Euler Angles compared with exp(-iu n.J) parameters PhL 11.19.16

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0. Goal of this document

I know two ways to represent a general rotation :

way1: $R = R_z(\psi)R_x(\theta)R_z(\varphi)$ Euler angles using x in the middle

way2: $R = e^{-iun\bullet J} = \exp(-iu\,\mathbf{n}\bullet\mathbf{J})$ Rotation of amount u about axis **n** (unit vector)

The goal is the following:

(1) express (ψ,θ,φ) in terms of (n_1,n_2,n_3,u)
(2) express (n_1,n_2,n_3,u) in terms of (ψ,θ,φ)

To get the results, I make use of a certain result from "exp nJ calc...doc" which is this

$$R_n(u) = \exp(-iu\mathbf{n}\bullet\mathbf{J}) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} + (\cos u - 1)\begin{pmatrix} 1-n_1^2 & -n_1n_2 & -n_1n_3 \\ -n_1n_2 & 1-n_2^2 & -n_2n_3 \\ -n_1n_3 & -n_2n_3 & 1-n_3^2 \end{pmatrix} + \sin u \begin{pmatrix} 0 & -n_3 & n_2 \\ n_3 & 0 & -n_1 \\ -n_2 & n_1 & 0 \end{pmatrix}$$

I derived the above in 2005 but had a wrong sign in the middle term, it is now corrected in that document and the correct result is stated above and used below.

The results are given in boxes in Sections 4 and 5 below which I copy to the next page :

I have always known there were such relations between the two parametrizations, but I had never figured them out until today.

In Section 1 I simply derive certain rotation matrices which appear in Goldstein's book.

In Section 2 I show that just looking at infinitesimal rotations does not solve the problem.

Section 3 is just setup for the following two sections where the results are obtained.

Results:

Summary for (1): express (ψ,θ,φ) in terms of (n_1,n_2,n_3,u)

$\cos\theta = 1 + (\cos u-1)(1-n_3^2)$ $\quad 0 \le \theta \le \pi$

$\sin\theta = \sqrt{1-\cos^2\theta}$ $\quad > 0$

$\sin\psi = [-(\cos u-1)n_1n_3 + \sin u\, n_2]/\sin\theta$ $\quad 0 \le \psi \le 2\pi$

$\cos\psi = [(\cos u-1)n_2n_3 + \sin u\, n_1]/\sin\theta$

$\sin\varphi = [-(\cos u-1)n_1n_3 - \sin u\, n_2]/\sin\theta$ $\quad 0 \le \psi \le 2\pi$

$\cos\varphi = [-(\cos u-1)n_2n_3 + \sin u\, n_1]/\sin\theta$

Summary for (2): express (n_1,n_2,n_3,u) in terms of (ψ,θ,φ)

$$\cos u = [\,(\cos\theta-1) + (\cos\theta+1)(\cos\psi\cos\varphi - \sin\psi\sin\varphi)\,]/2 = \cos^2(\theta/2)\cos(\psi-\varphi) - \sin^2(\theta/2)$$

From that you can get

$$\sin u = \cos(\theta/2)\sqrt{(\cos(\psi-\varphi)+1)[2-\cos^2(\theta/2)(\cos(\psi-\varphi)+1)]} \quad > 0$$

Then

$n_3 = [\cos\psi\sin\varphi + \sin\psi\cos\theta\cos\varphi + \sin\psi\cos\varphi + \cos\psi\cos\theta\sin\varphi]/2\sin u$

$n_1 = [\cos\psi\sin\theta + \sin\theta\cos\varphi]/2\sin u$

$n_2 = [\sin\psi\sin\theta - \sin\theta\sin\varphi]/2\sin u$

1. Derive Goldstein's rotation matrices shown on his page 109

I thought I had this somewhere but could not find it. So I will do this right here using Maple and using my sign conventions for active rotations where I have

$$R_x(\theta)=\begin{pmatrix}1 & 0 & 0\\ 0 & \cos\theta & -\sin\theta\\ 0 & \sin\theta & \cos\theta\end{pmatrix}\qquad R_y(\theta)=\begin{pmatrix}\cos\theta & 0 & \sin\theta\\ 0 & 1 & 0\\ -\sin\theta & 0 & \cos\theta\end{pmatrix}\qquad R_z(\theta)=\begin{pmatrix}\cos\theta & -\sin\theta & 0\\ \sin\theta & \cos\theta & 0\\ 0 & 0 & 1\end{pmatrix}$$

