CHEMISTRY 3BB3 1999/2000

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ASSIGNMENT 2

DUE: February 1, 2000

1. Using a spreadsheet, plot out part of the wavefunction for a $3d_{xy}$ hydrogen atom orbital. The formula for this orbital is proportional to $r^2 e^{-r} \sin^2\theta \cos 2\phi$. Plot this in the *xy* plane, so that $\sin\theta = 1$. Create a 100x100 grid of x and y points, and then use the fact that $r^2 = x^2 + y^2$ and that $\tan\phi = y/x$ (you will find the ATAN2 function useful here). Plot the value of the wavefunction using a surface plot, and then plot the one dimensional cross-sections along the x and y axes.

2. Suppose we use a function of the form Ae^{-cr^2} as a trial wavefunction for the radial part of the H atom.

(a) Evaluate the normalization constant, *A*.

(b) Using the variation principle, calculate the "best" value for the constant c. Use the radial Hamiltonian only.

$$H = \frac{-\hbar^2}{2m}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{e^2}{4\pi\varepsilon_0 r}$$

(c) Compare the expectation value of the Hamiltonian over this wavefunction with the true energy.

3. In spherical polar coordinates, the operator that corresponds to the square of the length of the angular momentum vector is

$$L^2 = \left(\frac{-1}{\sin\theta}\right)\frac{\partial}{\partial\theta}\left[\sin\theta\frac{\partial}{\partial\theta}\right] - \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}$$

Apply this operator to the (2,0), (2,1) and the (2,2) spherical harmonics (Harris & Bertolucci, page 113), and show that each is an eigenfunction of L^2 with eigenvalue *J(J+1)*, where *J* is the total angular momentum.

4. Calculate the eigenvalues of the following matrix

$$\begin{pmatrix} 17 & 13 & -2 \\ 13 & 4 & 7 \\ -2 & 7 & 25 \end{pmatrix}$$

To solve the associated cubic equation, use a solver program (for example, Matlab), or plot the function out using a spreadsheet, and estimate the roots to within +/- 0.05.