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Note added 2.24.17. This earlier App G version contains my best-so-far version of the ω calculation in Section G.4 which I will soon transcribe with edts into App G.7. Also the Generalizations section I think was written here for the first time. // Transcribed it into Section G.7. Also extracted the Generalizations section first into its own doc and then that got installed into Appendix G v2 doc.

So there is no further need for this file, it is then archived,

## Appendix G: Rotation Matrices and Goldstein's body-frame ω

Here we present still more information on rotation matrices and demonstrate some typical manipulations done with such matrices leading to a derivation of Goldstein body-frame **ω** vector expressions.

### G.1 Generators and finite rotation matrices

The general active rotation matrix for rotation by angle θ about some **n** *unit vector* axis is given by,

$$R_{\hat{\mathbf{n}}}(\varphi) = \exp(-i\,\theta\,\mathbf{n}\bullet\mathbf{J})\,, \qquad \text{(G.1.1)}$$

where the $J_k$ are 3x3 matrices known as the rotation **generator** matrices,

$$J_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix} \qquad J_2 = \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix} \qquad J_3 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad . \qquad \text{(G.1.2)}$$

The numbers in these three matrices can be summarized in this single statement,

$(J_a)_{bc} = -\,i\,\varepsilon_{abc}$ // for example, $(J_1)_{23} = -\,i\,\varepsilon_{123} = -i$

or

$$(iJ_a)_{bc} = \varepsilon_{abc} \qquad \text{(G.1.3)}$$

where the $\varepsilon_{abc}$ permutation tensor is described in (1.5.3).

Defining the commutator of two square matrices X,Y as [X, Y] = XY-YX, one can show that the above three matrices satisfy this "commutation relation",

$$[J_i, J_j] = i\varepsilon_{ijk}J_k \qquad \text{// for example, } [J_1,J_2] = iJ_3 \qquad \text{(G.1.4)}$$

Proof: These easily demonstrated facts will be used in the proof (implied sum on repeated indices) ,

$$\varepsilon_{abc}\varepsilon_{ABc} = \delta_{aA}\delta_{bB} - \delta_{aB}\delta_{bA} \qquad \delta_{ab} \equiv \delta_{a,b} \qquad \varepsilon_{abc} = \varepsilon_{bca} = \varepsilon_{cab} \tag{G.1.5}$$

$$LHS_{ac} = (J_i)_{ab}(J_j)_{bc} - (J_j)_{ab}(J_i)_{bc} = (-i)^2[\varepsilon_{iab}\varepsilon_{jbc} - \varepsilon_{jab}\varepsilon_{ibc}] = -[\varepsilon_{iab}\varepsilon_{cjb} - \varepsilon_{jab}\varepsilon_{cib}]$$

$$= -[(\delta_{ic}\delta_{aj} - \delta_{ij}\delta_{ac}) - (\delta_{jc}\delta_{ai} - \delta_{ji}\delta_{ac})] = \delta_{jc}\delta_{ai} - \delta_{ic}\delta_{aj} \ .$$

$$RHS_{ac} = i\varepsilon_{ijk}(J_k)_{ac} = i\varepsilon_{ijk}[-i\varepsilon_{kac}] = \varepsilon_{ijk}\varepsilon_{kac} = \varepsilon_{ijk}\varepsilon_{ack} = \delta_{ia}\delta_{jc} - \delta_{ja}\delta_{ic} \ . \qquad \text{QED}$$

The expression shown in (G.1.1) involves the exponentiation of a square matrix to produce a new square matrix of the same dimension. This notion of exponentiating a matrix is straightforward as we demonstrate with a simple example:

$$R_x(\theta) = \exp(-i\,\theta\,\hat{\mathbf{x}} \bullet \mathbf{J}) = \exp(-i\,\theta J_1) \equiv \Sigma_{n=0}^{\infty}(-i\theta)^n (J_1)^n/n!$$

$$= 1 + \Sigma_{2,4,6..}(-i\theta)^n (J_1)^n/n! + \Sigma_{1,3,5..}(-i\theta)^n (J_1)^n/n!$$

It is easy to show that $(J_1)^n = J_1$ for odd n, while $(J_1)^n = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ for even $n > 0$. Thus,

$$R_x(\varphi) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \Sigma_{2,4,6..}(-i\theta)^n/n! + \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix} \Sigma_{1,3,5..}(-i\theta)^n/n! \ .$$

But

$$\Sigma_{2,4,6..}(-i\theta)^n/n! = -\theta^2/2! + \theta^4/4! + \ldots = (\cos\theta - 1)$$
$$\Sigma_{1,3,5..}(-i\varphi)^n/n! = (-i\theta) + (-i\theta)^3/3! + \ldots = (-i)[\theta - \theta^3/3! + ..] = -i\sin\theta \tag{G.1.6}$$

and therefore

$$R_x(\varphi) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} (\cos\theta - 1) + \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix} (-i\sin\theta)$$

$$= \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & 0 \\ 0 & 0 & \cos\theta \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -\sin\theta \\ 0 & \sin\theta & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & -\sin\theta \\ 0 & \sin\theta & \cos\theta \end{pmatrix}. \tag{G.1.7}$$

The three axis-aligned rotations are found in this manner to be

$$R_x(\theta) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & -\sin\theta \\ 0 & \sin\theta & \cos\theta \end{pmatrix} \quad R_y(\theta) = \begin{pmatrix} \cos\theta & 0 & \sin\theta \\ 0 & 1 & 0 \\ -\sin\theta & 0 & \cos\theta \end{pmatrix} \quad R_z(\theta) = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} . \tag{G.1.8}$$

The general rotation (G.1.1) applied to a vector **v** produces a **forward** right-hand-rule rotation of vector **v** by an angle θ about an arbitrary $\hat{\mathbf{n}}$ axis to create **v'** = R**v**. We call this an **active rotation**. For example, if one applies $R_z(\theta)$ shown in (G.1.8) to the unit vector $\hat{\mathbf{x}}$ = (1,0,0) one gets (cosθ,sinθ,0) which for small θ is a vector in the first quadrant of the x,y plane.

Some authors define rotation matrices which rotate vectors **backwards** according to the right hand rule, with the connection to our matrices then being θ ↔ -θ. The motivation for doing this is the fact that, whereas **v'** = R**v** in the active view where the vector moves and the axes stay put, one can instead do $\mathbf{e'}_n = R^{-1}\mathbf{e}_n$ and have the vector stay put and the axes are back-rotated, which is the **passive** viewpoint. The definition of the rotation matrices is just a convention and (G.1.8) shows our definitions.

One says that the matrices $J_i$ "generate" the finite rotations when they are exponentiated.

An alternative approach: First, one can show that $R_i(d\theta) \approx 1 - id\theta J_i$ describes a 3x3 matrix which, when applied to a vector, causes that vector to rotate by the small amount dθ about the i axis (an "infinitesimal rotation"). Setting dθ = θ/n, one shows that $\lim_{n\to\infty} (1-i[\theta/n]J_i)^n = \exp(-i\theta J_i)$. This last limit is analogous to $\lim_{n\to\infty}(1+x/n)^n = e^x$ for a scalar value x.

**G.2 About the general rotation matrix**

An explicit expression for the general rotation matrix

We present this subsection as a Reader Exercise with a set of steps. The result is stated in (G.2.8).