I do this in Euler angle matrices.mws. First I enter the above matrices and verify against the above,

```
Rx := (a) -> matrix(3,3,[1,0,0,0,cos(a),-sin(a),0,sin(a),cos(a)]):
Rx(theta);
```

$$\begin{bmatrix}1 & 0 & 0\\ 0 & \cos(\theta) & -\sin(\theta)\\ 0 & \sin(\theta) & \cos(\theta)\end{bmatrix}$$

```
Ry := (a) -> matrix(3,3,[cos(a),0,sin(a), 0,1,0,-sin(a),0,cos(a)]):
Ry(theta);
```

$$\begin{bmatrix}\cos(\theta) & 0 & \sin(\theta)\\ 0 & 1 & 0\\ -\sin(\theta) & 0 & \cos(\theta)\end{bmatrix}$$

```
Rz := (a) -> matrix(3,3,[cos(a),-sin(a),0,sin(a),cos(a),0,0,0,1]):
Rz(theta);
```

$$\begin{bmatrix}\cos(\theta) & -\sin(\theta) & 0\\ \sin(\theta) & \cos(\theta) & 0\\ 0 & 0 & 1\end{bmatrix}$$

Then I think this should generate Goldstein's page 109 A matrix (here I use negative angles)

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

$$A:=\begin{bmatrix}\cos(\psi)\cos(\phi)-\sin(\psi)\cos(\theta)\sin(\phi) & \cos(\psi)\sin(\phi)+\sin(\psi)\cos(\theta)\cos(\phi) & \sin(\psi)\sin(\theta)\\ -\sin(\psi)\cos(\phi)-\cos(\psi)\cos(\theta)\sin(\phi) & -\sin(\psi)\sin(\phi)+\cos(\psi)\cos(\theta)\cos(\phi) & \cos(\psi)\sin(\theta)\\ \sin(\theta)\sin(\phi) & -\sin(\theta)\cos(\phi) & \cos(\theta)\end{bmatrix}$$

and this agrees with his (4-46), I checked every entry. The inverse is then

```
Ainv := inverse(A): simplify(%);
```

$$\begin{bmatrix}\cos(\psi)\cos(\phi)-\sin(\psi)\cos(\theta)\sin(\phi) & -\sin(\psi)\cos(\phi)-\cos(\psi)\cos(\theta)\sin(\phi) & \sin(\theta)\sin(\phi)\\ \cos(\psi)\sin(\phi)+\sin(\psi)\cos(\theta)\cos(\phi) & -\sin(\psi)\sin(\phi)+\cos(\psi)\cos(\theta)\cos(\phi) & -\sin(\theta)\cos(\phi)\\ \sin(\psi)\sin(\theta) & \cos(\psi)\sin(\theta) & \cos(\theta)\end{bmatrix}$$

and this agrees with his (4-47).

2. Compare $R_z(-\psi)R_x(-\theta)R_z(-\varphi)$ to $e^{-i\gamma n\bullet J}$ using infinitesimals only

The question here is this: can you relate (ψ,θ,φ) to (n_1,n_2,n_3,γ) merely by looking at a very small rotation? I once thought yes, but now I think no, there is not enough information in the infinitesimal.

Evaluate both sides to first order in small angles,

$$R_z(-\psi)R_x(-\theta)R_z(-\varphi) = [\,1 + i\psi J_3]\,[\,1 + i\theta J_1]\,[\,1 + i\varphi J_3]$$

$$= 1 + i\psi J_3 + i\theta J_1 + i\varphi J_3 + \text{order}(\text{angle}^2)$$

$$= 1 + i(\psi+\varphi)J_3 + i\theta J_1 + \text{order}(\text{angle}^2)$$

Let's construct this infinitesimal matrix in Maple as well using my data

$$J_x = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix} \qquad J_y = \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix} \qquad J_z = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

Here then are the generators and they verify with the above.

```
Jx := matrix(3,3,[0,0,0,0,0,-I,0,I,0]);
```

$$Jl := \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -I \\ 0 & I & 0 \end{bmatrix}$$

```
Jy := matrix(3,3,[0,0,I,0,0,0,-I,0,0]);
```

$$Jy := \begin{bmatrix} 0 & 0 & I \\ 0 & 0 & 0 \\ -I & 0 & 0 \end{bmatrix}$$

```
Jz := matrix(3,3,[0,-I,0,I,0,0,0,0,0]);
```

$$Jz := \begin{bmatrix} 0 & -I & 0 \\ I & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

Then $R_z(-\psi)R_x(-\theta)R_z(-\varphi)$ for small angles is this matrix,

```
X := evalm(ID + I*(psi+phi)*Jz + I*theta*Jx);
```

$$X := \begin{bmatrix} 1 & \psi+\phi & 0 \\ -\psi-\phi & 1 & \theta \\ 0 & -\theta & 1 \end{bmatrix}$$

