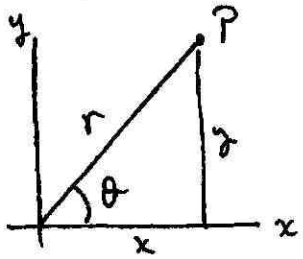
Problem Set #2 Chem 216

In polar (circular) coordinates



P is located at the point (x,y) where $x = r\cos\theta$ & $y = r\sin\theta$

① Consider the function $\psi_1 = e^{-r} r^2 \cos\theta \sin\theta$. Draw angular & radial diagrams for ψ_1. In the $1s$, $2p_z$, $3d_{x^2-y^2}$ etc... nomenclature what is the name of this orbital?

② Consider $\psi_2 = (1-r) r^2 \cos 2\theta$. Draw the angular & radial diagrams for this orbital. What is the name of this orbital?

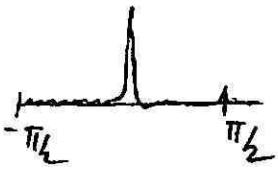
③ Consider the values of x ranging from $-\pi/2$ to $\pi/2$. Draw on the domain ranging from $-\pi/2$ to $\pi/2$ ($-\pi/2$, 0, $\pi/2$) the functions $\cos(x)$, $\cos(2x)$ & $\cos(3x)$.

ⓐ For those students without access to computer (programmable) draw the function $\psi_3 = \cos(x) + \cos(2x) + \cos(3x) + \ldots \cos(10x)$
For those with access to a programable computer draw

$$\psi_4 = \cos x + \cos(2x) + \cos(3x) + \ldots + \cos(1000x)$$

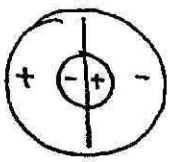
ⓑ In music the functions $\cos(x)$, $\cos(2x)$, ... correspond each to a pure musical note. If $\cos(x)$ is the note C ["doe a deer in Sound of Music] then $\cos(2x)$ corresponds to C one octave higher, $\cos(3x)$ is the G above this C etc...

(i) What do the functions ψ_3 or ψ_4 sound like to our ears?

(ii) ψ_4 looks something like this 

Recalling that ψ^2 corresponds to where the object is located, where is ψ_4 located in space? (Space here is one-dimensional)

(iii) [Heisenberg uncertainty Principle] If a particle (in 1-D) is located at the origin (see (ii) above) what is the "frequency" of this particle? Recalling that for a particle moving without interaction that energy = kinetic energy $= \frac{1}{2}mv^2$ where v is velocity, what are possible "velocities" for a particle located at the origin? The Heisenberg uncertainty principle states if the location of a particle is completely undetermined then its momentum (mv) is completely undetermined. How do our results in 3(a) support this conclusion?

④ In class we noted a $3p_x$ orbital would have node which looked as follows 

on a drum

Draw the $3d_{xy}$, $4d_{x^2-y^2}$ & 4s orbitals for a drum.

⑤ⓐ Which of the following molecules are attracted to a magnetic field : Be_2, S_2, N_2 & N_2^+ ?

ⓑ Why is Ne a noble gas ?

ⓒ Which molecule has the strongest bond (between the atoms) : C_2, N_2, O_2 or F_2 ? Which one is weakest ?

ⓓ In the model given in class would Be_2 be a stable molecule ? (In the real world there is 2s & 2p interaction) This interaction results in a weak Be - Be bond in Be_2)

⑥ Draw an MO diagram for Mo_2. Assume that the 5s valence orbital is slightly higher in energy than the 4d orbitals. Choose your axes as indicated

Mo Mo