We are interested in the following general rotation matrix:

$$R_n(\theta) = \exp(-i\,\theta\,\mathbf{n}\bullet\mathbf{J}) \equiv \Sigma_{n=0}^{\infty}(-i\theta)^n(\mathbf{n}\bullet\mathbf{J})^n/n! \quad . \quad \mathbf{n} = \hat{\mathbf{n}} \text{ = a unit vector} \qquad \text{(G.2.1)}$$

(a) using (G.1.3) and (G.1.5), show that $(\mathbf{n}\bullet\mathbf{J})^2 = T$ where $T_{ab} = (\delta_{ab} - n_a n_b)$ . (G.2.2)

(b) show that

$$(\mathbf{n}\bullet\mathbf{J})^n = (\mathbf{n}\bullet\mathbf{J})\,T \qquad \text{for } n = 3,5,7,....$$
$$(\mathbf{n}\bullet\mathbf{J})^n = T \qquad \text{for } n = 2,4,6... \qquad \text{(G.2.3)}$$

(c) show that $\exp(-i\theta\mathbf{n}\bullet\mathbf{J}) = \cos(\theta\mathbf{n}\bullet\mathbf{J}) - i\sin(\theta\mathbf{n}\bullet\mathbf{J})$ where each term is defined by its series

(d) show that

$$\cos(\theta\mathbf{n}\bullet\mathbf{J}) = 1 + T(\cos\theta - 1)$$

$$\sin(\theta\mathbf{n}\bullet\mathbf{J}) = (\theta\mathbf{n}\bullet\mathbf{J}) + (\mathbf{n}\bullet\mathbf{J})T(\sin\theta - \theta) \qquad \text{(G.2.4)}$$

(e) show therefore that

$$\exp(-i\theta \mathbf{n}\bullet\mathbf{J}) \;=\; 1 + T\,(\cos\theta - 1) \;-i\,(\mathbf{n}\bullet\mathbf{J})\{\,\theta + T\,(\sin\theta - \theta)\,\} \tag{G.2.5}$$

(f) show that the terms linear in θ all cancel leaving this simpler result

$$\exp(-i\theta \mathbf{n}\bullet\mathbf{J}) \;= 1 + (\cos\theta - 1)\,T \;+ \sin\theta[\,-i(\mathbf{n}\bullet\mathbf{J})] \tag{G.2.6}$$

(g) show that

$$T = \begin{pmatrix} 1-n_1^2 & -n_1n_2 & -n_1n_3 \\ -n_1n_2 & 1-n_2^2 & -n_2n_3 \\ -n_1n_3 & -n_2n_3 & 1-n_3^2 \end{pmatrix} \qquad -i(\mathbf{n}\bullet\mathbf{J}) = \begin{pmatrix} 0 & -n_3 & n_2 \\ n_3 & 0 & -n_1 \\ -n_2 & n_1 & 0 \end{pmatrix} \tag{G.2.7}$$

giving this final result,

$$R_{\mathbf{n}}(\theta) = \exp(-i\theta \mathbf{n}\bullet\mathbf{J}) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} + (\cos\theta - 1) \begin{pmatrix} 1-n_1^2 & -n_1n_2 & -n_1n_3 \\ -n_1n_2 & 1-n_2^2 & -n_2n_3 \\ -n_1n_3 & -n_2n_3 & 1-n_3^2 \end{pmatrix} + \sin\theta \begin{pmatrix} 0 & -n_3 & n_2 \\ n_3 & 0 & -n_1 \\ -n_2 & n_1 & 0 \end{pmatrix} . \tag{G.2.8}$$

Note that the first two terms are symmetric matrices, while the third is antisymmetric.

(h) verify the special cases shown in (G.1.8) above. These cases have **n** = (1,0,0), (0,1,0, (0,0,1).

Finding **n** and θ

**Problem**: One is handed a 9-element rotation matrix R and one wants to find **n**,θ so R = exp(-iθ**n**•**J**) .

Solution: We are unaware of a single magic formula that solves this problem, so we use brute force.

One can break R into the sum of two pieces, one symmetric and one antisymmetric by constructing

$$S_{ab} \equiv (R_{ab}+R_{ba})/2 \qquad A_{ab} \equiv (R_{ab}-R_{ba})/2 \qquad R_{ab} = S_{ab} + A_{ab} \qquad R = S + A\ . \tag{G.2.9}$$

Looking at (G.2.9) one then has,

$$S = \begin{pmatrix} S_{11} & S_{12} & S_{13} \\ S_{12} & S_{22} & S_{23} \\ S_{31} & S_{23} & S_{33} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} + (\cos\theta - 1) \begin{pmatrix} 1-n_1^2 & -n_1n_2 & -n_1n_3 \\ -n_1n_2 & 1-n_2^2 & -n_2n_3 \\ -n_1n_3 & -n_2n_3 & 1-n_3^2 \end{pmatrix}$$

$$A = \begin{pmatrix} 0 & A_{12} & A_{13} \\ -A_{12} & 0 & A_{23} \\ -A_{13} & -A_{23} & 0 \end{pmatrix} = \sin\theta \begin{pmatrix} 0 & -n_3 & n_2 \\ n_3 & 0 & -n_1 \\ -n_2 & n_1 & 0 \end{pmatrix} \tag{G.2.10}$$

which can be written as these nine equations

$$A_{12} = -n_3\sin\theta \qquad S_{11} = 1 + (\cos\theta-1)(1-n_1^2) \qquad S_{12} = (\cos\theta-1)(-n_1n_2)$$
$$A_{13} = n_2\sin\theta \qquad S_{22} = 1 + (\cos\theta-1)(1-n_2^2) \qquad S_{13} = (\cos\theta-1)(-n_1n_3)$$
$$A_{23} = -n_1\sin\theta \qquad S_{33} = 1 + (\cos\theta-1)(1-n_3^2) \qquad S_{23} = (\cos\theta-1)(-n_2n_3) \ . \qquad \text{(G.2.11)}$$

• If $\theta = 0$, then the original matrix must be R = 1 and then we have no work to do.

• If $\theta = \pi$, the entire A matrix vanishes according to (G.2.9) leaving only S. The equations above are then

$$S_{11} = 1 + (-2)(1-n_1^2) \qquad S_{12} = 2n_1n_2$$
$$S_{22} = 1 + (-2)(1-n_2^2) \qquad S_{13} = 2n_1n_3$$
$$S_{33} = 1 + (-2)(1-n_3^2) \qquad S_{23} = 2n_2n_3 \ .$$

Since $n_1^2 + n_2^2 + n_3^2 = 1$, not all three $n_i$ can vanish. The left column of equations says

$$n_i^2 = 1 - (1-S_{ii})/2 \qquad i = 1,2,3 \ .$$

Inspect the three $n_i^2$ and select one $n_r^2$ which is non-zero. Then select the plus sign to get,

$$n_r = +\sqrt{1 - (1-S_{rr})/2} \ .$$

To be specific, assume $n_r = n_1$. Then from the right column, $n_2 = S_{12}/(2n_1)$ and $n_2 = S_{13}/(2n_1)$ and we are done. So at least one of the following solutions must be viable:

$$\theta = \pi \qquad n_1 = \sqrt{1 - (1-S_{11})/2} \qquad n_2 = S_{12}/(2n_1) \qquad n_3 = S_{13}/(2n_1)$$
$$\theta = \pi \qquad n_2 = \sqrt{1 - (1-S_{22})/2} \qquad n_1 = S_{12}/(2n_2) \qquad n_3 = S_{23}/(2n_2)$$
$$\theta = \pi \qquad n_3 = \sqrt{1 - (1-S_{33})/2} \qquad n_1 = S_{13}/(2n_3) \qquad n_2 = S_{23}/(2n_3) \qquad \text{(G.2.12)}$$

• If $\theta \neq 0$ or $\pi$, then note from (G.2.10) that

$$A_{12}^2 + A_{13}^2 + A_{23}^2 = \sin^2\theta$$
$$S_{11} + S_{22} + S_{33} = 1 + 2\cos\theta \ . \qquad \text{(G.2.13)}$$

Using the sign ambiguity in the direction of **n**, we can assume that $0 < \theta < \pi$ so $\sin\theta > 0$. Then from (G.2.13) and the left column of (G.2.11) we have this solution,

$$\sin\theta = \sqrt{A_{12}^2 + A_{13}^2 + A_{23}^2}$$
$$\cos\theta = [\, S_{11} + S_{22} + S_{33} - 1]/2$$
$$n_1 = -A_{23}/\sin\theta$$
$$n_2 = A_{13}/\sin\theta$$
$$n_3 = -A_{12}/\sin\theta \qquad \text{(G.2.14)}$$

and thus a viable $\theta$ and **n** have been found such that $R = \exp(-i\theta\mathbf{n}\bullet\mathbf{J})$ .

Example: Let $R = \begin{pmatrix} \cos\alpha & -\sin\alpha & 0 \\ \sin\alpha & \cos\alpha & 0 \\ 0 & 0 & 1 \end{pmatrix}$ so then $S = \begin{pmatrix} \cos\alpha & 0 & 0 \\ 0 & \cos\alpha & 0 \\ 0 & 0 & 1 \end{pmatrix}$ and $A = \begin{pmatrix} 0 & -\sin\alpha & 0 \\ \sin\alpha & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ .

$\sin\theta = \sqrt{A_{12}^2 + A_{13}^2 + A_{23}^2} = \sqrt{\sin\alpha^2 + 0 + 0} = \sin\alpha$

$\cos\theta = [ S_{11} + S_{22} + S_{33} - 1]/2 = [\cos\alpha + \cos\alpha + 1 - 1]/2 = \cos\alpha \quad \Rightarrow \theta = \alpha$

$n_1 = -A_{23}/\sin\theta = 0$

$n_2 = A_{13}/\sin\theta = 0$

$n_3 = -A_{12}/\sin\theta = \sin\alpha/\sin\theta = 1 \quad \Rightarrow \quad \mathbf{n} = (0,0,1)$

Therefore $R = \exp(-i\alpha J_3) = R_z(\alpha)$ , as verified in (G.1.8).

**G.3 The CHB and Sandwich Formulas**

Statement and proof of the Campbell-Hausdorff-Baker (CHB) formula

We now quote a fascinating fact known as the Campbell-Hausdorff-Baker formula involving two square matrices A and B :

$$e^{-A}Be^{A} = B + [B,A]/1! + [[B,A],A]/2! + [[[B,A],A],A]/3! + \ldots\ldots \qquad (G.3.1)$$

*Outline of CHB proof:* LHS = RHS

(a) Show that LHS $= \Sigma_{n=0}^{\infty}\Sigma_{m=0}^{\infty} (-A)^n B A^m / (n!m!)$ .

(b) Set k = n+m to rewrite as LHS $= \Sigma_{k=0}^{\infty}\Sigma_{n=0}^{k} (-A)^n B A^{k-n} / (n![k-n]!)$ .

(c) Rewrite again as LHS $= \Sigma_{k=0}^{\infty} T_k/k!$ where $T_k \equiv \Sigma_{n=0}^{k} \binom{k}{n} (-A)^n B A^{k-n}$ .

(d) Define $C_0 = B$, $C_1 = [B,A]$, $C_2 = [[B,A],A]$ , etc. so that RHS $= \Sigma_{k=0} C_k/k!$ .
Note that $[C_k,A] = C_{k+1}$.

The proof LHS = RHS is complete if one can show that $T_k = C_k$.

(e) Show $T_k = C_k$ by induction: show $T_0 = C_0$ and $T_k = C_k \Rightarrow T_{k+1} = C_{k+1}$ . QED

Statement and proof of the Sandwich Formula

Now *using* this CHB formula, along with the commutation relation (G.1.4) that $[J_i, J_j] = i\varepsilon_{ijk}J_k$, one can show that

$$\exp(-i\theta \mathbf{n} \bullet \mathbf{J})\ \mathbf{J}\ \exp(+i\theta \mathbf{n} \bullet \mathbf{J}) = \cos\theta\ \mathbf{J} + \sin\theta\ \mathbf{J} \times \mathbf{n} + (1 - \cos\theta)\ \mathbf{n}(\mathbf{n} \bullet \mathbf{J}) . \qquad (G.3.2)$$

This "vector of matrices" notation is just a shorthand for the following equations for k = 1,2,3 :

$$\exp(-i\theta \mathbf{n}\bullet \mathbf{J})\ J_k \exp(+i\theta \mathbf{n}\bullet \mathbf{J}) = \cos\theta J_k + \sin\theta[\mathbf{J}\times\mathbf{n}]_k + (1-\cos\theta)\, n_k (\mathbf{n}\bullet \mathbf{J})$$

$$= \cos\theta\, J_k + \sin\theta\, \varepsilon_{kms} n_s J_m + (1-\cos\theta)\, n_k (\mathbf{n}\bullet \mathbf{J}) \ . \qquad \text{(G.3.3)}$$

This is the "sandwich formula" since $J_k$ on the left is sandwiched between two rotations.

*Outline of Sandwich proof:* LHS = RHS

(a) We will use the CHB formula with $A = i\theta\, \mathbf{n}\bullet \mathbf{J}$ and $B = J_k$. First, define $C_k$ as in (d) above.

(b) show that $C_0 = J_k$, $C_1 = -\theta n_i \varepsilon_{kij} J_j$, $C_2 = \theta^2 (n_k n_i J_i - J_k)$, $C_3 = -\theta^2 C_1$, $C_4 = -\theta^2 C_2$

(c) deduce (or use induction to show) that in general,

$$C_n = -(-1)^{n/2}\, \theta^n (n_k n_i J_i - J_k) \qquad n = 2,4,6....$$

$$C_n = -(-1)^{(n-1)/2}\, \theta^n\, n_i \varepsilon_{kij} J_j \qquad n = 1,3,,5...$$

At this point we have from the CHB formula,

$$\exp(-i\theta \mathbf{n}\bullet \mathbf{J})\ J_k \exp(+i\theta \mathbf{n}\bullet \mathbf{J}) = \Sigma_{n=0}^{\infty} C_n/n! \quad \text{with } C_n \text{ as in (c) above}$$

(d) Show that $\Sigma_{n=0}^{\infty} C_n/n! =$

$$= J_k - n_i \varepsilon_{kij} J_j \Sigma_{n=1,3,5..} (-1)^{(n-1)/2}\, \theta^n/n! - (n_k n_i J_i - J_k) \Sigma_{n=2,4,6..} (-1)^{n/2}\, \theta^n/n!$$

$$= J_k - n_i \varepsilon_{kij} J_j [\theta - \theta^3/3! + ...] - (n_k n_i J_i - J_k) [-\theta^2/2! + \theta^4/4! + .... ]$$

$$= J_k - n_i \varepsilon_{kij} J_j \sin\theta - (n_k n_i J_i - J_k)(\cos\theta - 1)$$

$$= J_k\cos\theta + \varepsilon_{kji} J_j n_i \sin\theta + n_k (\mathbf{n}\bullet\mathbf{J})(1-\cos\theta) \ . \qquad \text{QED}$$

Comments

A vector **v** (rank-1 tensor) transforms ("rotates") according to $\mathbf{v}' = R\mathbf{v}$.
For a matrix M (rank-2 tensor) the corresponding transformation is $M' = RMR^{-1}$, and this is what one sees on the left side of (G.3.3) where $M = J_k$ and $R = \exp(-i\theta\, \hat{\mathbf{n}} \bullet \mathbf{J})$. In the expression $RJ_kR^{-1}$ the rotation generator $J_k$ is "sandwiched" between the two rotations.

The above sandwich formulas play a major role in Magnetic Resonance Imaging. The connection is that protons in your body have magnetic moments (spins) which can be lined up by a strong magnetic field. When the proton spins are slammed with a certain radio frequency pulse, they do conical rotation (precession) about the magnetic field axis at the so-called Larmor frequency. After the pulse this proton

precession decays away (T1) and bulk-decoheres (T2) producing a certain return RF signal which can be analyzed. These return signals are sensitive to the local environment of the protons. The location of a particular response is determined by giving the magnetic field a spatial gradient which affects the Larmor frequency. In this manner, an image can be formed. The sandwich formulas are not applied directly to individual spin angular momenta **J**, but to the average spin (polarization) density in the object being scanned. The analysis is quite complicated since it must take into account thermal and statistical effects which are managed with the use of the density matrix formalism. See the excellent text of Levitt for all the details.