On the other hand we know that

$$\text{GEN} \equiv e^{-i\gamma \mathbf{n}\bullet\mathbf{J}} = 1 - i\gamma\, \mathbf{n}\bullet\mathbf{J} = 1 - i\gamma(n_1J_1 + n_2J_2 + n_3J_3)$$

```
Gen := evalm(ID - I*gamma*(n1*Jx+n2*Jy+n3*Jz));
```

$$Gen := \begin{bmatrix} 1 & -\gamma\, n3 & \gamma\, n2 \\ \gamma\, n3 & 1 & -\gamma\, n1 \\ -\gamma\, n2 & \gamma\, n1 & 1 \end{bmatrix}$$

These two matrices have to be the same to first order, so you find that

$\psi+\varphi = -\gamma\, n_3$

$n_2 = 0$

$\theta = -\gamma n_1$

$n_1^2 + n^3_3 = 1$ since $n_2 = 0$

So if we are given n_1 and n_3 with $n_2 = 0$, then we know that

$\psi+\varphi = -\gamma\, n_3$ any way you want to allocate

$\theta = -\gamma\, n_1$

On the other hand, if we are given ψ,θ,φ, now can we compute γ and **n** ? We have 2 in 2:

$\psi+\varphi = -\gamma\, n_3$
$\theta = -\gamma \sqrt{1-n_3^2}$

Rewrite

$(\psi+\varphi)^2 = \gamma^2 n_3^2$

$\theta^2 = \gamma^2(1-n_3^2) = \gamma^2 - \gamma^2 n_3^2 = \gamma^2 - (\psi+\varphi)^2$

Then we have an expression for γ ,

$\gamma^2 = \theta^2 + (\psi+\varphi)^2$

and then

$n_1 = -\theta/\gamma \qquad n_2 = 0 \qquad n_3 = -(\psi+\varphi)/\gamma$

But since angles are very small, I guess we can say

$\gamma^2 = \theta^2 + \psi^2 + \varphi^2$

So this seems to be the solution to the problem when all angles are very small

$\gamma = \sqrt{\theta^2 + \psi^2 + \varphi^2}$
$n_1 = -\theta/\gamma \qquad n_2 = 0 \qquad n_3 = -(\psi+\varphi)/\gamma$

I could check this later for a small rotation, but the point is that this does NOT tell you the connection between (ψ,θ,φ) to (n_1,n_2,n_3,γ) for finite values of things. You learn nothing by doing this!

3. Compare $R_z(\psi)R_x(\theta)R_z(\varphi)$ to $e^{-iun\bullet J}$ using finite rotations

I know from exp nJ calculation.doc the following finite matrix (after I corrected 2nd term sign !!!!)

$$R_n(u) = \exp(-iu\mathbf{n}\bullet\mathbf{J}) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} + (C_u - 1)\begin{pmatrix} 1-n_1^2 & -n_1n_2 & -n_1n_3 \\ -n_1n_2 & 1-n_2^2 & -n_2n_3 \\ -n_1n_3 & -n_2n_3 & 1-n_3^2 \end{pmatrix} + S_u\begin{pmatrix} 0 & -n_3 & n_2 \\ n_3 & 0 & -n_1 \\ -n_2 & n_1 & 0 \end{pmatrix}$$

And I have from above that, going back to my usual active notation,

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

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

I am going to set these two matrices equal thereby find out how (ψ,θ,φ) to (n_1,n_2,n_3,γ) are related. There are a total of 9 equations that can be used. The R matrix only has 6 independent elements, but it is convenient nevertheless to make use of all 9 equations to obtain simple forms for expressions.

Top row:

$1 + (\cos u - 1)(1-n_1^2) = \cos\psi\cos\varphi - \sin\psi\cos\theta\sin\varphi \qquad (1)$

$-(\cos u - 1)(n_1n_2) - \sin u\, n_3 = -\cos\psi\sin\varphi - \sin\psi\cos\theta\cos\varphi \qquad (2)$

$-(\cos u - 1)n_1n_3 + \sin u\, n_2 = \sin\psi\sin\theta \qquad (3)$

Second row:

$$-(\text{cosu}-1)n_1n_2 + \text{sinu}\, n_3 = \sin\psi\cos\varphi + \cos\psi\cos\theta\sin\varphi \quad (4)$$

$$1 + (\text{cosu}-1)(1-n_2^2) = -\sin\psi\sin\varphi + \cos\psi\cos\theta\cos\varphi \quad (5)$$

$$-(\text{cosu}-1)n_2n_3 - \text{sinu}\, n_1 = -\cos\psi\sin\theta \quad (6)$$

Last row:

$$-(\text{cosu}-1)n_1n_3 - \text{sinu}\, n_2 = \sin\theta\sin\varphi \quad (7)$$

$$-(\text{cosu}-1)n_2n_3 + \text{sinu}\, n_1 = \sin\theta\cos\varphi \quad (8)$$

$$1 + (\text{cosu}-1)(1-n_3^2) = \cos\theta \quad (9)$$

Finally

$$n_1^2+n_2^2+n_3^2 = 1 \quad (10)$$

4. Direction (n,u) → (ψ,θ,φ)

Since angle θ only ranges 0 to π. equation (9) fully determines cosθ, so we have

$$\cos\theta = 1 + (\text{cosu}-1)(1-n_3^2) \qquad 0 \le \theta \le \pi$$

$$\sin\theta = \sqrt{1-\cos^2\theta} \qquad > 0$$

Then from (3) and (6) we have

$$-(\text{cosu}-1)n_1n_3 + \text{sinu}\, n_2 = \sin\psi\, \sin\theta \quad (3)$$
$$(\text{cosu}-1)n_2n_3 + \text{sinu}\, n_1 = \cos\psi\sin\theta \quad (6)$$

and this then tells us sinψ and cosψ.

Then from (7) and (8),

$$-(\text{cosu}-1)n_1n_3 - \text{sinu}\, n_2 = \sin\theta\sin\varphi \quad (7)$$

$$-(\text{cosu}-1)n_2n_3 + \text{sinu}\, n_1 = \sin\theta\cos\varphi \quad (8)$$

and this tells us sinφ and cosφ. So here is the solution in this direction:

Summary: Compute

$\cos\theta = 1 + (\cos u - 1)(1 - n_3^2)$ $\quad 0 \le \theta \le \pi$

$\sin\theta = \sqrt{1 - \cos^2\theta}$ $\quad > 0$

$\sin\psi = [-(\cos u - 1)n_1 n_3 + \sin u\, n_2]/\sin\theta$ $\quad 0 \le \psi \le 2\pi$

$\cos\psi = [(\cos u - 1)n_2 n_3 + \sin u\, n_1]/\sin\theta$

$\sin\varphi = [-(\cos u - 1)n_1 n_3 - \sin u\, n_2]/\sin\theta$ $\quad 0 \le \psi \le 2\pi$

$\cos\varphi = [-(\cos u - 1)n_2 n_3 + \sin u\, n_1]/\sin\theta$

You can see that **n**,u $\rightarrow$ a specific solution (ψ,θ,φ) with no ambiguity.

Test this result for $n_1 = 1$ and $n_2 = n_3 = 0$:

$\cos\theta = 1 + (\cos u - 1)(1) = \cos u$ $\quad \Rightarrow\ \theta = u$

$\sin\theta = \sin u$

$\sin\psi = 0$

$\cos\psi = [\sin u\, n_1]/\sin\theta = 1$ $\quad \Rightarrow\ \psi = 0$

$\sin\varphi = 0 \qquad 0 \le \psi \le 2\pi$

$\cos\varphi = [\ + \sin u\, n_1]/\sin\theta = 1$ $\quad \Rightarrow\ \varphi = 0$

and this is the desired result.

Let's verify that this is correct for the R_{11} matrix element. That element is this:

LHS = $R_{11} = 1 + (\cos u - 1)(1 - n_1^2)$

RHS = $R_{11} = \cos\psi\cos\varphi - \sin\psi\cos\theta\sin\varphi$

So

RHS = $\cos\psi\cos\varphi - \sin\psi\cos\theta\sin\varphi$

$= [(\cos u - 1)n_2 n_3 + \sin u\, n_1]/\sin\theta * [-(\cos u - 1)n_2 n_3 + \sin u\, n_1]/\sin\theta$

$- [-(\cos u - 1)n_1 n_3 + \sin u\, n_2]/\sin\theta * [1 + (\cos u - 1)(1 - n_3^2)] * [-(\cos u - 1)n_1 n_3 - \sin u\, n_2]/\sin\theta$

Multiply through by $\sin^2\theta$ to get

A = $\sin^2\theta$ RHS =

$= [(\text{cosu}-1)n_2n_3 + \text{sinu}\ n_1] * [-(\text{cosu}-1)n_2n_3 + \text{sinu}\ n_1]$

$- [-(\text{cosu}-1)n_1n_3 + \text{sinu}\ n_2] * [1 + (\text{cosu}-1)(1-n_3^2)] * [-(\text{cosu}-1)n_1n_3 - \text{sinu}\ n_2]$

