MATH 728A, BIOMOLECULAR GEOMETRY, HOMEWORK #7

Problem 1 (Rotation Matrices). Define SO(3) to be the set of all rotation matrices R, i.e. 3×3 real matrices such that $R^T R = I$ (I denotes the 3×3 identity matrix) and $\det R = 1$. Show that there exists a pair $(e^{i\theta}, \mathbf{u})$, uniquely determined up to reflection $(e^{-i\theta}, -\mathbf{u})$, where θ is real and $\mathbf{u} \in \mathbb{R}^3$ is a unit vector, such that for all $\mathbf{x} \in \mathbb{R}^3$ we have

$$R\mathbf{x} = \mathbf{u}(\mathbf{u} \cdot \mathbf{x}) + [\mathbf{x} - \mathbf{u}(\mathbf{u} \cdot \mathbf{x})] \cos\theta + (\mathbf{u} \times \mathbf{x}) \sin\theta.$$

Problem 2 (Quaternions for rotations). Define the complex matrices

$$\sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

If $\mathbf{x} = \langle x_1, x_2, x_3 \rangle \in \mathbb{R}^3$ then define $X(\mathbf{x}) = \sigma_1 x_1 + \sigma_2 x_2 + \sigma_3 x_3$. If $\mathbf{u} = \langle u_1, u_2, u_3 \rangle \in \mathbb{R}^3$ is a unit vector and θ is a real number, define $H(e^{i\theta}, \mathbf{u}) = \sigma_0 \cos(\theta/2) - i(\sigma_1 u_1 + \sigma_2 u_2 + \sigma_3 u_3) \sin(\theta/2)$. If H is a 2×2 complex matrix let $H^\dagger$ denote its complex conjugate transpose. Suppose R is a rotation matrix as in problem 1 above. Then show that $X(R\mathbf{x}) = H(e^{i\theta}, \mathbf{u}) X(\mathbf{x}) H(e^{i\theta}, \mathbf{u})^\dagger$, where $(e^{i\theta}, \mathbf{u})$ correspond to R as in problem 1.

Problem 3 (Internal coordinates via coordinate transformations). Define the following matrices:

$$T_0(l) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ l & 0 & 0 & -1 \end{pmatrix}, T_1(c) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -c & 0 & s \\ 0 & 0 & -1 & 0 \\ 0 & s & 0 & c \end{pmatrix}, T_2(z) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & x & -y & 0 \\ 0 & y & x & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix},$$

where $l > 0$, $-1 < c < 1$, $s = \sqrt{1 - c^2}$, $z = x + iy$, and $x^2 + y^2 = 1$. If $\mathcal{X}(A) \in \mathbb{R}^3$ denotes the position of atom A recall we defined the conformed pose, pose(A, b, t), where A is an atom contained in the bond b, which is in turn contained in the triangle t, by the rule: pose$(A, b, t) = (\mathbf{e}_0, \mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)$, where $\mathbf{e}_0 = \mathcal{X}(A)$,

$$\mathbf{e}_3 = \frac{\mathcal{X}(A') - \mathcal{X}(A)}{\|\mathcal{X}(A') - \mathcal{X}(A)\|}, \qquad \mathbf{e}_1 = \frac{\mathcal{X}(A'') - \mathcal{X}(A) - \mathbf{e}_3\{\mathbf{e}_3 \cdot [\mathcal{X}(A'') - \mathcal{X}(A)]\}}{\|\mathcal{X}(A'') - \mathcal{X}(A) - \mathbf{e}_3\{\mathbf{e}_3 \cdot [\mathcal{X}(A'') - \mathcal{X}(A)]\}\|},$$

$\mathbf{e}_2 = \mathbf{e}_3 \times \mathbf{e}_1$, where $b = \{A, A'\}$ and $t = \{A, A', A''\}$. These formulae make sense provided the triangle t is noncollinear in the configuration $\mathcal{X}$. Verify the following assertions.

1. If the bond b has length l then pose$(A', b, t) =$ pose$(A, b, t) T_0(l)$.
2. If an angle $a = \{b_1, b_2\}$ has the common atom A, and bond angle cosine $c = \cos\theta$, then pose$(A, b', t(a)) =$ pose$(A, b, t(a)) T_1(c)$.
3. If a wedge $w = \{t_1, t_2\}$ has the common bond $b = \{A, A'\}$, and the wedge angle coordinate is $z = e^{i\phi}$ relative to the orientation $[A_1'', A, A', A_2'']$, where $A_j'' \in t_j \setminus b$, $j = 1, 2$, then pose$(A, b, t_2) =$ pose$(A, b, t_1) T_2(e^{i\phi})$.