Special cases of the sandwich formula

We shall have our own purposes for the sandwich formulas in the next Section. For rotations about the i axis we set

$$n_s = \delta_{s,i} \quad \Rightarrow \quad \mathbf{n} \bullet \mathbf{J} = J_i \qquad \text{and} \qquad \varepsilon_{kms} J_m n_s = \varepsilon_{kmi} J_m = \varepsilon_{ikm} J_m \tag{G.3.4}$$

Then from the sandwich formula (G.3.3),

$$\exp(-i\theta \mathbf{n}\bullet \mathbf{J})\ J_k \exp(+i\theta \mathbf{n}\bullet \mathbf{J}) = \cos\theta\, J_k + \sin\theta\, \varepsilon_{kms} n_s J_m + (1 - \cos\theta)\, n_k (\mathbf{n}\bullet \mathbf{J}) \tag{G.3.3}$$

we find that (there is no implied sum on i in the rightmost term and $\varepsilon_{kmi} = \varepsilon_{ikm}$ )

$$\exp(-i\theta J_i)\ J_k \exp(+i\theta J_i) = \cos\theta\, J_k + \sin\theta \varepsilon_{ikm} J_m + (1 - \cos\theta)\, \delta_{k,i}\, J_i$$

so then

$$R_i(\theta)\, J_k\, R_i(-\theta) = \cos\theta\, J_k + \sin\theta\, \varepsilon_{ikm}\, J_m + (1 - \cos\theta)\, \delta_{k,i}\, J_i\ . \tag{G.3.5}$$

In the case i = k we know that the left side is just $J_k$ since everything then commutes. This is verified on the right since $\varepsilon_{iim} = 0$ and the other two terms then add up to $J_k$. So although obvious, we state:

$$R_k(\theta)\, J_k\, R_k(-\theta) = J_k \qquad i = k \tag{G.3.6}$$

In the case $i \neq k$ the third term in (G.3.5) does not contribute and we have

$$R_i(\theta)\, J_k\, R_i(-\theta) = \cos\theta\, J_k + \varepsilon_{ikm} \sin\theta\, J_m \qquad i \neq k$$

We shall now construct a table of all the cases for which $i \neq k$ : (G.3.7)

$$\begin{aligned}
R_1(\theta)\, J_2 R_1(-\theta) &= \cos\theta\, J_2 + \varepsilon_{12m} \sin\theta\, J_m = \cos\theta\, J_2 + \sin\theta\, J_3 \\
R_1(\theta)\, J_3 R_1(-\theta) &= \cos\theta\, J_3 + \varepsilon_{13m} \sin\theta\, J_m = \cos\theta\, J_3 - \sin\theta\, J_2 \\
\\
R_2(\theta)\, J_1 R_2(-\theta) &= \cos\theta\, J_1 + \varepsilon_{21m} \sin\theta\, J_m = \cos\theta\, J_1 - \sin\theta\, J_3 \\
R_2(\theta)\, J_3 R_2(-\theta) &= \cos\theta\, J_3 + \varepsilon_{23m} \sin\theta\, J_m = \cos\theta\, J_3 + \sin\theta\, J_1
\end{aligned}$$

$$R_3(\theta)\, J_1 R_3(-\theta) = \cos\theta\, J_1 + \varepsilon_{31m} \sin\theta\, J_m = \cos\theta J_1 + \sin\theta\, J_2$$
$$R_3(\theta)\, J_2 R_3(-\theta) = \cos\theta\, J_2 + \varepsilon_{32m} \sin\theta\, J_m = \cos\theta J_2 - \sin\theta\, J_1 \ . \qquad \text{(G.3.8)}$$

## G.4 The Euler Angles and Goldstein's body-frame ω formula

Here we are first going to formulate a problem, then we shall solve the problem.

In problems involving rigid-body dynamics, a non-inertial reference frame is often glued to the rigid body. In our non-swap notation we would call this Frame S', whereas Goldstein aptly calls it the Body Frame. The object exists in a space which has some inertial frame of reference we would call Frame S and Goldstein calls the Space frame. For example, for an axially-symmetric top that is spinning, precessing and nutating, the body frame would be selected to align with the top symmetry axis. One wants to hop into the Body Frame and analyze the problem taking into account fictitious forces and torques.

The orientation of any rigid body can be described by three Euler Angles which can be chosen in a variety of ways. These angles then describe the orientation of the Frame S' axes relative to the Frame S axes.

In our Section 1 we noted that the Frame S and Frame S' basis vectors are related in this way

$$\mathbf{e}_n = R\, \mathbf{e}'_n \qquad \textit{(1.1.1)} \qquad \text{(G.4.1)}$$

where R is some rotation. Here we shall take that rotation to be

$$R = R_z(\psi)\, R_x(\theta)\, R_z(\varphi) = R(\mathbf{\Phi}) = \exp(-i\, \mathbf{\Phi} \bullet \mathbf{J}) = \exp(-i\, \Phi\, \mathbf{n} \bullet J) \qquad \text{(G.4.2)}$$

where we have made a particular selection for the meaning of the **Euler angles** ψ,θ,φ. Some authors use other letters, and some put $R_y$ in the middle in place of $R_x$. Maple is happy to compute this matrix R. We enter the rotation matrices shown above in (G.1.8) then have Maple multiply according to (G.4.1) to get

```
R := evalm(Rz(psi) &* Rx(theta) &* Rz(phi));
```

$$R := \begin{bmatrix} \cos(\psi)\cos(\phi) - \sin(\psi)\cos(\theta)\sin(\phi) & -\cos(\psi)\sin(\phi) - \sin(\psi)\cos(\theta)\cos(\phi) & \sin(\psi)\sin(\theta) \\ \sin(\psi)\cos(\phi) + \cos(\psi)\cos(\theta)\sin(\phi) & -\sin(\psi)\sin(\phi) + \cos(\psi)\cos(\theta)\cos(\phi) & -\cos(\psi)\sin(\theta) \\ \sin(\theta)\sin(\phi) & \sin(\theta)\cos(\phi) & \cos(\theta) \end{bmatrix} \qquad \text{(G.4.3)}$$

If we carry out the procedure outlined in (G.2.14), things are rather unpleasant. The expression for sinΦ is a huge mess, but that for cosΦ is not *too* bad,

$$\cos(\Phi) = \frac{1}{2}\cos(\psi)\cos(\phi) - \frac{1}{2}\sin(\psi)\cos(\theta)\sin(\phi) - \frac{1}{2}\sin(\psi)\sin(\phi) + \frac{1}{2}\cos(\psi)\cos(\theta)\cos(\phi) + \frac{1}{2}\cos(\theta) - \frac{1}{2}$$

At least when ψ=θ=φ=0 we get the right answer cos(Φ) = 1 so Φ = 0. Certainly a detailed calculation of the angle Φ and the direction **n** is complicated and we shall have no need for those results.

We now turn to our Problem Statement. The basis vector relation between Frame S and Frame S' was given in (1.1.1) and (G.4.1) above which we rewrite as

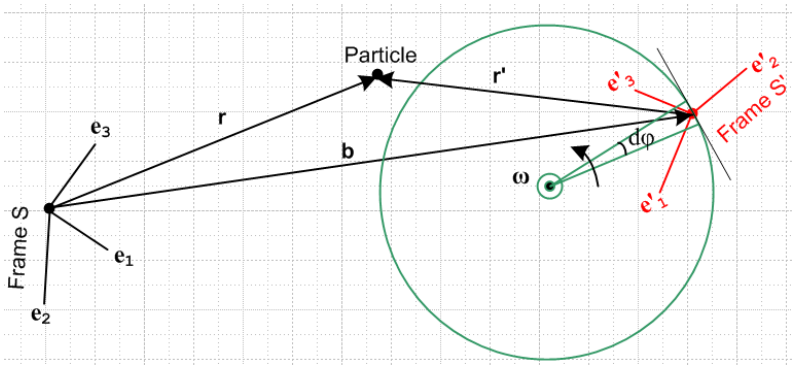
$$\mathbf{e}_n = R(\mathbf{\Phi})\,\mathbf{e}'_n = R_z(\psi)R_x(\theta)R_z(\varphi)\,\mathbf{e}'_n \qquad \text{(G.4.4)}$$

We now imagine that all three Euler angles are changing in time. As we observe things from the rotating Frame S' we see that the inertial Frame S basis vectors $\mathbf{e}_n$ are *moving* due to changing Euler angles. Within Frame S', this movement is described by (1.7.4),

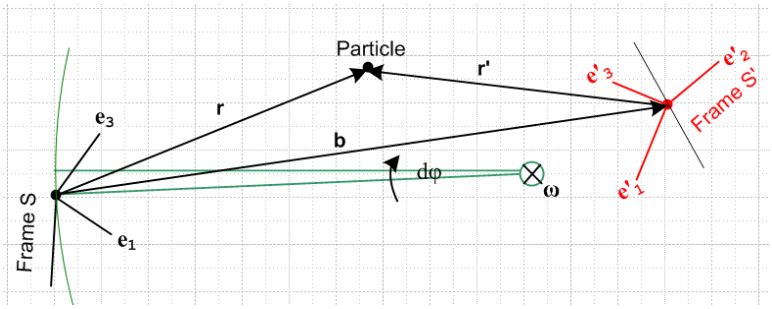
$$(d\mathbf{e}_n/dt)_{S'} = -\,\boldsymbol{\omega} \times \mathbf{e}_n \,. \qquad \textit{(1.7.4)} \qquad \text{(G.4.5)}$$

The problem is to compute **ω**! In particular, we want to know the components of **ω** evaluated in Frame S' because this is where we intend to do physics.

