MATH 728B, WATER MOLECULE, HOMEWORK PROBLEMS II

Rigid water molecule. If a system of particles has zero linear momentum and angular momentum $\Lambda = A\lambda$ then we have computed its total energy to be:

$$\frac{1}{2}\mathbf{i}^{-1}\lambda \cdot \lambda + \frac{1}{2}\sum_{a=0}^{2} M_a \|\dot{r}_a\|^2 - \frac{1}{2}\mathbf{i}^{-1}j \cdot j + \frac{1}{2}(q - q_0)^T K (q - q_0),$$

where $\mathbf{i}$ is the moment of inertia tensor in the body frame. $\omega = \mathbf{i}^{-1}\lambda$ is the angular velocity vector in the body frame. Since $\dot{\Lambda} = 0$ we have that $\dot{\lambda} = -A^T \dot{A}\lambda = -\tilde{\omega} \times \lambda = \lambda \times \tilde{\omega}$. Since we have also seen that $\lambda = \mathbf{i}\omega = \mathbf{i}\tilde{\omega} + j$ we have that $\dot{\lambda} = \lambda \times \mathbf{i}^{-1}(\lambda - j)$.

An important simplifying assumption which is often made in the simulation of water molecules (especially when there are many of them) is that the geometry q is constrained to be equal to the equilibrium geometry q_0. The effect of this assumption is that nothing moves in the body frame and hence $\dot{r}_a = 0$ and $j = 0$. Hence the total energy is given by $E = \frac{1}{2}\mathbf{i}^{-1}\lambda \cdot \lambda$. Show that if $\dot{\lambda} = \lambda \times \mathbf{i}^{-1}\lambda$ then both E and $\|\lambda\|^2$ are conserved on any trajectory.

Principal Axes. Since $\mathbf{i}$ is a symmetric matrix it can be diagonalized via an orthogonal matrix: $\mathbf{i}P = P\delta$, where $PP^T = P^T P = I$ and δ is a diagonal matrix. If the water molecules has the equilibrium geometry q_0 then compute the matrix P and the diagonal matrix δ; assume that $\delta_{11} \geq \delta_{22} \geq \delta_{33}$. The columns of P are called principal axes. Draw a diagram of the water molecule with the principal axes labeled.

Let $\lambda = P\tilde{\lambda}$. Show that $E = \frac{1}{2}\delta^{-1}\tilde{\lambda} \cdot \tilde{\lambda}$, and $\|\tilde{\lambda}\|^2 = \|\Lambda\|^2$. The constant energy surface is an ellipsoid in $\tilde{\lambda}$ space. Show that $\dot{\tilde{\lambda}} = \tilde{\lambda} \times \delta^{-1}\tilde{\lambda}$. These are called *Euler's equations of rigid body motion.* Trajectories of these equations lie on the intersection between the constant energy ellipsoid and the sphere $\|\tilde{\lambda}\|^2 = \|\Lambda\|^2$. This fact can be used to geometrically classify the trajectories. Use Maple to integrate Euler's equations with initial conditions of the form

$$\tilde{\lambda}(0) = \begin{pmatrix} \tilde{\lambda}_1 \\ 0 \\ \sqrt{2E\delta_{33}\left(1 - \frac{(\tilde{\lambda}_1)^2}{2E\delta_{11}}\right)} \end{pmatrix}, \qquad |\tilde{\lambda}_1| \leq \sqrt{2E\delta_{11}}.$$

(Choose a finite set of values of $\tilde{\lambda}_1$ satisfying the above inequality.) Plot these trajectories on a three dimensional plot. They will all lie on the same energy ellipsoid, but different trajectories will have different values of $\|\tilde{\lambda}\|^2$. Classify and describe these trajectories. Identify the critical values of $\tilde{\lambda}_1$ where the qualitative features of the trajectories change.

Recovering the rotational motion. The above description of rigid body motion is entirely from the standpoint of the body frame, i.e. we find out how $\lambda(t) = P\tilde{\lambda}(t)$ evolves, but we have not yet discovered how the water molecule rotates relative to the inertial frame. We know that $\tilde{\omega} = \mathbf{i}^{-1}[\lambda(t) - j(t)]$, and $[\tilde{\omega}\, \times\,] = A(t)^{-1}\dot{A}(t)$, where $A(t)$ is a time-dependent rotation matrix relating the body and inertial frames. Thus we can find $A(t)$

by solving the differential equation $\dot{A} = A[\tilde{\omega} \times] = A[\mathbf{i}^{-1}\{\lambda(t) - j(t)\} \times]$. This assumes we have already found $\lambda(t)$ and $j(t)$ in a previous step. In the case of a rigid water molecule $j(t) = 0$ and $\lambda(t)$ is found by solving Euler's equations as above.

Thus our task is to solve the system of differential equations $\dot{A} = A[\mathbf{i}^{-1}\lambda(t) \times]$. If A is represented as 3×3 matrix this is a coupled system of 9 equations in 9 unknowns; straightforward but messy to solve numerically. However we know that it is possible to write $A = R(\mathbf{u}, e^{i\theta})$. Define $\mathbf{v} = \mathbf{u}\theta$. Show that

$$R(\mathbf{u}, e^{i\theta}) = R_1(\mathbf{v}) = \mathbf{1}\cos(\sqrt{\mathbf{v}^T\mathbf{v}}) + \mathbf{v}\mathbf{v}^T \frac{[1 - \cos\sqrt{\mathbf{v}^T\mathbf{v}}]}{\mathbf{v}^T\mathbf{v}} + [\mathbf{v} \times] \frac{\sin\sqrt{\mathbf{v}^T\mathbf{v}}}{\sqrt{\mathbf{v}^T\mathbf{v}}}.$$

Notice that the functions $(1 - \cos\theta)/\theta^2$ and $(\sin\theta)/\theta$ are well-behaved functions of θ near $\theta = 0$. Using Maple compute $\dot{A} = \nabla_{\mathbf{v}} R_1 \cdot \dot{\mathbf{v}}$ and derive 3 ODEs for the components of $\mathbf{v}$. Use Maple to solve this system numerically using two of the different types of $\lambda(t)$ trajectories computed earlier.