# MATH 728A, BIOMOLECULAR GEOMETRY, HOMEWORK #12

**Problem 1 (Facts about SU$(2)$).** Let SU$(2)$ denote the set of all $2\times 2$ matrices $U$ with complex entries such that $U^\dagger U = UU^\dagger = I$ and $\det U = 1$. Show that for all real $\theta$ and real unit vectors $\mathbf{u}$ the matrix $H(e^{i\theta},\mathbf{u})$ is in SU$(2)$. Show that any matrix $U = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}$ in SU$(2)$ satisfies $a_{21} = -\bar{a}_{12}$, $a_{22} = \bar{a}_{11}$, and $|a_{11}|^2 + |a_{12}|^2 = 1$, and hence $U = H(e^{i\theta},\mathbf{u})$ for some pair $(e^{i\theta},\mathbf{u})$ as above. (*Hint:* Use the relation $a_{11}a_{22} - a_{21}a_{12} = 1$ and the first row of the equation $U^\dagger U = I$.) Show that if $U_1, U_2 \in \mathrm{SU}(2)$ then $U_1^{-1}U_2 \in \mathrm{SU}(2)$.

**Problem 2 (Axis and angle for products of rotations).** Show how to find a real unit vector $\mathbf{u}$ and a real angle $0 \le \theta \le \pi$ such that $H(e^{i\theta/2},\mathbf{u}) = H(e^{i\theta_1/2},\mathbf{u}_1)H(e^{i\theta_2/2},\mathbf{u}_2)$.

**Problem 3 (Active and passive rotations).** Let $R(e^{i\theta},\mathbf{u}) = \mathbf{u}\mathbf{u}^T + [I - \mathbf{u}\mathbf{u}^T]\cos\theta + [\mathbf{u}\times\,]\sin\theta$, where

$$[\mathbf{u}\times\,] = \begin{pmatrix} 0 & -u_3 & u_2 \\ u_3 & 0 & -u_1 \\ -u_2 & u_1 & 0 \end{pmatrix},$$

provided $\mathbf{u} = \langle u_1, u_2, u_3\rangle$. Show that $R(e^{i\theta},\mathbf{u}) \in \mathrm{SO}(3)$. Suppose $B \in \mathrm{SO}(3)$. Show that $R(e^{i\theta}, B\mathbf{u})B = BR(e^{i\theta},\mathbf{u})$. If $B = (\mathbf{b}_1,\mathbf{b}_2,\mathbf{b}_3)$ is interpreted as a right-handed orthonormal basis of $\mathbb{R}^3$ then $R(e^{i\theta}, B\mathbf{u})$ is considered an *active rotation* whereas $R(e^{i\theta},\mathbf{u})$ is considered a *passive rotation*. The effect of these two types of rotations on the basis $B$ is the same (that is what you are asked to show above). If $B' = R(e^{i\theta}, B\mathbf{u})(\mathbf{b}_1,\mathbf{b}_2,\mathbf{b}_3) = (\mathbf{b}_1',\mathbf{b}_2',\mathbf{b}_3')$ is the rotated basis, and $\mathbf{v} = \langle v_1, v_2, v_3\rangle$, then show that $R(e^{i\eta}, B'\mathbf{v})R(e^{i\theta}, B\mathbf{u})B = BR(e^{i\theta},\mathbf{u})R(e^{i\eta},\mathbf{v})$. Thus active and passive rotations are composed in opposite orders.

**Problem 4 (Rigid Motions).** If $A \in \mathrm{SO}(3)$ and $\mathbf{b},\mathbf{x} \in \mathbb{R}^3$ then let $M(b,A)$ and $\tilde{\mathbf{x}}$ denote

$$M(\mathbf{b},A) = \begin{pmatrix} 1 & \mathbf{0}^T \\ \mathbf{b} & A \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ b_1 & a_{11} & a_{12} & a_{13} \\ b_2 & a_{21} & a_{22} & a_{23} \\ b_3 & a_{31} & a_{32} & a_{33} \end{pmatrix}, \qquad \tilde{\mathbf{x}} = \begin{pmatrix} 1 \\ \mathbf{x} \end{pmatrix} = \begin{pmatrix} 1 \\ x_1 \\ x_2 \\ x_3 \end{pmatrix}.$$

$M(\mathbf{b},A)$ is called a *rigid motion* of $\mathbb{R}^3$. Show that $M(\mathbf{b},A)\tilde{\mathbf{x}} = (\mathbf{b} + A\mathbf{x})\tilde{}$. This is interpreted as the effect of the rigid motion on the point $\mathbf{x}$ in space. Show that $M(\mathbf{b},A)^{-1} = M(-A^T\mathbf{b}, A^T)$, and that $M(\mathbf{b}_1,A_1)M(\mathbf{b}_2,A_2) = M(\mathbf{b}_1 + A_1\mathbf{b}_2, A_1A_2)$.

**Problem 5 (T-matrices as rigid motions).** Show that $T_0(l) = M(\hat{\mathbf{e}}_3 l, R(e^{i\pi},\hat{\mathbf{e}}_1))$, $T_1(\cos\theta) = M(\mathbf{0}, R(e^{i\theta},\hat{\mathbf{e}}_2)R(e^{i\pi},\hat{\mathbf{e}}_3))$, and $T_2(e^{i\phi}) = M(\mathbf{0}, R(e^{i\phi},\hat{\mathbf{e}}_3))$, where $(\hat{\mathbf{e}}_1,\hat{\mathbf{e}}_2,\hat{\mathbf{e}}_3)$ denote the three columns of the identity matrix.