Recall our earlier pictures,




(G.4.6)




(G.4.7)

In Fig (G.4.6) the Frame S' axes rotate at **ω** relative to the Frame S axes. We then hop on a camera platform (located on the **ω** axis) which rotates at rate **ω** and observe (G.4.6). This freezes the rotation of Frame S' and causes Frame S to rotate instead, as shown in Fig (G.4.7). In this lower picture then the axes of Frame S rotate at **-ω** relative to those of Frame S'.

It is the **ω** shown in (G.4.6) which appears in (G.4.5), but we want its components evaluated in Frame S'.

Solution: We want to compute the $(d\mathbf{e}_n/dt)_{S'}$ which appears in (G.4.5). We start this way,

$$\mathbf{e}_n = R(\mathbf{\Phi})\,\mathbf{e'}_n \qquad (G.4.4)$$

$$(d\mathbf{e}_n)_{S'} = R(\mathbf{\Phi}+d\mathbf{\Phi})\mathbf{e'}_n - R(\mathbf{\Phi})\mathbf{e'}_n$$

$$= R_z(\psi+d\psi)\,R_x(\theta+d\theta)\,R_z(\varphi+d\varphi)\,\mathbf{e'}_n - R_z(\psi)\,R_x(\theta)\,R_z(\varphi)\,\mathbf{e'}_n$$

$$= [\,R_z(\psi+d\psi)\,R_x(\theta+d\theta)\,R_z(\varphi+d\varphi) - R_z(\psi)\,R_x(\theta)\,R_z(\varphi)\,]\mathbf{e'}_n$$

$$\equiv dR'\,\mathbf{e'}_n \qquad (G.4.8)$$

where

$$dR' \equiv [\,R_z(\psi+d\psi)\,R_x(\theta+d\theta)\,R_z(\varphi+d\varphi) - R_z(\psi)\,R_x(\theta)\,R_z(\varphi)\,] \ . \qquad (G.4.9)$$

We put a prime on dR' because we are working in Frame S' and dR' is a rank-2 tensor in Frame S'.

We now replace $\mathbf{e'}_n$ in (G.4.8) using (G.4.4) to get

$$(d\mathbf{e}_n)_{S'} = dR'\,\mathbf{e'}_n = dR'\,[R^{-1}(\mathbf{\Phi})\mathbf{e}_n\,] = [dR'\,R^{-1}(\mathbf{\Phi})\,]\,\mathbf{e}_n \ . \qquad (G.4.10)$$

Next, divide by dt to get

$$(d\mathbf{e}_n/dt)_{S'} = [(dR'/dt)_{S'}R^{-1}(\mathbf{\Phi})\,]\,\mathbf{e}_n$$

$$\equiv A'\,\mathbf{e}_n \qquad A' \equiv [(dR'/dt)_{S'}R^{-1}(\mathbf{\Phi})\,] \ . \qquad (G.4.11)$$

This left equation looks a bit like (G.4.5) which says $(d\mathbf{e}_n/dt)_{S'} = -\,\boldsymbol{\omega} \times \mathbf{e}_n$, so that is hopeful.

The next step is to process dR' as follows (all to first order in the infinitesimal angles),

$$dR' = [\,R_z(\psi+d\psi)\,R_x(\theta+d\theta)\,R_z(\varphi+d\varphi) - R_z(\psi)\,R_x(\theta)\,R_z(\varphi)\,]$$

$$= [\,R_z(\psi)R_z(d\psi)\,R_x(\theta)\,R_x(d\theta)R_z(\varphi)R_z(d\varphi) - R_z(\psi)\,R_x(\theta)\,R_z(\varphi)]$$

$$= [\,R_z(\psi)\{1-id\psi J_3\}\,R_x(\theta)\{1-id\theta J_1\}R_z(\varphi)\{1-id\varphi J_3\} - R_z(\psi)\,R_x(\theta)\,R_z(\varphi)]$$

$$= [-id\psi\,R_z(\psi)J_3R_x(\theta)R_z(\varphi) - id\theta\,R_z(\psi)\,R_x(\theta)J_1R_z(\varphi) - id\varphi\,R_z(\psi)\,R_x(\theta)R_z(\varphi)J_3\,] \ . \qquad (G.4.12)$$

Then,

$$(dR'/dt)_{S'} = [\,-i\dot{\psi}\,R_z(\psi)J_3R_x(\theta)R_z(\varphi) - i\dot{\theta}\,R_z(\psi)R_x(\theta)J_1R_z(\varphi) - i\dot{\varphi}\,R_z(\psi)R_x(\theta)R_z(\varphi)J_3\,] \ . \qquad (G.4.13)$$

We are now going to show every single step. The trivial sandwich rule (G.3.6) will be used three times as shown in blue:

$$A' = [\, -i\dot{\psi}\ R_z(\psi)J_3\, R_x(\theta)R_z(\varphi)\ -\ i\dot{\theta}\ R_z(\psi)\, R_x(\theta)J_1R_z(\varphi)\ -\ i\dot{\varphi}\, R_z(\psi)\, R_x(\theta)R_z(\varphi)J_3\,]R_z(-\varphi)\, R_x(-\theta)\, R_z(-\psi)$$

$$= [\, -i\dot{\psi}\ R_z(\psi)J_3\, R_x(\theta)\ -\ i\dot{\theta}\ R_z(\psi)\, R_x(\theta)J_1\ -\ i\dot{\varphi}\, R_z(\psi)\, R_x(\theta)\color{blue}{R_z(\varphi)J_3R_z(-\varphi)}\,]\, R_x(-\theta)\, R_z(-\psi)$$

$$= [\, -i\dot{\psi}\ R_z(\psi)J_3\, R_x(\theta)\ -\ i\dot{\theta}\ R_z(\psi)\, R_x(\theta)J_1\ -\ i\dot{\varphi}\, R_z(\psi)\, R_x(\theta)\color{blue}{J_3}\,]\, R_x(-\theta)\, R_z(-\psi)$$

$$= [\, -i\dot{\psi}\ R_z(\psi)J_3\ -\ i\dot{\theta}\ R_z(\psi)\, \color{blue}{R_x(\theta)J_1R_x(-\theta)}\ -\ i\dot{\varphi}\, R_z(\psi)\, R_x(\theta)J_3R_x(-\theta)\,]\, R_z(-\psi)$$

$$= [\, -i\dot{\psi}\ R_z(\psi)J_3\ -\ i\dot{\theta}\ R_z(\psi)\, \color{blue}{J_1}\ -\ i\dot{\varphi}\, R_z(\psi)\, R_x(\theta)J_3R_x(-\theta)\,]\, R_z(-\psi)$$

$$= [\, -i\dot{\psi}\ \color{blue}{R_z(\psi)J_3\, R_z(-\psi)}\ -\ i\dot{\theta}\ R_z(\psi)\, J_1\, R_z(-\psi)\ -\ i\dot{\varphi}\, R_z(\psi)\, R_x(\theta)J_3R_x(-\theta)\, R_z(-\psi)\,]$$

$$= [\, -i\dot{\psi}\ \color{blue}{J_3}\ -\ i\dot{\theta}\ R_z(\psi)\, J_1\, R_z(-\psi)\ -\ i\dot{\varphi}\, R_z(\psi)\, R_x(\theta)J_3R_x(-\theta)\, R_z(-\psi)\,]$$

$$= [\, -i\dot{\psi}\ J_3\ -\ i\dot{\theta}\ M_1\ -\ i\dot{\varphi}\, M_2\,] \qquad \text{(G.4.14)}$$

where

$$M_1 \equiv R_z(\psi)\, J_1R_z(-\psi) \qquad = [\, R_3(\psi)\, J_1R_3(-\psi)]$$

$$M_2 \equiv R_z(\psi)\, R_x(\theta)J_3R_x(-\theta)R_z(-\psi) \qquad = R_3(\psi)\, [\, R_1(\theta)J_3R_1(-\theta)\,]\, R_3(-\psi)\ . \qquad \text{(G.4.15)}$$

We now call upon our non-trivial sandwich formulas in (G.3.8) to simplify thing further :

$$M_1 = R_3(\psi)\, J_1R_3(-\psi) = \cos\psi J_1 + \sin\psi\, J_2 \qquad \text{// (G.3.8) line 5} \qquad \text{(G.4.16)}$$

$$M_2 = R_3(\psi)\, [\, R_1(\theta)J_3R_1(-\theta)\,]\, R_3(-\psi)$$

$$= R_3(\psi)\, [\, \cos\theta\, J_3 - \sin\theta\, J_2\,]\, R_3(-\psi) \qquad \text{// (G.3.8) line 2}$$

$$= \cos\theta\, [\, R_3(\psi)\, J_3\, R_3(-\psi)]\ - \sin\theta\, [R_3(\psi)J_2R_3(-\psi)]$$

$$= \cos\theta\, J_3\ - \sin\theta\, (\cos\psi J_2 - \sin\psi\, J_1) \qquad \text{// (G.3.6) and (G.3.8) line 6}$$

$$= \sin\theta\sin\psi J_1 - \sin\theta\cos\psi J_2 + \cos\theta\, J_3\ . \qquad \text{(G.4.17)}$$

Then

$$A' = [\, -i\dot{\psi}\ J_3 \ - \ i\dot{\theta}\ M_1 \ - i\dot{\varphi}\, M_2\,]$$

$$= [\, -i\dot{\psi}\ J_3 \ - \ i\dot{\theta}\,(\cos\psi J_1 + \sin\psi\, J_2) \ - i\dot{\varphi}\,(\sin\theta c\sin\psi J_1 - \sin\theta\cos\psi J_2 + \ \cos\theta\, J_3)\,]$$

$$= [\, -i\dot{\psi}\ J_3 \ - \ i\dot{\theta}\,\cos\psi J_1 \ - \ i\dot{\theta}\,\sin\psi\, J_2 \ - i\dot{\varphi}\,\sin\theta\sin\psi J_1 + \ i\dot{\varphi}\sin\theta\cos\psi J_2 - i\dot{\varphi}\ \cos\theta\, J_3\,]$$

$$= (-i)[\, \dot{\psi}\ J_3 \ + \dot{\theta}\,\cos\psi J_1 \ + \dot{\theta}\,\sin\psi\, J_2 \ + \dot{\varphi}\,\sin\theta\sin\psi J_1 - \dot{\varphi}\sin\theta\cos\psi J_2 \ + \dot{\varphi}\ \cos\theta\, J_3\,]$$

$$= (-i)[\, (\,\dot{\theta}\,\cos\psi + \dot{\varphi}\,\sin\theta\sin\psi)J_1 \ + (\dot{\theta}\,\sin\psi - \dot{\varphi}\sin\theta\cos\psi)J_2 + (\dot{\psi} + \dot{\varphi}\,\cos\theta)J_3\,]$$

$$= -\,[\, (\,\dot{\theta}\,\cos\psi + \dot{\varphi}\,\sin\theta\sin\psi)(iJ_1) \ + (\dot{\theta}\,\sin\psi - \dot{\varphi}\sin\theta\cos\psi)(iJ_2) + (\dot{\psi} + \dot{\varphi}\,\cos\theta)(iJ_3)\,] \qquad \text{(G.4.18)}$$

We now take the ij element of this matrix using the fact (G.1.3) that $(iJ_k)_{ij} = \varepsilon_{kij}$ :

$$A'_{ij} = -\,[\, (\,\dot{\theta}\,\cos\psi + \dot{\varphi}\,\sin\theta\sin\psi)\varepsilon_{1ij} \ + (\dot{\theta}\,\sin\psi - \dot{\varphi}\sin\theta\cos\psi)\varepsilon_{2ij} + (\dot{\psi} + \dot{\varphi}\,\cos\theta)\varepsilon_{3ij}\,] \,. \qquad \text{(G.4.19)}$$

The tensor $\varepsilon_{kij}$ is antisymmetric in i↔j and therefore the entire matrix A' is antisymmetric and thus has only three distinct matrix elements. They are:

$$A'_{23} = -\,(\,\dot{\theta}\,\cos\psi + \dot{\varphi}\,\sin\theta\sin\psi)\varepsilon_{123} \ = \ -\,(\,\dot{\theta}\,\cos\psi + \dot{\varphi}\,\sin\theta\sin\psi)$$

$$A'_{31} = -\,(\dot{\theta}\,\sin\psi - \dot{\varphi}\sin\theta\cos\psi)\varepsilon_{231} = -\,(\dot{\theta}\,\sin\psi - \dot{\varphi}\sin\theta\cos\psi)$$

$$A'_{12} = -\ (\dot{\psi} + \dot{\varphi}\,\cos\theta)\ \varepsilon_{312} \ = \ -\ (\dot{\psi} + \dot{\varphi}\,\cos\theta)\,. \qquad \text{(G.4.20)}$$

The work is now nearly done. In order to determine **ω**, we now want to compare,

$$(d\mathbf{e}_n/dt)_{S'} \ = \ A'\,\mathbf{e}_n \qquad \textit{(G.4.11)}$$

$$(d\mathbf{e}_n/dt)_{S'} \ = -\,\boldsymbol{\omega}\ \mathrm{x}\ \mathbf{e}_n\,. \qquad \textit{(G.4.5)}$$

Since the left sides are the same, we take Frame S' components of the right sides and set them equal,

$$[A'\,\mathbf{e}_n]'_i = -\,[\boldsymbol{\omega}\ \mathrm{x}\ \mathbf{e}_n]'_i$$

or

$$A'_{ij}\,(\mathbf{e}_n)'_j \ = \ -\,\varepsilon_{ikj}\,(\omega)'_k(\mathbf{e}_n)'_j$$

or

$$A'_{ij} = -\,\varepsilon_{ikj}\,(\omega)'_k \ = \ \varepsilon_{ijk}\,(\omega)'_k$$

so

$$A'_{12} = \ \varepsilon_{123}(\omega)'_3 \ = (\omega)'_3$$

$$A'_{23} = \varepsilon_{231}(\omega)'_1 = (\omega)'_1$$
$$A'_{31} = \varepsilon_{312}(\omega)'_2 = (\omega)'_2 \ . \qquad \text{(G.4.21)}$$

Therefore our final result for the components of **ω** in rotating Frame S' is:

$$(\omega)'_1 = A'_{23} = -(\dot\theta\cos\psi + \dot\varphi\sin\theta\sin\psi) = -\dot\varphi\sin\theta\sin\psi - \dot\theta\cos\psi$$
$$(\omega)'_2 = A'_{31} = -(\dot\theta\sin\psi - \dot\varphi\sin\theta\cos\psi) = \dot\varphi\sin\theta\cos\psi - \dot\theta\sin\psi$$
$$(\omega)'_3 = A'_{12} = -(\dot\psi + \dot\varphi\cos\theta) = -\dot\varphi\cos\theta - \dot\psi \ . \quad \text{// our result} \qquad \text{(G.4.22)}$$

Below (G.1.8) we discuss the different conventions for defining rotation matrices. Goldstein defines his $R_i(\alpha)$ matrices in the passive sense whereas we use the active sense. This can be seen by comparing our matrices (G.1.8) to his/their matrices (G page 109, GPS page 153). The upshot is the in order to compare results, we have to negate each Euler angle since $R_i^{G}(\alpha) = R_i^{us}(-\alpha)$. Doing this, the above results become,

$$(\omega)'_1 = \dot\varphi\sin\theta\sin\psi + \dot\theta\cos\psi$$
$$(\omega)'_2 = \dot\varphi\sin\theta\cos\psi - \dot\theta\sin\psi$$
$$(\omega)'_3 = \dot\varphi\cos\theta + \dot\psi \quad \text{// our result converted to Goldstein convention} \qquad \text{(G.4.23)}$$

which we can now compare to GPS page 174,

$$\omega_{x'} = \dot\phi\sin\theta\sin\psi + \dot\theta\cos\psi$$
$$\omega_{y'} = \dot\phi\sin\theta\cos\psi - \dot\theta\sin\psi$$
$$\omega_{z'} = \dot\phi\cos\theta + \dot\psi. \qquad (4.87)$$
(G.4.24)

Goldstein's derivation of these equations involves staring carefully at a picture of the three Euler rotations (where the middle rotation θ is about a "line of nodes") and considering them one at a time and adding the **ω** vectors that arise from each Euler angle's contribution. This explanation has always seemed a bit difficult to follow which is one of our motivations for this section in which we verify the result by brute force. The second motivation is of course to exercise all our rotation matrix machinery.

