Physics 309 - Solving the Three Dimensional Schroedinger Equation 1

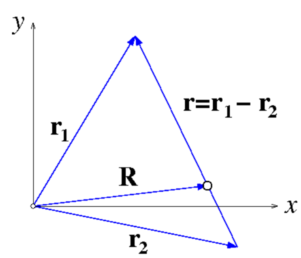
1. A water molecule consists of an oxygen atom with two hydrogen atoms bound to it. The angle between the two bonds is $\theta = 106°$. If the bonds are 1.0 Å long, then where is the center of mass?

2. An airplane of mass $m = 12000\ kg$ flies over the Midwestern plains at an altitude $h = 4.3\ km$ with velocity $v = 175\ m/s$ west. What is the airplane's angular momentum vector relative to a farmer on the ground directly below the plane? Does this value change as the plane continues its motion in a straight line?

3. In studying rotational motion, we take advantage of the center-of-mass system to make life easier. Consider the two-particle system shown in the figure including the center-of-mass vector **R**. For convenience we will place our origin at the center-of-mass of the system ($\mathbf{R} = \mathbf{0}$). Show the classical mechanical energy of the two-particle system in the center-of-mass frame can be written as

$$E_{cm} = \frac{1}{2}\mu v^2 + V(r) \qquad \text{where} \qquad \mu = \frac{m_1 m_2}{m_1 + m_2} \qquad \text{and} \qquad v = \frac{dr}{dt}$$

and r is the relative coordinate between the two particles as shown in the figure. Notice that $V(r)$ depends only on the relative coordinate.



4. The three-dimensional Schroedinger equation can be written in spherical coordinates as

$$\frac{-\hbar^2}{2\mu}\left\{\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right\}\psi + V(r)\psi = E\psi$$

where μ is the reduced mass. We want to show that the Schroedinger equation is separable, *i.e.,* that it can be broken down into a different equation that each of the three coordinates, r, θ, and ϕ, must satisfy. To do this assume that the wave function is of the form

$$\psi = R(r)\Theta(\theta)\Phi(\phi)$$

and rearrange the Schroedinger equation to obtain the following result.

$$-\left\{\frac{\sin^2\theta}{R}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right) + \frac{\sin\theta}{\Theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Theta}{\partial\theta}\right) + \frac{2\mu r^2\sin^2\theta}{\hbar^2}(E - V)\right\} = \frac{1}{\Phi}\frac{\partial^2\Phi}{\partial\phi^2}$$

5. Starting with the result from the previous problem show

$$-\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)+\frac{m^2}{\sin^2\theta}\Theta = A\Theta$$

where Θ is the solution to the angular part and A is a new separation constant.

6. Make the substitution $z = \cos\theta$ in the equation from the previous problem and show that z must satisfy Legendre's differential equation

$$(1-z^2)\frac{d^2\Theta}{dz^2} - 2z\frac{d\Theta}{dz} + \left(A - \frac{m^2}{1-z^2}\right)\Theta = 0 \qquad .$$

7. Now consider the result from Problem 5. For the case $m = 0$ what is the recursion relationship for the series solution to Legendre's differential equation? In other words, let $\Theta = \sum a_k z^k$, set $m = 0$, and show that Legendre's differential equation leads to

$$a_{k+2} = \frac{k(k+1) - A}{(k+2)(k+1)}\, a_k \qquad .$$

What must the constant A equal if we want to terminate the series at some arbitrary value of $k = l$?