$B = \sin^2\theta$ LHS $= \sin^2\theta\ [\ 1 + (\text{cosu}-1)(1-n_1^2)\ ]$

$= (1 - \cos^2\theta)\ [\ 1 + (\text{cosu}-1)(1-n_1^2)\ ]$

$= (\ 1 - [1 + (\text{cosu}-1)(1-n_3^2)]^2)\ [\ 1 + (\text{cosu}-1)(1-n_1^2)\ ]$

So I want to show that A-B = 0. So I will make Maple do this:

```
A := sin(theta)^2*(cospsi*cosphi-sinpsi*costheta*sinphi);
```

$$A := \sin(\theta)^2\ (cospsi\ cosphi - sinpsi\ costheta\ sinphi)$$

```
costheta := 1 + (cos(u)-1)*(1-n3^2);
```

$$costheta := 1 + (\cos(u) - 1)\ (1 - n3^2)$$

```
sinpsi := (-(cos(u)-1)*n1*n3 + sin(u)*n2)/sin(theta);
```

$$sinpsi := \frac{-(\cos(u) - 1)\ n1\ n3 + \sin(u)\ n2}{\sin(\theta)}$$

```
cospsi := ((cos(u)-1)*n2*n3 + sin(u)*n1)/sin(theta);
```

$$cospsi := \frac{(\cos(u) - 1)\ n2\ n3 + \sin(u)\ n1}{\sin(\theta)}$$

```
cosphi := (-(cos(u)-1)*n2*n3 + sin(u)*n1)/sin(theta);
```

$$cosphi := \frac{-(\cos(u) - 1)\ n2\ n3 + \sin(u)\ n1}{\sin(\theta)}$$

```
sinphi := (-(cos(u)-1)*n1*n3 - sin(u)*n2)/sin(theta);
```

$$sinphi := \frac{-(\cos(u) - 1)\ n1\ n3 - \sin(u)\ n2}{\sin(\theta)}$$

```
A := simplify(A);
```

$$:= -2\ n2^2\ n3^2\ \cos(u)^2 + n2^2\ n3^2\ \cos(u) + n1^2 - n1^2\ \cos(u)^2 - n1^2\ n3^2\ \cos(u)^3 + 2\ n1^2\ n3^2\ \cos(u)^2 + n1^2\ n3^4\ \cos(u)^3 - 3\ n1^2\ n3^4\ \cos(u)^2 + 3\ n1^2\ n3^4\ \cos(u) - n1^2\ n3^2\ \cos(u) - n1^2\ n3^4 + n2^2\ \cos(u) - n2^2\ \cos(u)^3 + n2^2\ n3^2\ \cos(u)^3$$

```
B := (1 - (1 + (cos(u)-1)*(1-n3^2))^2)*(1 + (cos(u)-1)*(1-n1^2));
```

$$B := \left(1 - (1 + (\cos(u) - 1)\ (1 - n3^2))^2\right)\ (1 + (\cos(u) - 1)\ (1 - n1^2))$$

```
simplify(A-B);
```

$$0$$

And so I have verified just the R_{11} element.

5. Direction (ψ,θ,φ) → (n,u)

Consider these 3 equations from above

$1 + (\text{cosu}-1)(1-n_1^2) = \cos\psi\cos\varphi - \sin\psi\cos\theta\sin\varphi$ (1)

$1 + (\cos u-1)(1-n_2^2) = -\sin\psi\sin\varphi + \cos\psi\cos\theta\cos\varphi$ (5)

$1 + (\cos u-1)(1-n_3^2) = \cos\theta$ (9)

If you add these up you get the left side being

$3 + (\cos u-1)[\,3 - n^2] = 3 + (\cos u-1)[\,3 - 1] = 3 + 2(\cos u-1) = 1 + 2\cos u$

You then know that

$1 + 2\cos u = \cos\psi\cos\varphi - \sin\psi\cos\theta\sin\varphi - \sin\psi\sin\varphi + \cos\psi\cos\theta\cos\varphi + \cos\theta$

Rewrite as

$1 + 2\cos u = \cos\psi\cos\varphi(1+\cos\theta) - \sin\psi\sin\varphi(1+\cos\theta) + \cos\theta$

$= (\cos\theta+1)(\cos\psi\cos\varphi - \sin\psi\sin\varphi) + \cos\theta$

Then

$1 + 2\cos u = (\cos\theta+1)(\cos\psi\cos\varphi - \sin\psi\sin\varphi) + \cos\theta$

$2\cos u = -1 + (\cos\theta+1)(\cos\psi\cos\varphi - \sin\psi\sin\varphi) + \cos\theta$

$\cos u = [\,(\cos\theta-1) + (\cos\theta+1)(\cos\psi\cos\varphi - \sin\psi\sin\varphi)\,]/2$

Try one angle at a time. If $\psi=\varphi = 0$ and $\theta = \theta$ get

$\cos u = [\,(\cos\theta-1) + (\cos\theta+1)(\,1)\,]/2 = \cos\theta$ // correct

Consider now,

$(1-\cos u)(n_1n_2) + \sin u\, n_3 = \cos\psi\sin\varphi + \sin\psi\cos\theta\cos\varphi$ (2)

$-(1-\cos u)n_1n_2 + \sin u\, n_3 = \sin\psi\cos\varphi + \cos\psi\cos\theta\sin\varphi$ (4)