**G.9 Generalizations of the Rotation Group**

Here we consider some generalizations of the ideas presented above in Section G.1

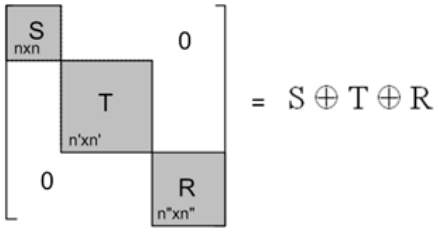
N dimensional representations of the rotation group

The generators $J_i$ shown in (G.1.2) are a special case of a more general idea which starts with the commutation relation

$$[J_i, J_j] = i\varepsilon_{ijk}J_k \ . \quad \text{// for example, } [J_1,J_2] = iJ_3 \qquad \textit{(G.1.4)} \qquad \text{(G.2.1)}$$

One first thinks of the $J_i$ as abstract "operators" in some abstract "operator space". One can show that it is possible to find a set of three NxN matrices of any integer dimension N which satisfy (G.1.4). The matrices are not unique, so (G.1.2) for the $J_i$ in three dimensions is not unique, but it is a standard form.

The three NxN generator matrices $J_i$ are said to form an N-dimensional "irreducible representation" of the abstract generators $J_i$. One can always create new viable generator matrices by taking a "direct sum" of existing viable generator matrices, such as in this block-diagonal-form picture




(G.2.2)

This generator matrix is "reducible" into a direct sum of S, T and R. An "irreducible" representation is one that cannot be reduced in this manner. The same comment applies to rotation matrices.

The commutation relation (G.2.1) is an example of a **Lie Algebra**. Our particular Lie Algebra is called so(3), so we can represent the algebra elements $J_i$ of this algebra by three NxN matrices $J_i$. It is possible to write down a formula analogous to (G.1.3) $(iJ_a)_{bc} = \varepsilon_{abc}$ which works for any N, but (G.1.3) itself only applies to N = 3. This is so because $\varepsilon_{abc}$ has no meaning for $N \neq 3$. But it always has meaning in (G.2.1) because there are only three generators regardless of the value of N.

For general N, the object $R_i(\theta) = \exp(-i\theta \mathbf{J}_i)$ is an NxN matrix which represents the action of a rotation of an N-vector in a Euclidean space $E^N$. The set of such rotation matrices forms an "irreducible representation" of the rotation group SO(3) in N dimensions. The integer N is usually written N = 2j+1 where j = 0, 1/2, 1, 3/2 ... and this j then serves as a label for a given matrix representation.

The value of j in N = 2j+1 is associated with "angular momentum" or "spin". In the case N=2 (having j=1/2) the generator matrices are the 2x2 "Pauli matrices". In this case the 2x2 matrices $\exp(-i\theta J_i)$ describe the rotations of spin-1/2 particles such as electrons or protons. Here are the details for N=2 :

$$J_x = (1/2)\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad J_y = (1/2)\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad J_z = (1/2)\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$R_x = \begin{pmatrix} \cos\frac{\theta}{2} & -i\sin\frac{\theta}{2} \\ -i\sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{pmatrix} \qquad R_y = \begin{pmatrix} \cos\frac{\theta}{2} & -\sin\frac{\theta}{2} \\ \sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{pmatrix} \qquad R_z = \begin{pmatrix} \exp(-i\frac{\theta}{2}) & 0 \\ 0 & \exp(+i\frac{\theta}{2}) \end{pmatrix}$$

(G.2.2)

The "vectors" for spin-1/2 particles have two components $\begin{pmatrix} u \\ d \end{pmatrix}$. The special case $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ is called "spin up" and $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$ is "spin down".

For the Lie Algebra so(3) one can show that $J^2 \equiv J_1^2 + J_2^2 + J_3^2$ and any particular $J_i$ commute with each other, so $[J^2, J_i] = 0$. $J^2$ is called a Casimir operator of this Algebra, and fancier Lie Algebras can have several such Casimirs.

A Differential operator representation of the rotation group

It is also possible to "represent" the three rotation generators $J_i$ by three differential operators in spherical coordinates θ and φ. These operators satisfy $[J_i, J_j] = i\varepsilon_{ijk}J_k$ and in this context they are usually called $L_i$ but we shall stick with $J_i$. In this case, one can compute the differential operator $J^2$ and one can ponder differential equations which take the form $J^2\, f_{jm}(\theta,\varphi) = j(j+1)\, f_{jm}(\theta,\varphi)$ and $J_z\, f_{jm}(\theta,\varphi) = m\, f_{jm}(\theta,\varphi)$. [The facts that the eigenvalue of $J^2$ is j(j+1) and not $j^2$, and that m runs from -j to j, derive from the structure of the Lie Algebra.] The solutions $f_{jm}(\theta,\varphi)$ are able to have well-defined eigenvalues j(j+1) and m *because* $[J^2, J_3] = 0$. If we instead had $[J^2, J_3] \neq 0$, then $[J^2, J_3]\, f_{jm}(\theta,\varphi) = j(j+1)m - mj(j+1) = 0$ is a contradiction and the two eigenfunction equations could not exist. The solutions $f_{jm}(\theta,\varphi)$ of these equations are called the **spherical harmonics** and are usually written $Y_{jm}(\theta,\varphi)$. Just for the record, here is what the differential operators look like, where C = cos and S = sin (for example, $S_\varphi = \sin\varphi$ and $\partial_\varphi = \partial/\partial\varphi$) :

$$J_1 = i\,[\, S_\varphi\, \partial_\theta + \cot\theta\, C_\varphi\, \partial_\varphi] \qquad J_\pm = e^{\pm i\varphi}\, [\, \pm\partial_\theta + i\, \cot\theta\, \partial_\varphi\,]$$
$$J_2 = -i\,[\, C_\varphi\, \partial_\theta - \cot\theta\, S_\varphi\, \partial_\varphi] \qquad J^2 = -[\, \partial_\theta^2 + \cot\theta\, \partial_\theta + (1/S_\theta)^2\, \partial_\varphi^2]$$
$$J_3 = -i\, \partial_\varphi \qquad J^2 = -[\, (1/S\theta)\, \partial_\theta\, [\, S_\theta\, \partial_\theta\,] + (1/S_\theta)^2\, \partial_\varphi^2\,] \qquad \text{(G.2.3)}$$

Reader Exercise: Verify that the three operators on the left satisfy the Lie Algebra $[J_i, J_j] = i\varepsilon_{ijk}J_k$.

For the hydrogen atom with a spinless electron, there are three mutually commuting quantities H, $J^2$ and $J_3$ where H is the Hamiltonian. This means that the solution eigenfunctions can have well defined E, j and m values and these eigenfunctions are those painful "orbitals" appearing in chemistry books. When the Hamiltonian commutes with some other operator like $J^2$, that operator is called a "symmetry". Solution functions then bear a label for each such symmetry, such as j for $J^2$.

The Lie Algebra so(3) is isomorphic (one-to-one related) to another Lie Algebra called su(2).
The Lie Group SO(3) is isomorphic to another Lie Group called SU(2).

In the above we discuss only the Lie Group SO(3) with its three generators $J_i$. There are many other Lie Groups which have physics applications.

Some Other Lie Groups of Interest

The group SO(n) is the **orthogonal group** in n dimensions and it has n(n-1)/2 generators.

The group SO(3,1) is the **Lorentz Group** which has 6 generators $J_i$ and $K_i$ which generate 3 rotations and 3 "boosts" (velocity transformations). The Lie Algebra is this,

$$[\, J_i, J_j] = +i\, \varepsilon_{ijk}J_k$$

$$[\,J_i, K_j] = +i\,\varepsilon_{ijk}\,K_k$$
$$[\,K_i, K_j] = -i\,\varepsilon_{ijk}J_k \qquad \text{(G.2.4)}$$

There are two Casimirs : $J^2 - K^2$ and $\mathbf{J}\bullet\mathbf{K}$ .

