Problem Set PS04

ISSUED: 9/19/02 **Due: 9/26/02**

Prof. Darin J. Ulness Name _____

Instructions. Complete all questions before class on the due date. You are encouraged to work together. Be sure to struggle with the problem before seeking help. Many of the exercises are very similar to problems in the book. Understanding the solution to these problems will be helpful in completing the assigned exercises.

Mathematical Exercises

1. Convert the following points on a 2D plane from Cartesian to polar coordinates

   (a) (1,1)
   (b) (3,4)

2. Convert the following points in a 3D space from Cartesian to spherical polar coordinates

   (a) (1,1,1)
   (b) (1,1,0)

Exercises

3. Using your handout on hydrogenic wavefunctions and average values, plot $\langle r \rangle$ for each value of n and l up through $n = 5$ (work in units of Bohr radius, i.e., set $a_0 = 1$).

4. Using your handout on hydrogenic wavefunctions and average values, plot $\langle r^2 \rangle$ for each value of n and l up through $n = 5$ (work in units of Bohr radius, i.e., set $a_0 = 1$).

5. Plot the uncertainty in the position of the electron of a hydrogen atom, $\delta r = \sqrt{\langle r^2 \rangle - \langle r \rangle^2}$, for each value of n and l up through $n = 5$ (work in units of Bohr radius, i.e., set $a_0 = 1$).

6. Derive the $3\mathrm{d}_2$ and $3\mathrm{d}_{-2}$ wavefunctions from the $3\mathrm{d}_{xy}$ and $3\mathrm{d}_{x^2+y^2}$ wavefunctions.

Conceptual Problems

7. The parity operator, $\hat{\pi}$, is defined by replacing $\vec{r}$ with $-\vec{r}$. That is, the parity operator inverts the wavefunction through the origin. Sketch a picture of the result of

   (a) $\hat{\pi}\psi_{1\mathrm{s}}$
   (b) $\hat{\pi}\psi_{2\mathrm{p}_z}$
   (c) $\hat{\pi}\psi_{3\mathrm{d}_{xy}}$
   (d) $\hat{\pi}\psi_{3\mathrm{d}_{x^2+y^2}}$

8. Suppose we lived in a two dimensional world. Ignoring spin altogether, how many quantum numbers would emerge when one solves the 2D hydrogen atom? Would two dimensional freshmen learn about the same periodic table as we do?

Computer Problems

9. Use MATHEMATICA to make a density plot of the $|\psi_{1s}|^2$ and $|\psi_{2s}|^2$. What do these plots tell us? (Hint: Define $\sigma = \sqrt{x^2 + y^2}$ and plot versus x and y. