another. An orthogonal coordinate system can be defined by a spherical triangle with each side being 90° of arc. The vertices of the triangle are the points where the three axes x, y, and z of the system poke through the unit sphere. In fact it is easy to see that just *one* directed 90° arc (say the $x \rightarrow y$ arc) is enough to define a system. Now if we have two such arcs, one for each of two systems, we can find a **T** on the slide rule which rotates the great circle of one into that of the other. This is followed by a rotation along the new great circle in order to bring the old arc on top of the new one. The combination of **T** and this last rotation is the desired coordinate transformation.

Three orthogonal 90° arcs and the 180° rotations associated with them can be thought of as the basis of Hamilton's theory. In fact the three matrices,

$$Q_x = \langle \mathbf{R}(-90°\ 180°\ 90°)\rangle = -i\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} \equiv -i\langle\sigma_x\rangle,$$

$$Q_y = \langle \mathbf{R}(0\ 180°\ 0)\rangle = -i\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix} \equiv -i\,\langle\sigma_y\rangle,$$

$$Q_z = \langle \mathbf{R}(180°\ 0\ 0)\rangle = -i\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} \equiv -i\,\langle\sigma_z\rangle, \qquad (4.5)$$

are the famous quaternion matrices which satisfy the well-known multiplication rules

$$Q_x^2 = Q_y^2 - Q_z^2 = -1,\ Q_xQ_y = Q_z = -Q_yQ_x \quad \cdots (xyz \text{ cyclic}), \qquad (4.6)$$

of the quaternion group. Many interesting mathematical properties of these "hypercomplex" quantities are discussed by Biedenharn and Louck.[3]

V. TIME BEHAVIOR OF SPIN-1/2 STATES

We now briefly review a solution of the Schrödinger equation for a spin-1/2 system and indicate how the rotational slide rule may be used to calculate it. The Schrödinger equation is written

$$i\frac{\partial}{\partial t}\begin{pmatrix}\langle 1\,|\psi(t)\rangle\\ \langle 2\,|\psi(t)\rangle\end{pmatrix} = \begin{pmatrix}H_{11} & H_{12}\\ H_{12}^* & H_{22}\end{pmatrix}\begin{pmatrix}\langle 1\,|\psi(t)\rangle\\ \langle 2\,|\psi(t)\rangle\end{pmatrix}, \qquad (5.1)$$

where $|1\rangle$ stands for the state of "spin-up" ($\langle 1|J_z|1\rangle = 1/2$) and $|2\rangle$ stands for "spin-down" ($\langle 2|J_z|2\rangle = -1/2$), and H_{ij} are components of the Hamiltonian matrix.

If the H_{ij} are constant, we may use the well known[5,6] exponential solution to Eq. (5.1). This solution has the form

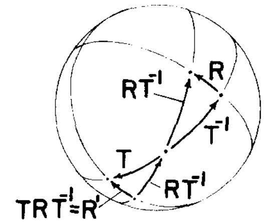


Fig. 6. Showing class equivalence and coordinate transformations using Hamilton arc vectors.

$$\begin{pmatrix}\langle 1|\psi(t)\rangle\\ \langle 2|\psi(t)\rangle\end{pmatrix} = \exp\left[\frac{t}{i}\begin{pmatrix}H_{11} & H_{12}\\ H_2^* & H_{22}\end{pmatrix}\right]\begin{pmatrix}\langle 1|\psi(o)\rangle\\ \langle 2|\psi(o)\rangle\end{pmatrix}, \qquad (5.2a)$$

where we expand the matrix exponent in terms of spin angular momentum operators $\mathbf{J}_x$, $\mathbf{J}_y$, and $\mathbf{J}_z$

$$\begin{pmatrix}H_{11} & H_{12}\\ H_{12}^* & H_{22}\end{pmatrix} = (H_{11} + H_{22})/2\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} + (H_{12} + H_{12}^*)\begin{pmatrix}0 & 1/2\\ 1/2 & 0\end{pmatrix} + i(H_{12} - H_{12}^*)\begin{pmatrix}0 & -i/2\\ 1/2 & 0\end{pmatrix} + (H_{11} - H_{22})\begin{pmatrix}1/2 & 0\\ 0 & -1/2\end{pmatrix} \qquad (5.2b)$$

$$= H_0\langle\mathbf{1}\rangle + \omega_x\,\langle\mathbf{J}_x\rangle + \omega_y\langle\mathbf{J}_y\rangle + \omega_z\langle\mathbf{J}_z\rangle,$$

and where we let

$$H_0 = (H_{11} + H_{22})/2,\ \omega_x = \mathrm{Re}\,H_{12},\quad \omega_y = -\mathrm{Im}\,H_{12},\quad \omega_z = H_{11} - H_{22}. \qquad (5.2c)$$

Rewriting the solution in terms of the $\boldsymbol{\omega}$ vector we have

$$\begin{pmatrix}\langle 1|\psi(t)\rangle\\ \langle 2|\psi(t)\rangle\end{pmatrix} = e^{H_0t/i}\,e^{\boldsymbol{\omega}\cdot\langle\mathbf{J}\rangle t/i}\begin{pmatrix}\langle 1|\psi(o)\rangle\\ \langle 2|\psi(o)\rangle\end{pmatrix} = e^{H_0t/i}\,e^{(\omega t/i)\langle\mathbf{J}_\omega\rangle}\begin{pmatrix}\langle 1|\psi(o)\rangle\\ \langle 2|\psi(o)\rangle\end{pmatrix} \qquad (5.3)$$

which, except for the overall phase $e^{H_0t/i}$, is just a rotation $\mathbf{R}[\omega t]$ of the initial state $|\psi(0)\rangle$. [Recall Eq. (3.1).]

$$|\psi(t)\rangle = e^{H_0t/i}\,\mathbf{R}[\omega t]\,|\psi(o)\rangle. \qquad (5.4)$$

Following Refs. 5 and 6 one may show that all states $|\psi(0)\rangle \cdots |\psi(t)\rangle$ can be written as rotations $\mathbf{R}(\alpha_0\beta_0\gamma_0)\cdots\mathbf{R}(\alpha_t\beta_t\gamma_t)$ of some single state, say "spin-up" $|1\rangle$. For any given $|\psi\rangle$ may be set equal to

$$|\psi\rangle = \mathbf{R}(\alpha\beta\gamma)\,|1\rangle, \qquad (5.5a)$$

or [using Eq. (3.3)]

$$\begin{pmatrix}\langle 1|\psi\rangle\\ \langle 2|\psi\rangle\end{pmatrix} = \begin{pmatrix}e^{-i(\alpha+\gamma)/2}\cos(\beta/2) & -e^{i(\gamma-\alpha)/2}\sin(\beta/2)\\ e^{i(\alpha-\gamma)/2}\sin(\beta/2) & e^{i(\alpha+\gamma)/2}\cos(\beta/2)\end{pmatrix}\begin{pmatrix}1\\ 0\end{pmatrix} \qquad (5.5b)$$

$$= e^{-i\gamma/2}\begin{pmatrix}e^{-i\alpha/2}\cos(\beta/2)\\ e^{i\alpha/2}\sin(\beta/2)\end{pmatrix},$$

for some Euler angles α, β, and γ. Furthermore the expectation values of the spin angular momentum vector in this state are

$$\langle\psi|\,\mathbf{J}_x\,|\psi\rangle = \begin{pmatrix} e^{-i\alpha/2}\cos(\beta/2) \\ e^{i\alpha/2}\sin(\beta/2) \end{pmatrix}^* \times \begin{pmatrix} 0 & 1/2 \\ 1/2 & 0 \end{pmatrix} \begin{pmatrix} e^{-i\alpha/2}\cos\beta/2 \\ e^{i\alpha/2}\sin\beta/2 \end{pmatrix} \tag{5.6}$$

$$= [(e^{i\alpha} + e^{-i\alpha})/4]\sin(\beta/2)\cos(\beta/2)$$

$$= (1/2)\cos\alpha\,\sin\beta,$$

$$\langle\psi|\,\mathbf{J}_y\,|\psi\rangle = (1/2)\sin\alpha\,\sin\beta,\ \langle\psi|\mathbf{J}_z|\psi\rangle = (1/2)\cos\beta,$$

i.e., a spin-½ vector with polar angles $\Phi = \alpha$ and $\Theta = \beta$. (The "twist angle" γ is just the overall phase multiplied by 2.) We see here how Euler angles provide a convenient description of a state while axis angles $[\omega]$ provide a convenient description of an operator.

Putting these two descriptions [Eqs. (5.4) and (5.5a) together we have

$$|\psi(t)\rangle \equiv \mathbf{R}(\alpha_t\beta_t\gamma_t)\,|1\rangle$$

$$= e^{H_0t/i}\,\mathbf{R}[\omega t]\cdot\mathbf{R}(\alpha_0\beta_0\gamma_0)\,|1\rangle$$

$$= \mathbf{R}[\omega t]\cdot\mathbf{R}(\alpha_0\beta_0\gamma_0 - 2H_0t)\,|1\rangle. \tag{5.7}$$

Now the problem of finding the final state $|\psi(t)\rangle$ reduces to computing the α_t, β_t, and γ_t of the product operator

$$\mathbf{R}(\alpha_t\beta_t\gamma_t) = \mathbf{R}[\omega t]\cdot\mathbf{R}(\alpha_0\beta_0\gamma_0 - 2H_0t), \tag{5.8}$$

given ωt, H_0t [Eq. (5.2c)], α_0, β_0, and γ_0 [Eq. (5.5b)]. The procedure for doing this on the slide rule has been described in the preceding section. The physical effect of $\mathbf{R}[\omega t]$ is the well-known precession of the spin vector $\langle\mathbf{J}(\alpha\beta)\rangle$ around the axis vector $\boldsymbol{\omega}$ as time goes on.

In article II we shall do some numerical examples in detail for the analogous optical activity problem. The physical interpretation of the various angles α, β, γ, and ωt is probably easier to understand there.

VI. FINITE ROTATIONAL SYMMETRIES

Just as the integers are a subset of all numbers, so are the finite or molecular point symmetries a subset of all spatial rotations. In fact, it is common practice to write multiplication tables for the finite groups that remind one of the "times tables" for arithmetic. Now we shall see how simple nomograms can be made which contain all possible products of symmetry rotations. We use as our examples the two most complicated finite symmetries in nature, the cubic-octahedral symmetry (O), and the icosahedral-dodecahedral symmetry (I).

Figure 7(a) shows the octahedral rotations as they appear according to Hamilton's prescription for assigning arcs that are each half the corresponding angle of rotation. There are five classes of rotations: the null or identity operator, and four classes of nonzero rotations. The 120° rotations ($\mathbf{r}_1$, $\mathbf{r}_2$, $\mathbf{r}_3$, $\mathbf{r}_4$) in the counterclockwise direction around (111), ($\underline{1}\underline{1}1$), ($1\underline{1}\underline{1}$) and ($\underline{1}1\underline{1}$) axes, respectively, are in the same class with 240° rotations ($\mathbf{r}_1^2$, $\mathbf{r}_2^2$, $\mathbf{r}_3^2$, $\mathbf{r}_4^2$) about the same axes. Similarly, the 90° rotations ($\mathbf{R}_1$, $\mathbf{R}_2$, $\mathbf{R}_3$) around x, y, and z [i.e., (100), (010), and (001)] axes, respectively, are in the same class with the 270° rotations ($\mathbf{R}_1^3$, $\mathbf{R}_2^3$, $\mathbf{R}_3^3$) about the same axes. However, the 180° x, y, and z rotations ($\mathbf{R}_1^2$, $\mathbf{R}_2^2$, $\mathbf{R}_3^2$) are in a class by themselves as are the 180° rotations ($\mathbf{i}_1$, $\mathbf{i}_2$, $\mathbf{i}_3$, $\mathbf{i}_4$, $\mathbf{i}_5$, $\mathbf{i}_6$) around the (101), ($10\underline{1}$), (110), ($1\underline{1}0$), ($0\underline{1}1$), and (011) axes.

One should note that for ordinary (nonspin 1/2) transformation a rotation like the 270° $\mathbf{R}_3^3$ around (001) has the same effect as a 90° rotation around (001), i.e., the same as a 90° *clockwise* rotation around (001). So its easy to see that $\mathbf{R}_3$ and $\mathbf{R}_3^3$ are in the same class since they are both 90° rotations around octahedral vertices, as are $\mathbf{R}_1$, $\mathbf{R}_2$, $\cdots$ etc. To be more precise, the six operators $\mathbf{R}_1$, $\mathbf{R}_2$, $\cdots$, $\mathbf{R}_3^3$ belong to six equivalent vertices of the octahedron and there exist octahedral transformations $\mathbf{T}$ to transform them into each other.

$$\mathbf{R}_1 = \mathbf{T}\mathbf{R}_2\mathbf{T}^{-1} \quad (\text{for } \mathbf{T} = \mathbf{r}_1^2, \mathbf{R}_3, \cdots)$$

$$= \mathbf{T}\mathbf{R}_3\mathbf{T}^{-1} \quad (\text{for } \mathbf{t}, \mathbf{r}_1, \mathbf{R}_2, \cdots). \tag{6.1}$$

Class relations like the preceding can be derived by direct inspection, on the rotational slide rule, or most easily using the nomogram in Fig. 7(a)–(c).

To construct the nomogram, we first superimpose the great circles of each rotation as shown in the stereopicture in Fig. 7(b). A hemispherical projection of Fig. 7(b), with the arrows labeled, is the desired nomogram in Fig. 7(c). Note that we have labeled many of the elements with minus signs. For electrons or spin-½ states, we will have, for example, that the rotation $\mathbf{R}_3^3$ by 270° around (001) is not quite the same as the 90° clockwise rotation $\mathbf{R}_3^{-1}$. In fact we have [from Eq. (4.1)]

$$\mathbf{R}_j^{-1} = -\mathbf{R}_j^3, \tag{6.2}$$

and this is how we have labeled all rotations that would have otherwise given arrows longer than 90°.

Thus the nomogram gives not just the O group table, but all 48 × 48 = 3304 entries of the so called "double group" of O. However, we shall show in Sec. VII that there is no need to deal with double groups, and that in fact the physical applications of symmetry to half-integral spin should be roughly half as much work instead of double trouble!

Our last example of finite symmetry is the icosahedral group I. This is the most complex multiaxial three-dimensional point symmetry, and includes 59 nonzero rotations indicated in Fig. 8. We label each one by the permutation which it performs on integers 1 through 5 attached to the icosahedron. For example, (153) means all 1's jump to where 5's were, 5's jump to where 3's were, 3's jump to where 1's were, but 2's go into 2's and 4's into 4's. This corresponds to a 120° rotation around the axis labeled (153) in Fig. 8. In this way the multiplication rules for permutations give the group multiplication for I symmetry. (An octahedron can be numbered so that all the rotations in O correspond to permutations of 1 through 4.)

However, to combine rotations for half-integral spin states easily, we need to make a nomogram using Hamilton's rules. The great circle arcs corresponding to various classes of I are shown on the stereo drawing of Fig. 9(a)–(c), and they are superimposed in Fig. 9(d). It is interesting to see which part of the Hamilton arcs make up the basic Fuller geodesic[11] dome which is shown in Fig. 9(e). The dark arcs are the 72°–144° class circles, while the lighter lines are segments of the 180° class circles, which are projections of the edges of the icosahedron onto the sphere.

A projection of one side of Fig. 9(d) is the I nomogram shown by Fig. 10. Each permutations symbol corresponds to a given counterclockwise rotation around the axis indicated in Fig. 9 by the angle written there. Rotations by more than 180° are replaced by shorter clockwise arrows and a minus sign as usual. One difference between this nomogram and the cubic one (Fig. 7(c)) is the order of products ab instead of ba. This is because the operations of I are defined

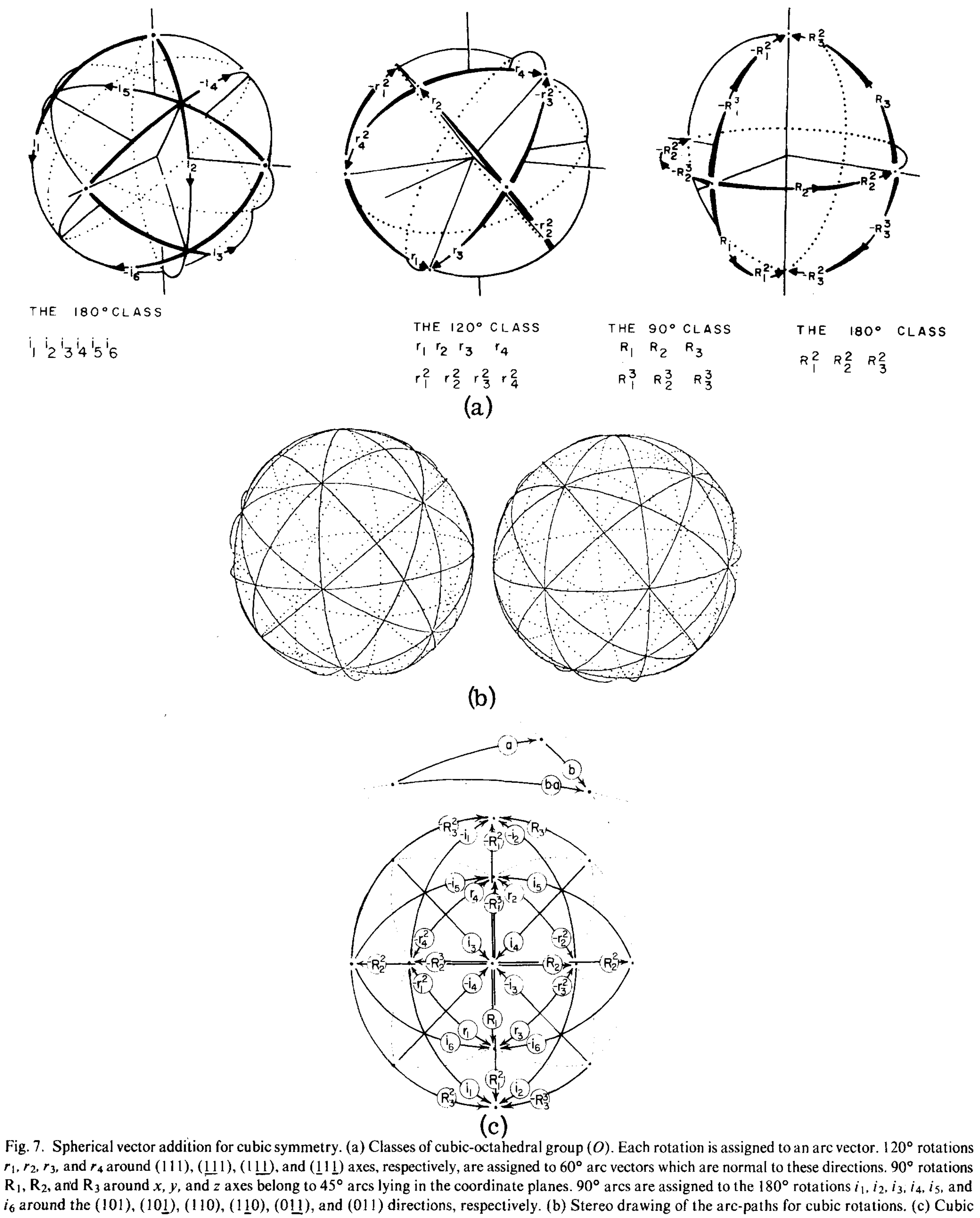


Fig. 7. Spherical vector addition for cubic symmetry. (a) Classes of cubic-octahedral group (O). Each rotation is assigned to an arc vector. 120° rotations r_1, r_2, r_3, and r_4 around (111), ($\underline{1}\underline{1}$1), (1$\underline{1}\underline{1}$), and ($\underline{1}1\underline{1}$) axes, respectively, are assigned to 60° arc vectors which are normal to these directions. 90° rotations R_1, R_2, and R_3 around x, y, and z axes belong to 45° arcs lying in the coordinate planes. 90° arcs are assigned to the 180° rotations i_1, i_2, i_3, i_4, i_5, and i_6 around the (101), (10$\underline{1}$), (110), (1$\underline{1}$0), (0$\underline{1}\underline{1}$), and (011) directions, respectively. (b) Stereo drawing of the arc-paths for cubic rotations. (c) Cubic symmetry nomograms. To multiply rotations using the nomogram, one imagines moving their vectors into a head-to-tail position as shown in the key above the figure. The desired product corresponds to the resultant or vector sum. One ignores the signs written in the labeling circles when operating on integral-spin (Bose) systems, but they must be included in any calculation involving half-integral (Fermi) systems.

with respect to the body frame, i.e., the integers 1–5 are glued to the icosahedron and ride with it.

A nomogram can be constructed and used for any of the other molecular point groups in the same way. Many of the point groups contain "improper" reflections or rotation reflections, however, as long as the proper rotation products are known, the improper ones are easily found. Each improper operation S is always a product

$$\mathbf{S} = \mathbf{I} \cdot \mathbf{R} = \mathbf{R} \cdot \mathbf{I} \tag{6.3}$$

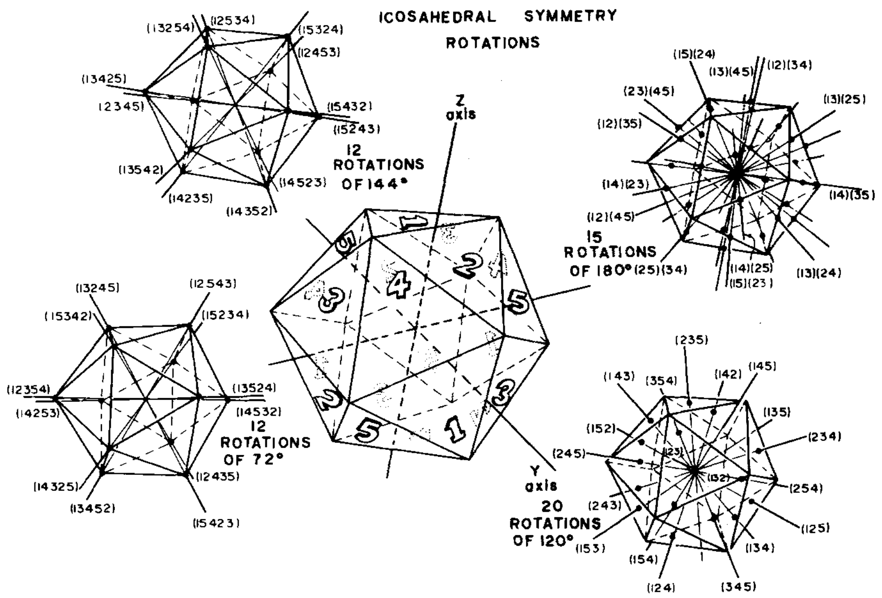


Fig. 8. Icosahedral symmetry rotations. Each rotation corresponds to an even permutation of the integers 1–5 which are written on the icosahedron.

of a proper rotation and the inversion **I** ($x \rightarrow -x, y \rightarrow -y$, and $z \rightarrow -z$). Furthermore, inversion commutes with all rotations and $\mathbf{I}^2 = \mathbf{1}$. Finally, one may assume that inversion has no effect on spin functions.

There is one very interesting observation about plane reflections which is part of a development of Hamilton's rules. For any two planes in space, a reflection through plane 1 followed by a reflection through plane 2 is the same as a rotation by twice the dihedral angle (1 2) of intersection between the two planes. The Hamilton arc (1 2) = $\omega/2$ is precisely the great circle arc perpendicular to the two planes and extending from 1 to 2.

VII. SIMPLIFIED DERIVATION OF HALF-INTEGRAL SPIN CHARACTERS

The derivation of ordinary (integral spin) characters of irreducible representations (IR) of point groups is based

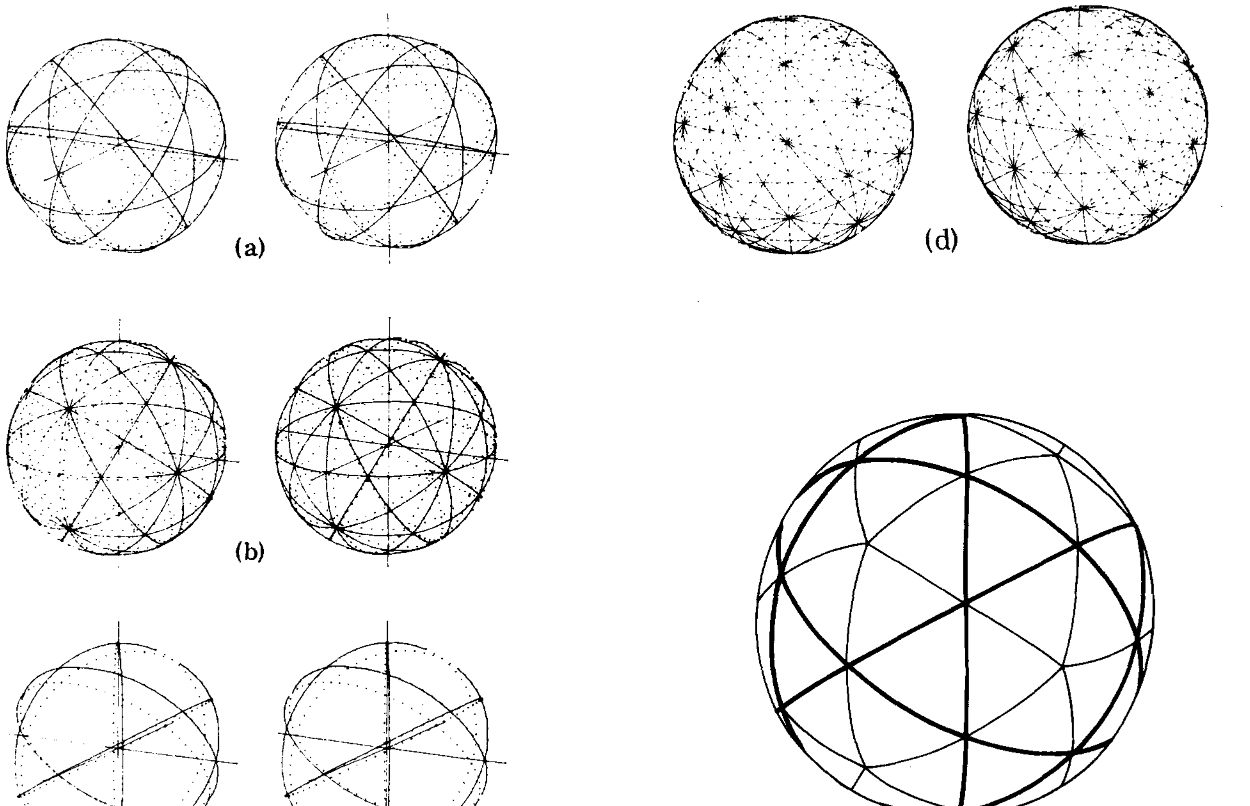


Fig. 9. Hamilton arcs for icosahedral symmetry. Stereo drawings of arcs paths for (a) 120°, (b) 180°, (c) 72° and 144° rotations all show icosahedral symmetry. All the arcs are drawn together in (d). This forms the icosahedral "lattice" which is projected to make the nomogram (Fig. 10). (e) The 72° arc paths are selected parts of the 180° arc paths form the elementary geodesic dome structure of Fuller.

Table I. Partial group table of cubic rotations (half-integer spin).

1	r_1	r_2	r_3	r_4	$-r_1^2$	$-r_2^2$	$-r_3^2$	$-r_4^2$	R_1	R_2	R_3	$-R_1^3$	$-R_2^3$	$-R_3^3$
r_1					1								R_1	
r_2						1								
r_3							1			R_1				
r_4								1						
$-r_1^2$	1				$-r_1$									
$-r_2^2$		1					r_1				R_1			
$-r_3^2$			1					r_1						
$-r_4^2$				1		r_1								R_1
R_1										r_1		1		
R_2											r_1		1	
R_3									r_1					1
$-R_1^3$									1					
$-R_2^3$										1				
$-R_3^3$											1			

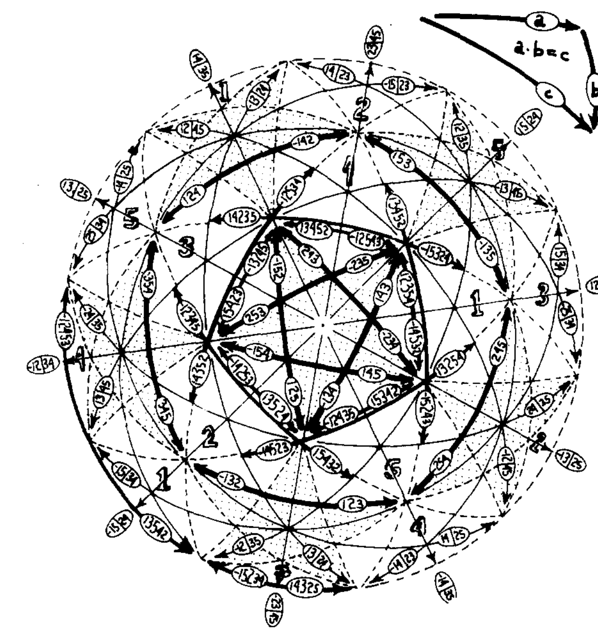


Fig. 10. Icosahedral vector addition nomogram.

upon the theory of class algebras. The number of independent IR of any group $\mathcal{G}$ must equal the number of classes which $\mathcal{G}$ has. As we mentioned in Sec. IV, operators h and h' belong to the same class of $\mathcal{G}$ if

$$h' = ghg^{-1} \quad (7.1)$$

for some g in $\mathcal{G}$. The key algebraic quantities in any IR character derivation are the independent class sums $\mathbf{c}_h$ defined by

$$\mathbf{c}_h = N_h \sum_{g \text{ in } \mathcal{G}} ghg^{-1}, \quad (7.2)$$

where N_h is a "normalization" factor. (N_h is the ratio of the number operators in the class of h to the number in $\mathcal{G}$.)

We give now a way to find the characters needed to analyze half-integer as well as integer spin representations of a finite group $\mathcal{G}$. The representations needed for the half-integer cases are called irreducible ray representations (IRR) of $\mathcal{G}$, or "double-group" representations. The procedure we describe is simpler than conventional ones which deal with a whole double group. Working with double the number of operators generally means having four times as much algebra to do.

In order to calculate characters for either IR or IRR, we may use a $\mathcal{G}$ nomogram such as Figs. 7(c) and 10 to derive the class sums by Eq. (7.2). To obtain IR characters we ignore the minus signs in the nomograms, but we will include them in all products needed for the IRR case.

For example, without the signs we find the following five independent class sums for cubic octahedral symmetry:

$$\mathbf{c}_1 = \mathbf{1}, \quad \mathbf{c}_r = r_1 + r_2 + r_3 + r_4 + r_1^2 + r_2^2 + r_3^2 + r_4^2,$$
$$\mathbf{c}_R = R_1 + R_2 + R_3 + R_1^3 + R_2^3 + R_3^3$$
$$\mathbf{c}_{R^2} = R_1^2 + R_2^2 + R_3^2,$$
$$\mathbf{c}_i = i_1 + i_2 + i_3 + i_4 + i_5 + i_6. \quad (7.3)$$

However, if we include the signs, then only the following independent class sums exist:

$$\mathbf{c}_1 = \mathbf{1}, \quad \mathbf{c}_r = r_1 + r_2 + r_3 + r_4 - r_1^2 - r_2^2 - r_3^2 - r_4^2,$$
$$\mathbf{c}_R = R_1 + R_2 + R_3 - R_1^3 - R_2^3 - R_3^3. \quad (7.4)$$

We note that the classes $\mathbf{c}_{R^2}$ and $\mathbf{c}_i$ of 180° rotations "die" when the spin-$\frac{1}{2}$ signs are used. It can be proved that this will happen in general.

To derive the three independent IRR characters of cubic symmetry we must find and solve the algebra of $\mathbf{c}_1$, $\mathbf{c}_r$, and $\mathbf{c}_R$. We use the O-nomogram [Fig. 7(c)] to construct the partial group table in Table I. The class sum algebra given by Table II is deduced just from the 1, r_1, and R_1 entries in the partial group table.

To reduce a class algebra we construct the lowest-order polynomial equation satisfied by key elements, such as the following for $\mathbf{c}_R$.

$$\mathbf{c}_{R^3} - 18\mathbf{c}_R = \mathbf{0}. \quad (7.5)$$

(These equations must involve powers of the key element and $\mathbf{c}_1 = \mathbf{1}$ only. They are called minimal equations of the element.) Such equations may be factored in all cases to give distinct roots or eigenvalues[8] as in the following factorization of Eq. (7.5).

$$(\mathbf{c}_R - 3\sqrt{2}\,\mathbf{1})(\mathbf{c}_R + 3\sqrt{2}\,\mathbf{1})(\mathbf{c}_R) = \mathbf{0}. \quad (7.6)$$

Then we use spectral decomposition formulas described in Appendix C to compute class projection operators. From $\mathbf{c}_R$ we obtain

$$\mathbf{P}^{E_1} = \frac{(\mathbf{c}_R + 3\sqrt{2}\,\mathbf{1})\mathbf{c}_R}{(3\sqrt{2} + 3\sqrt{2})(3\sqrt{2})} = \frac{1}{6}\mathbf{1} + \frac{1}{12}\mathbf{c}_r + \frac{2}{12}\mathbf{c}_R$$
$$\mathbf{P}^{E_2} = \frac{(\mathbf{c}_R - 3\sqrt{2}\,\mathbf{1})\mathbf{c}_R}{(-3\sqrt{2} - 3\sqrt{2})(-3\sqrt{2})}$$
$$= (1/6)\,\mathbf{1} + (1/12)\,\mathbf{c}_r - (2/12)\,\mathbf{c}_R$$
$$\mathbf{P}^{G} = \frac{(\mathbf{c}_R - 3\sqrt{2}\,\mathbf{1})(\mathbf{c}_R + 3\sqrt{2}\,\mathbf{1})}{(-3\sqrt{2})(3\sqrt{2})}$$
$$= (2/3)\,\mathbf{1} - (1/6)\,\mathbf{c}_r \quad (7.7)$$

Table II. Cubic class algebra (half-integer spin). Just the upper half of the table is shown since class algebras commute ($\mathbf{c}'\mathbf{c} = \mathbf{c}\mathbf{c}'$).

	$\mathbf{c}_1 = \mathbf{1}$	$\mathbf{c}_r$	$\mathbf{c}_R$
$\mathbf{c}_1$	$\mathbf{1}$	$\mathbf{c}_r$	$\mathbf{c}_R$
$\mathbf{c}_r$		$8\,\mathbf{1} + 2\mathbf{c}_r$	$4\mathbf{c}_R$
$\mathbf{c}_R$			$6\,\mathbf{1} + 3\mathbf{c}_r$

Table III. Cubic IRR characters.

x_G^A:	$g =$	1	r	R
A	$= E_1$	2	1	2
	E_s	2	1	−2
	G	4	−1	0

where Table II is used to simplify the products, and the notations E_1, E_2, and G are the conventional labels for the roots $3\sqrt{2}$, $-3\sqrt{2}$, and 0, respectively, of $\mathbf{C}_R$.

Now when we have n projection operators $\mathbf{P}^A$ expressed as n linearly independent combinations of the n class sums $\mathbf{c}_g$, i.e.,

$$\mathbf{P}^a = \sum_g^{(n)} d_g^A \, \mathbf{c}_g, \tag{7.8}$$

then we may compare the expansion with the standard[9] general expression for the irreducible projection operator.

$$\mathbf{P}^A = \sum_g^{(n)} (l^A/n_{\mathcal{G}}) \, x_g^{A*} \, \mathbf{c}_g. \tag{7.9}$$

Here, x_g^A are the desired characters, $l^A = x_1^A$ is the dimension of the irreducible representation (A), and $n_{\mathcal{G}}$ is the number of operators in the group $\mathcal{G}$. The characters are found by equating the coefficients in Eqs. (7.8) and (7.9).

$$x_g^A = (n_{\mathcal{G}}/l^A) \, d_g^{A*}. \tag{7.10}$$

The dimensions l^A are found using a simple formula

$$l^A = (n_{\mathcal{G}} \, d_1^A)^{1/2} \tag{7.11}$$

as, for example, from Eq. (7.7).

$$l^{E_1} = \left(24\frac{1}{6}\right)^{1/2} = l^{E_2} = 2, \, l^G = \left(24\frac{2}{3}\right)^{1/2} = 4.$$

Finally, we obtain the cubic IRR characters which are assembled in Table III.

All half-integral angular momentum levels ($J = 1/2, 3/2, 5/2, \cdots$) will split into some number of E_1, E_2, or G levels in cubic crystal fields.

Icosahedral symmetry has a rather formidable structure, however, the methods just described are surprisingly easy to carry out in the derivation of its IR or IRR characters. We shall do the latter.

Let us denote the 72° rotations as follows:

$$R_1 = (14325), \quad R_2 = (15423), \quad R_3 = (13524),$$
$$R_4 = (15342), \quad R_5 = (12354), \quad R_6 = (13452);$$

and the 120° rotations as follows:

$$r_1 = (123), r_2 = (245), r_3 = (153), r_4 = (124), r_5 = (345)$$
$$r_6 = (125), r_7 = (145), r_8 = (143), r_9 = (243), r_{10} = (253).$$

The only independent IRR class sums are the following:

$$\mathbf{c}_1 = 1, \quad \mathbf{c}_R = \sum_{a=1}^{6} (R_a - R_a^4),$$

$$\mathbf{c}_{R^2} = \sum_{a=1}^{6} (R_a^2 - R_a^3), \quad \mathbf{c}_r = \sum_{a=1}^{10} (r_a - r_a^2).$$

Table IV. Icosahedral class algebra (half-integer spin).

$\mathbf{c}_1$	$\mathbf{c}_R$	$\mathbf{c}_{R^2}$	$\mathbf{c}_r$
$\mathbf{c}_R$	$12\mathbf{c}_1 + 5\mathbf{c}_R + \mathbf{c}_{R^2} + 3\mathbf{c}_r$	$\mathbf{c}_R - \mathbf{c}_{R^2} + 3\mathbf{c}_r$	$5\mathbf{c}_R + 5\mathbf{c}_{R^2} + 3\mathbf{c}_r$
$\mathbf{c}_{R^2}$		$12\mathbf{c}_1 - \mathbf{c}_R - 5\mathbf{c}_{R^2} + 3\mathbf{c}_r$	$5\mathbf{c}_R + 5\mathbf{c}_{R^2} + 3\mathbf{c}_r$
$\mathbf{c}_r$			$20\mathbf{c}_1 + 5\mathbf{c}_R - 5\mathbf{c}_{R^2} + 5\mathbf{c}_r$

The algebra of these class sums is found using the nomogram in Fig 10, and is given in Table IV.

The minimal equation of the class sum $\mathbf{c}_R$ is found by computing powers of $\mathbf{c}_R$ using Table IV, and checking for linear dependence each time. The results is

$$\mathbf{c}_{R^4} - 7\mathbf{c}_{R^3} - 36\mathbf{c}_{R^2} + 72\mathbf{c}_R + 216\mathbf{c}_1 = 0,$$

which has roots $m_1 = 3(1+\sqrt{5})$, $m_2 = 3(1-\sqrt{5})$, $m_3 = 3$, and $m_4 = -2$. Using the formulas given in Appendix C we derive the following projection operators:

$$\mathbf{P}^1 = (4\mathbf{c}_1 + (1+\sqrt{5})\,\mathbf{c}_R - (1-\sqrt{5})\,\mathbf{c}_{R^2} + 2\mathbf{c}_r)/60,$$
$$\mathbf{P}^2 = (4\mathbf{c}_1 + (1-\sqrt{5})\,\mathbf{c}_R - (1+\sqrt{5})\,\mathbf{c}_{R^2} + 2\mathbf{c}_r)/60,$$
$$\mathbf{P}^3 = (4\mathbf{c}_1 + \mathbf{c}_R - \mathbf{c}_{R^2} - \mathbf{c}_r)/15,$$
$$\mathbf{P}^4 = (6\mathbf{c}_1 - \mathbf{c}_R + \mathbf{c}_{R^2})/10.$$

Using Eqs. (7.10) and (7.11) the icosahedral IRR characters follow immediately. These are given in Table V.

The application of these and related symmetry quantities are beyond the scope of this article. Some particularly interesting applications of the theory in this article have been made quite recently[12] in molecular spectroscopy.

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APPENDIX A. EXPONENTIAL FORM FOR ROTATION OPERATORS

Let the orbital wave function of an electron in state $|\psi\rangle$ be given by

$$\langle xyz|\psi\rangle = \psi(xyz). \tag{A1}$$

Let the wave function of the electron in the rotated state $\mathbf{R}(\alpha\beta\gamma)|\psi\rangle$ be given by

$$\langle xyz|\mathbf{R}(\alpha\beta\gamma)|\psi\rangle = \psi^R(xyz). \tag{A2}$$

For z-axis rotations $\mathbf{R}(\delta\alpha 00)$ by an infinitesimal angle $\delta\alpha$,

Table V. Icosahedral IRR characters [$G_\pm = (1 \pm \sqrt{5})/2$].

x_g^A:	$g =$	1	R	R^2	r
A	= 1	2	G_+	G_-	1
	2	2	G_-	G_+	1
	3	4	1	−1	−1
	4	6	−1	1	0

we obtain the following Taylor expansion for the rotated wave $\psi^R(xyz)$.

$$\psi^R(xyz) = \psi(x + y\delta\alpha, y - x\delta\alpha, z)$$

$$= \psi(xyz) + y\frac{\partial\psi}{\partial x}\delta\alpha - x\frac{\partial\psi}{\partial y}\delta\alpha\cdots$$

$$= \left[\mathbf{1} - \delta\alpha\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) + \cdots\right]\psi(xyz). \quad \text{(A3)}$$

The standard representation of the z component of angular momentum is

$$\langle xyz|\mathbf{J}_z|\psi\rangle = \langle xyz|\mathbf{xp}_y - \mathbf{yp}_x|\psi\rangle$$

$$= (-i)\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)\psi(xyz). \quad \text{(A4)}$$

Comparison of Eqs. (A3) and (A4) suggests that we may write

$$\mathbf{R}(\delta\alpha\, 00) = \mathbf{1} + \delta\alpha \mathbf{J}_z/i \quad \text{(A5)}$$

for infinitesimal z rotations. For z rotations by a finite angle $\alpha = n(\alpha/n) = n(\delta\alpha)$, $(n \to \infty)$, we imagine an infinite product of infinitesimal rotations.

$$\mathbf{R}(\alpha 00) = \lim_{n\to\infty} (\mathbf{R}(\alpha/n\, 00))^n$$

$$= \lim_{n\to\infty} (\mathbf{1} + (\alpha/n)\mathbf{J}_z/i)^n. \quad \text{(A6)}$$

Then we apply the well-known definition of the exponential: $e^x = \lim_{n\to\infty}(1 + (x/n))^n$ to obtain the formula

$$\mathbf{R}(\alpha 00) = e^{\alpha \mathbf{J}_z/i} = \mathbf{R}(00\alpha). \quad \text{(A7)}$$

Similarly, we would have the following y-rotation operator:

$$\mathbf{R}(0\beta 0) = e^{\beta \mathbf{J}_y/i} \quad \text{(A8)}$$

and similarly for rotations around any axis $\boldsymbol{\omega}$.

APPENDIX B. MATRIX SPECTRAL DECOMPOSITION AND EXPONENTIAL FORM EVALUATION.

In order to evaluate specific examples of the exponential forms [Eqs. (A7) and (A8)] we shall use the spectral decomposition

$$\mathbf{M} = \mathrm{m}_1\mathbf{P}_1 + \mathrm{m}_2\mathbf{P}_2 + \cdots + \mathrm{m}_n\mathbf{P}_n \quad \text{(B1)}$$

of an nxn matrix $\mathbf{M}$ having n distinct eigenvalues $m_1, m_2, \cdots, m_n$, where the $\mathbf{P}_j$ are defined by

$$\mathbf{P}_i = \left(\prod_{j\neq i}(\mathbf{M} - m_j\mathbf{1})\right) \Big/ \left(\prod_{j\neq i}(m_i - m_j)\right). \quad \text{(B2)}$$

The $\mathbf{P}_i$ are projection operators satisfying orthonormality relations

$$\mathbf{P}_i\mathbf{P}_k = 0 \quad (\text{if } k \neq i), \quad \text{(B3a)}$$

$$\mathbf{P}_i\mathbf{P}_i = \mathbf{P}_i, \quad \text{(B3b)}$$

as well as the following eigenvalue equations.

$$\mathbf{MP}_i = m_i\mathbf{P}_i = \mathbf{P}_i\mathbf{M}. \quad \text{(B4)}$$

The spectral decomposition equations [Eqs. (B1) to (B4)] follow from the fact that a matrix satisfies its own eigenvalue (secular) equation, i.e.,

$$(\mathbf{M} - \mathrm{m}_1\mathbf{1})(\mathbf{M} - \mathrm{m}_2\mathbf{1})\cdots(\mathbf{M} - \mathrm{m}_n\mathbf{1}) = \mathbf{0}. \quad \text{(B5)}$$

(This is essence of the Hamilton-Cayley Theorem.) To verify the relations we isolate the (ith) factor in Eq. (B5) so that it reads

$$(\mathbf{M} - m_i\mathbf{1})\mathbf{p}_i = \mathbf{0}, \quad \text{(B6)}$$

where

$$\mathbf{p}_i = \prod_{j\neq i}(\mathbf{M} - m_j\mathbf{1}). \quad \text{(B7)}$$

Thus we have

$$\mathbf{Mp}_i = m_i\mathbf{p}_i, \quad \text{(B8)}$$

which is the same as Eqs. (B2) and (B4) except for a constant factor. Next we may prove (B3) using, in turn, (B7) and (B8).

$$\mathbf{p}_i\mathbf{p}_k = \prod_{j\neq i}(\mathbf{M} - m_j\mathbf{1})\,\mathbf{p}_k$$

$$= \prod_{j\neq i}(m_k - m_j)\,\mathbf{p}_k = \mathbf{0}\ (\text{if } k \neq i).$$

This proves (B3) if we divide $\mathbf{p}_i$ by the constant factor which makes it into $\mathbf{P}_i$. [See Eq. (B2).]

Finally, to prove (B1) we use the completeness relation

$$\mathbf{1} = \mathbf{P}_1 + \mathbf{P}_2 + \cdots + \mathbf{P}_n. \quad \text{(B9)}$$

This is a general algebraic result. It is easy to verify for $n = 2$:

$$\mathbf{P}_1 + \mathbf{P}_2 = (\mathbf{M} - m_2\mathbf{1})/(m_1 - m_2) + (\mathbf{M} - m_1\mathbf{1})/(m_2 - m_1)$$

$$= (\mathbf{M} - m_2\mathbf{1} - \mathbf{M} + m_1\mathbf{1})/(m_1 - m_2)$$

$$= \mathbf{1}.$$

and similarly for $n = 3$, but it is more difficult to prove in general. [Eq. (B9) holds for all values of m_i, not just the M eigenvalues.] Now Eq. (B1) follows if we operate on both sides of (B9) and use (B4).

We may evaluate matrix exponentials $e^{\mathbf{M}}$ and other functions using decomposition (B1). For the exponential we have

$$e^{\mathbf{M}} = e^{m_1}\mathbf{P}_1 + e^{m_2}\mathbf{P}_2 + \cdots + e^{m_n}\mathbf{P}_n \quad \text{(B10)}$$

which follows directly from (B1) if we expand $e^M = 1 + M + M^2/2! + \cdots$ and use (B3) to eliminate the cross terms. In the case of the y rotation $\mathbf{R}(0\beta 0)$ we need the spectral decomposition of the y component $(\mathbf{J}_y)$ of angular momentum. The spin-½ representation of $\mathbf{J}_y$ is the (Yth) Pauli spinor multiplied by 1/2. Its eigenvalues are $m_1 = 1/2$ and $m_2 = -1/2$. From (B1) we derive

$$\langle\mathbf{J}_y\rangle = \begin{pmatrix} 0 & -i/2 \\ i/2 & 0 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1/2 & -i/2 \\ i/2 & 1/2 \end{pmatrix} - \frac{1}{2}\begin{pmatrix} 1/2 & i/2 \\ -i/2 & 1/2 \end{pmatrix}.$$

Then from (B10) we derive Eq. (3.2b)

$$e^{-i\beta\langle\mathbf{J}_y\rangle} = e^{-i\beta/2}\begin{pmatrix} 1/2 & -i/2 \\ i/2 & 1/2 \end{pmatrix} + e^{i\beta/2}\begin{pmatrix} 1/2 & i/2 \\ -i/2 & 1/2 \end{pmatrix}$$

$$= \begin{pmatrix} (e^{-i\beta/2} + e^{i\beta/2})/2 & (e^{-i\beta/2} - e^{i\beta/2})/2i \\ -(e^{-i\beta/2} - e^{i\beta/2})/2i & (e^{-i\beta/2} + e^{i\beta/2})/2 \end{pmatrix}$$

$$= \begin{pmatrix} \cos(\beta/2) & -\sin(\beta/2) \\ \sin(\beta/2) & \cos(\beta/2) \end{pmatrix}.$$

APPENDIX C. REDUCTION OF CLASS ALGEBRAS

The same techniques which give the spectral decomposition of a matrix in Appendix B may also be used to decompose a class operator **c**. Suppose that we are given the minimal equation of **c**:

$$\mathbf{c}^n + a_1\mathbf{c}^{n-1} + a_2\mathbf{c}^{n-2} + \cdots + a_n\mathbf{1} = 0.$$

It can be shown[8] that the roots $c_1, c_2, \cdots$, and c_n of this equation must be distinct. Therefore we may construct a set of orthonormal projection operators using the same formula (B2) which worked for matrices.

$$\mathbf{P}_i = \prod_{j\neq i} (\mathbf{c} - c_j\mathbf{1}) \Big/ \prod_{j\neq i} (c_i - c_j). \qquad \text{(C1)}$$

These operators will satisfy the completeness relation

$$\mathbf{1} = \mathbf{P}_1 + \mathbf{P}_2 + \cdots + \mathbf{P}_n, \qquad \text{(C2)}$$

the eigenvalue equations ($\mathbf{c}\mathbf{P}_i = c_i\mathbf{P}_i$), and the spectral decomposition relations

$$\mathbf{c} = c_1\mathbf{P}_1 + c_2\mathbf{P}_2 + \cdots + c_n\mathbf{P}_n. \qquad \text{(C3)}$$

If we are lucky enough to have a class sum **c** for which the degree n of its minimal equation is equal to the number of class sum operators, then Eqs. (C1)–(C3) give the complete reduction of the class algebra. Otherwise, we may combine them with different spectral decompositions

$$\mathbf{d} = \mathrm{d}_1\mathrm{Q}_1 + \mathrm{d}_2\mathrm{Q}_2 + \cdots (\mathbf{1} = \mathrm{Q}_1 + \mathrm{Q}_2 + \cdots)$$

until a complete one is achieved.

$$\mathbf{1} = \mathbf{1}\cdot\mathbf{1} = (\mathrm{Q}_1 + \mathrm{Q}_2 + \cdots)(\mathbf{P}_1 + \mathbf{P}_2 + \cdots + \mathbf{P}_n)$$
$$= \mathrm{Q}_1\mathbf{P}_1 + \mathrm{Q}_1\mathbf{P}_2 + \cdots + \mathrm{Q}_1\mathbf{P}_n$$
$$+ \mathrm{Q}_2\mathbf{P}_1 + \mathrm{Q}_2\mathbf{P}_2 + \cdots + \mathrm{Q}_2\mathbf{P}_n \cdots.$$

Since all class algebras are commutative ($\mathbf{cd} = \mathbf{dc}$, $\mathrm{Q}_i\mathbf{P}_j = \mathbf{P}_j\mathrm{Q}_i$, etc.) these multiplications must yield bona-fide spectral decompositions each time. Furthermore, it can be shown that the final result is unique.[8]

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