In the "vector representation" known as 1/2⊗1/2 the generators are represented as 4x4 matrices. When these are exponentiated, one obtains the finite rotation and boost matrices used in special relativity. For example, with space-time vectors ordered $x^\mu$ = (ct,x,y,z) one has

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \cos(r) & -\sin(r) \\ 0 & 0 & \sin(r) & \cos(r) \end{pmatrix} = \exp(-irJ_1) \qquad \text{where } (J_1)^\mu{}_\nu = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \end{pmatrix} \qquad \text{// rotation } R_x(r)$$

$$\begin{pmatrix} \cosh(b) & \sinh(b) & 0 & 0 \\ \sinh(b) & \cosh(b) & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = \exp(-ibK_1) \quad \text{where } (K_1)^\mu{}_\nu = \begin{pmatrix} 0 & i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \qquad \text{// boost } B_x(b) \qquad \text{(G.2.5)}$$

The **Poincare Group** is basically the Lorentz group SO(3,1) bolted onto the group T(4) of translations in four directions ct,x,y,z. It thus has 10 generators $J_i$, $K_i$ and $P_\mu$ where these last four are momentum and energy. The Poincare algebra has two Casimir operators whose eigenvalues are associated with mass and spin. For example, the mass Casimir is $P^\mu P_\mu$ . The irreducible representations of the Poincare Group are associated with "elementary particles" which have well defined mass and spin.

The group **SU(3)** has 8 generators and 2 Casimirs. In one key representation the generators are represented by 3x3 matrices which act on 3-vectors. Instead of having up and down states as with spin-1/2 noted above, these vectors have up, down and strange states called u,d.s which are associated with quarks. The full symmetry group for the Standard Model of elementary particles is SU(3) x SU(2) x U(1) in which SU(3) plays its part.

Special Groups have Traceless Generators

It is desirable that "rotation matrices" have unit determinant because such matrices then do not change the "length" of a vector on which they act. When the representation matrices are restricted to have unit determinant, they are called "special" and the group name is prefixed by the letter S, as in SO(3) for the rotation group. For the 3x3 representation of the rotation group we know that the matrices are real orthogonal which means $RR^T = 1$ which in turn means $[\det(R)]^2 = 1$ and in SO(3) we select only those R with det(R) = +1. A "rotation" which just negates z (reflection) still satisfies $RR^T = 1$ but has det(R) = -1.

An elegant theorem concerning exponentiated square matrices is this (proved below):

$$\det(e^A) = e^{tr(A)} \qquad \text{(G.2.6)}$$

where det is the determinant and $\mathrm{tr}(A) \equiv \Sigma_i A_{ii}$ is the "trace" or "spur" of the matrix A -- the sum of the diagonal elements. If we want the matrix $\exp(-i\,\theta\,\hat{\mathbf{n}} \bullet \mathbf{J})$ to have unit determinant so it is "Special", the exponent must be traceless, and in this case that means that the generators $J_i$ must all be traceless. One can see from examples (G.1.2) and (G.2.2) and (G.2.5) that this is indeed the case.

Offhand, the matrix identity $\det(e^{\mathbf{A}}) = e^{\mathbf{tr(A)}}$ seems very unlikely and almost too simple. For that reason, we include here a straightforward proof which we feel is "one for the Book".

Proof of (G.2.6) There are no implied sums in this proof!

Write $A = \Sigma_{ij} A_{ij}\, s^{(ij)}$ where $[s^{(ij)}]_{ab} \equiv \delta_{ia}\delta_{jb}$ . To verify,

$$A_{ab} = \Sigma_{ij} A_{ij}\, [s^{(ij)}]_{ab} = \Sigma_{ij} A_{ij} \delta_{ia}\delta_{jb} = A_{ab} \quad .$$

The matrix $s^{(ij)}$ is all zeros except for a single 1 located in row a and column b. Using $e^{x+y\cdots} = e^x e^y \ldots$ we can write

$$e^{\mathbf{A}} = \exp(\Sigma_{ij} A_{ij}\, s^{(ij)}) = \Pi_{i,j} \exp(A_{ij}\, s^{(ij)}) \quad .$$

Then using det(XY..) = det(X)det(Y).... ,

$$\det(e^{\mathbf{A}}) = \det\{\Pi_{i,j} \exp(A_{ij}\, s^{(ij)})\} = \Pi_{i,j} \det[\exp(A_{ij}\, s^{(ij)})] \quad . \qquad \text{(G.2.7)}$$

[Case $i \neq j$ :] We first note that $[s^{(ij)}]^2 = 0$ :

$$[s^{(ij)}]^2_{ac} = \Sigma_b [s^{(ij)}]_{ab} [s^{(ij)}]_{bc} = \Sigma_b \delta_{ia}\delta_{jb}\, \delta_{ib}\delta_{jc} = \delta_{ia}\delta_{ji}\delta_{jc} = 0 \text{ since } i \neq j$$

Then $[s^{(ij)}]^n = 0$ for $n \geq 2$. In this case we have

$$[\exp(A_{ij}\, s^{(ij)}) = \Sigma_{n=0}^{\infty} (A_{ij})^n [\, s^{(ij)}]^n/n! = 1 + A_{ij} [\, s^{(ij)}]$$

and so

$$\det[\exp(A_{ij}\, s^{(ij)})] = \det[\, 1 + A_{ij}\, s^{(ij)}] = 1 \, .$$

This is so because the matrix in question has all 1's on the diagonal and one non-vanishing off-diagonal element at (i,j) In fact, *any* triangular matrix (one side all zeros) with 1's on the diagonal has det = 1.

[Case i=j : ] In this case we have $[s^{(ii)}]^2 = [s^{(ii)}]$ :

$$[s^{(ii)}]^2_{ac} = \Sigma_b [s^{(ii)}]_{ab} [s^{(ii)}]_{bc} = \Sigma_b \delta_{ia}\delta_{ib}\, \delta_{ib}\delta_{ic} = \delta_{ia}\delta_{ii}\delta_{ic} = \delta_{ia}\delta_{ic} = [s^{(ii)}]_{ac} \quad .$$

Note that $[s^{(ii)}]_{ab} = \delta_{ia}\delta_{ib} = 1$ only when a = b = i, so $s^{(ii)}$ is an all-zero matrix with a single 1 at location i on the diagonal.

Since $[s^{(ii)}]^2 = s^{(ii)}$ it follows that $[s^{(ii)}]^n = s^{(ii)}$ for $n \geq 1$. Then,

$$\exp(A_{ii}\, s^{(ii)}) = \Sigma_{n=0}^{\infty} (A_{ii})^n [\, s^{(ii)}]^n / n! = 1 + s^{(ii)} [\Sigma_{n=1}^{\infty}(A_{ii})^n / n!]$$

$$= 1 + s^{(ii)} [\, -1 + \Sigma_{n=0}^{\infty}(A_{ii})^n/n! \,] = 1 + s^{(ii)}[-1 + \exp(A_{ii})] \ .$$

This last item is the unit matrix with the $i^{th}$ diagonal 1 replaced by $\exp(A_{ii})$ . Therefore,

$$\det [\exp(A_{ii}\, s^{(ii)}) ] = \det \{ 1 + s^{(ii)}[-1 + \exp(A_{ii})] \} = \exp(A_{ii}) \ .$$

Now go back to (G.2.7),

$$\det(e^{A}) = \Pi_{i,j} \det [\exp(A_{ij}\, s^{(ij)}) ] \qquad \textit{(G.2.7)}$$

$$= (\Pi_{i\neq j} \det [\exp(A_{ij}\, s^{(ij)}) ] ) \ * \ (\Pi_{i=j} \det [\exp(A_{ij}\, s^{(ij)}) ] )$$

$$= (1*1*1*1..... \quad ....*1*1) * ( \ \exp(A_{11})\exp(A_{22}) ..... \quad )$$

$$= 1 * \exp(A_{11} + A_{22} + ...) = \exp (\mathrm{tr}(A))$$

$$= e^{tr(A)} \qquad \text{QED}$$