Chemistry 20262 | Spring 2018
Professor J. Daniel Gezelter | Due Fri. 4/6/2018

Problem Set 7
(3-D integration and Matrices)

1. The *electron density* for an electron in a 1s orbital of a hydrogen atom is:

$$P(r,\theta,\phi) = \frac{1}{\pi a_0^3} e^{-2r/a_0}$$

This function is the square of that electron's wavefunction. The constant a_0 is the Bohr radius:

$$a_0 = 0.529\text{Å}$$

Complete the following:

(a) The *average value* for r for the electron is given by

$$\int d\mathbf{r}\; rP(r,\theta,\phi)$$

where $\int d\mathbf{r}$ is the integral over all space in spherical coordinates ($d\mathbf{r} = r^2 \sin\theta dr d\theta d\phi$). Show that

$$\int d\mathbf{r}\; rP(r,\theta,\phi) = \frac{3}{2}a_0$$

(Use an integral table or other integration aid!)

(b) The radial distribution function $Q(r)$ is given by

$$Q(r) = \int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta d\theta\; r^2 P(r,\theta,\phi)$$

The *most likely* value for r is the value where $Q(r)$ is maximized. Show that $r_{\max} = a_0$

2. Does $A = \begin{bmatrix} 4 & 3 \\ 2 & 5 \end{bmatrix}$ satisfy the equation $3A^2 - 2A = \begin{bmatrix} 40 & 21 \\ 8 & 65 \end{bmatrix}$?

Explain why A does or does not satisfy the equation. Note: For real numbers, a multiplied by itself n times can be written as a^n. Similarly, the matrix A multiplied by itself n times can be written as A^n. Therefore, A^2 means $A \cdot A$.

3. Extra credit: A system of linear equations,

$$\begin{array}{ccccccccc} a_{11}x_1 & + & a_{12}x_2 & + & \dots & + & a_{1n}x_n & = & b_1 \\ a_{21}x_1 & + & a_{22}x_2 & + & \dots & + & a_{2n}x_n & = & b_2 \\ \vdots & & \vdots & & \ddots & & \vdots & & \vdots \\ a_{m1}z_1 & + & a_{m2}x_2 & + & \dots & + & a_{mn}x_n & = & b_m \end{array}$$

can be written as a matrix-vector problem.

$$\begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \ddots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_m \end{bmatrix}$$

That is, $A\vec{x} = \vec{b}$, and can be solved easily by multiplying both sides of the equation by the matrix inverse (A^{-1}) from the left. Use what you have learned about matrices to solve the system of equations below:

$$\begin{aligned} 2v + 5w - 8x + 1y + 2z &= 0 \\ 6v + 2w - 10x + 6y + 8z &= 6 \\ 1v + 6w + 2x + 3y + 5z &= 6 \\ 3v + 2w + 5x + 3y + 5z &= 3 \\ 6v + 7w - 3x + 6y + 9z &= 9 \end{aligned}$$

for the values v, w, x, y, and z. You may find Mathematica to be a helpful tool.