Add these to get

$2n_3\sin u = \cos\psi\sin\varphi + \sin\psi\cos\theta\cos\varphi + \sin\psi\cos\varphi + \cos\psi\cos\theta\sin\varphi$

Then consider

$(\cos u-1)n_2n_3 + \sin u\, n_1 = \cos\psi\sin\theta$ (6)

$-(\cos u-1)n_2n_3 + \sin u\, n_1 = \sin\theta\cos\varphi$ (8)

Add these to get

$$2\sin u\, n_1 = \cos\psi\sin\theta + \sin\theta\cos\varphi$$

Then consider

$$-(\cos u-1)n_1n_3 + \sin u\, n_2 = \sin\psi\sin\theta \qquad (3)$$
$$-(\cos u-1)n_1n_3 - \sin u\, n_2 = \sin\theta\sin\varphi \qquad (7)$$

Subtract these to get

$$2\sin u\, n_2 = \sin\psi\sin\theta - \sin\theta\sin\varphi$$

At this point I then know that

$$2n_3\sin u = \cos\psi\sin\varphi + \sin\psi\cos\theta\cos\varphi + \sin\psi\cos\varphi + \cos\psi\cos\theta\sin\varphi$$
$$2n_1\sin u = \cos\psi\sin\theta + \sin\theta\cos\varphi$$
$$2n_2\sin u = \sin\psi\sin\theta - \sin\theta\sin\varphi$$

If I square and add, this tells me $\sin^2 u$ but no sign for sinu. So no better than knowing just cosu as earlier.

OK, I guess I can consider $0 < u < \pi$ and allow the n_i to have arbitrary sign and that is fully general. Then I determine u first as follows:

$$\cos u = [\,(\cos\theta-1) + (\cos\theta+1)(\cos\psi\cos\varphi - \sin\psi\sin\varphi)\,]/2$$

$$\cos u = [\,-2\sin^2(\theta/2) + 2\cos^2(\theta/2)\cos(\psi-\varphi)]/2$$

$$\cos u = \cos^2(\theta/2)\cos(\psi-\varphi) - \sin^2(\theta/2)$$

Maple tells me that

$$1 - \cos^2 u = \cos^2(\theta/2)(\cos(\psi-\varphi) + 1)[2-\cos^2(\theta/2)(\cos(\psi-\varphi) + 1)]$$

So sinu is just a big mess

$$\sin u = \cos(\theta/2)\sqrt{(\cos(\psi-\varphi) + 1)[2-\cos^2(\theta/2)(\cos(\psi-\varphi) + 1)]}$$

If $\psi = \varphi = 0$, however, we get

$$\sin u = \cos(\theta/2)\sqrt{(1 + 1)[2-\cos^2(\theta/2)(1 + 1)]} = \cos(\theta/2)\sqrt{2[2-\cos^2(\theta/2)2]}$$

$$= 2\cos(\theta/2)\sqrt{[1-\cos^2(\theta/2)]} = 2\cos(\theta/2)\sin(\theta/2) = \sin\theta \qquad \text{// which is correct}$$

Then I use the above three to get the n_i

$n_3 = [\cos\psi\sin\varphi + \sin\psi\cos\theta\cos\varphi + \sin\psi\cos\varphi + \cos\psi\cos\theta\sin\varphi] / 2\sin u$

$n_1 = [\cos\psi\sin\theta + \sin\theta\cos\varphi]/2\sin u$

$n_2 = [\sin\psi \sin\theta - \sin\theta\sin\varphi]/2\sin u$

Summary: Compute

$$\cos u = [(\cos\theta-1) + (\cos\theta+1)(\cos\psi\cos\varphi - \sin\psi\sin\varphi)]/2 = \cos^2(\theta/2)\cos(\psi-\varphi) - \sin^2(\theta/2)$$

From that you can get

$$\sin u = \cos(\theta/2)\sqrt{(\cos(\psi-\varphi)+1)[2-\cos^2(\theta/2)(\cos(\psi-\varphi)+1)]} \quad > 0$$

Then

$n_3 = [\cos\psi\sin\varphi + \sin\psi\cos\theta\cos\varphi + \sin\psi\cos\varphi + \cos\psi\cos\theta\sin\varphi] / 2\sin u$

$n_1 = [\cos\psi\sin\theta + \sin\theta\cos\varphi]/2\sin u$

$n_2 = [\sin\psi \sin\theta - \sin\theta\sin\varphi]/2\sin u$

In theory, you should be able to insert these into

$$R_n(u) = \exp(-iu\mathbf{n}\bullet\mathbf{J}) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} + (C_u-1)\begin{pmatrix} 1-n_1^2 & -n_1n_2 & -n_1n_3 \\ -n_1n_2 & 1-n_2^2 & -n_2n_3 \\ -n_1n_3 & -n_2n_3 & 1-n_3^2 \end{pmatrix} + S_u\begin{pmatrix} 0 & -n_3 & n_2 \\ n_3 & 0 & -n_1 \\ -n_2 & n_1 & 0 \end{pmatrix}$$

and you should end up with

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

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

As before, let's try the first element and see what happens ,

$$R_{11} = 1 + (\cos u-1)(1-n_1^2)$$

$$= 1 + (\cos u-1)\left(1 - [\cos\psi\sin\theta + \sin\theta\cos\varphi]^2/(2\sin u)^2\right) \qquad ?$$

Multiply through by $4\sin^2 u$ to get,

$$RHS = 4\sin^2 u\, R_{11} = 4\sin^2 u + (\cos u-1)(4\sin^2 u - [\cos\psi\sin\theta + \sin\theta\cos\varphi]^2)$$

$$= 4 - 4\cos^2 u + (\cos u-1)(4 - 4\cos^2 u - [\cos\psi\sin\theta + \sin\theta\cos\varphi]^2)$$

LHS = $4\sin^2 u\,(\cos\psi\cos\varphi - \sin\psi\cos\theta\sin\varphi)$

$= (4 - 4\cos^2 u)\,(\cos\psi\cos\varphi - \sin\psi\cos\theta\sin\varphi)$

If these really are equal, I should find RHS - LHS = 0. Here is Maple on the subject:

```
restart;
RHS := 4 - 4*cosu^2 +(cosu-1)*(4 - 4*cosu^2  - (cos(psi)*sin(theta)+sin(theta)*cos(phi))^2 );
```

$$RHS := 4 - 4\,cosu^2 + (cosu - 1)\,(4 - 4\,cosu^2 - (\cos(\psi)\sin(\theta) + \sin(\theta)\cos(\phi))^2)$$

```
LHS := (4 - 4*cosu^2)*(cos(psi)*cos(phi)- sin(psi)*cos(theta)*sin(phi));
```

$$LHS := (4 - 4\,cosu^2)\,(\cos(\psi)\cos(\phi) - \sin(\psi)\cos(\theta)\sin(\phi))$$

```
cosu := (cos(theta)-1 +(cos(theta)+1)*(cos(psi)*cos(phi)-sin(psi)*sin(phi)))/2;
```

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

```
> expand(RHS-LHS);
```

$$-\cos(\psi)\cos(\phi)\sin(\psi)\sin(\phi) - \cos(\theta)\cos(\psi)\sin(\theta)^2\cos(\phi) - \frac{1}{2}\cos(\theta)\cos(\psi)^3\cos(\phi)\sin(\theta)^2 - \cos(\theta)\cos(\psi)^2\cos(\phi)^2\sin(\theta)^2$$
$$- \frac{1}{2}\cos(\theta)\cos(\psi)\cos(\phi)^3\sin(\theta)^2 - \frac{1}{2}\cos(\psi)^2\cos(\phi)^2\sin(\psi)\sin(\phi) - \frac{1}{2}\cos(\psi)\cos(\phi)\sin(\psi)^2\sin(\phi)^2 + \frac{1}{2}\sin(\psi)\sin(\phi)\cos(\psi)^2\sin(\theta)^2$$
$$+ \frac{1}{2}\sin(\psi)\sin(\phi)\sin(\theta)^2\cos(\phi)^2 - \frac{1}{2}\sin(\psi)\cos(\theta)\sin(\phi) + \frac{1}{2}\sin(\psi)\cos(\theta)\sin(\phi)\cos(\psi)^2\sin(\theta)^2 + \sin(\psi)\cos(\theta)\sin(\phi)\cos(\psi)\sin(\theta)^2\cos(\phi)$$
$$+ \frac{1}{2}\sin(\psi)\cos(\theta)\sin(\phi)\sin(\theta)^2\cos(\phi)^2 + \sin(\psi)\sin(\phi)\cos(\psi)\sin(\theta)^2\cos(\phi) - \frac{1}{2}\cos(\theta)\cos(\psi)^2\cos(\phi)^2\sin(\psi)\sin(\phi) + \frac{1}{2}\cos(\theta)^3\cos(\psi)^2\cos(\phi)^2\sin(\psi)\sin(\phi)$$
$$+ \frac{1}{2}\cos(\theta)^2\cos(\psi)^2\cos(\phi)^2\sin(\psi)\sin(\phi) + \frac{1}{2}\cos(\theta)^3\cos(\psi)\cos(\phi)\sin(\psi)^2\sin(\phi)^2 + \frac{1}{2}\cos(\theta)^2\cos(\psi)\cos(\phi)\sin(\psi)^2\sin(\phi)^2 - \frac{1}{2}\sin(\psi)^3\cos(\theta)^3\sin(\phi)^3$$
$$- \frac{1}{2}\sin(\psi)^3\cos(\theta)^2\sin(\phi)^3 + \frac{1}{2}\sin(\psi)^3\cos(\theta)\sin(\phi)^3 - \frac{1}{2}\cos(\psi)^3\cos(\phi)\sin(\theta)^2 - \cos(\psi)^2\cos(\phi)^2\sin(\theta)^2 - \frac{1}{2}\cos(\psi)\cos(\phi)^3\sin(\theta)^2$$
$$+ \cos(\theta)^3\cos(\psi)\cos(\phi)\sin(\psi)\sin(\phi) + \cos(\theta)^2\cos(\psi)\cos(\phi)\sin(\psi)\sin(\phi) - \cos(\theta)\cos(\psi)\cos(\phi)\sin(\psi)\sin(\phi) - \frac{1}{2}\cos(\theta)^3$$
$$- \frac{1}{2}\cos(\theta)\cos(\psi)\cos(\phi)\sin(\psi)^2\sin(\phi)^2 - \frac{3}{2} + \frac{3}{2}\cos(\theta)\cos(\psi)\cos(\phi) + \frac{5}{2}\cos(\theta)^2\cos(\psi)\cos(\phi) + \frac{1}{2}\sin(\psi)\cos(\theta)^2\sin(\phi) + \frac{1}{2}\cos(\theta)^2\cos(\psi)^2\cos(\phi)^2$$
$$- \frac{1}{2}\cos(\theta)^2\cos(\psi)^3\cos(\phi)^3 + \frac{3}{2}\cos(\theta)\cos(\psi)^2\cos(\phi)^2 - \frac{3}{2}\sin(\psi)^2\cos(\theta)^2\sin(\phi)^2 - \frac{1}{2}\sin(\psi)^2\cos(\theta)\sin(\phi)^2 + 3\cos(\psi)\sin(\theta)^2\cos(\phi)$$
$$- \frac{3}{2}\cos(\theta)^3\cos(\psi)\cos(\phi) + \frac{1}{2}\sin(\psi)\cos(\theta)^3\sin(\phi) - \frac{3}{2}\cos(\theta)^3\cos(\psi)^2\cos(\phi)^2 + \frac{1}{2}\sin(\psi)^2\cos(\theta)^3\sin(\phi)^2 - \frac{1}{2}\cos(\theta)\cos(\psi)^2\sin(\theta)^2$$
$$- \frac{1}{2}\cos(\theta)\sin(\theta)^2\cos(\phi)^2 + \frac{3}{2}\cos(\theta)^2 - \frac{1}{2}\cos(\psi)^2\cos(\phi)^2 + \frac{3}{2}\sin(\psi)^2\sin(\phi)^2 + \frac{3}{2}\cos(\psi)^2\sin(\theta)^2 + \frac{3}{2}\sin(\theta)^2\cos(\phi)^2 + \frac{1}{2}\cos(\psi)^3\cos(\phi)^3 + \frac{1}{2}\sin(\psi)^3\sin(\phi)^3$$
$$- \frac{5}{2}\cos(\psi)\cos(\phi) - \frac{1}{2}\sin(\psi)\sin(\phi) + \frac{1}{2}\cos(\theta) - \frac{1}{2}\cos(\theta)^3\cos(\psi)^3\cos(\phi)^3 + \frac{1}{2}\cos(\theta)\cos(\psi)^3\cos(\phi)^3$$

```
> simplify(%);
```

$$0$$

So there you have it, for the R_{11} it really works.

Footnote: Look back at my conclusion above that

1 + 2cosu = cosψcosφ - sinψcosθsinφ -sinψsinφ + cosψcosθcosφ+ cosθ

with

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

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

Goldstein p 123 notes that you can write $Q\mathbf{n} = \hat{\mathbf{z}}$ for some rotation Q, and then

$$R\mathbf{n} = \mathbf{n} \quad \Rightarrow \quad QR\mathbf{n} = \hat{\mathbf{z}} \quad \Rightarrow \quad QRQ^{-1}\hat{\mathbf{z}} = \hat{\mathbf{z}} \quad \Rightarrow \quad QRQ^{-1} = R_{\mathbf{z}}(u)$$

Here you have rotated your coordinate system so the rotation by amount u is about the z axis. But then you know that $\mathrm{tr}(R) = \mathrm{tr}(R_{\mathbf{z}}(u)) = 1 + 2\cos u$. Thus you would claim that

$$1 + 2\cos u = \Sigma_i R_{ii}$$

In our R matrix that means

$$1 + 2\cos u = \cos\psi\cos\varphi - \sin\psi\cos\theta\sin\varphi - \sin\psi\sin\varphi + \cos\psi\cos\theta\cos\varphi + \cos\theta$$

and this agrees with what I found above by brute force.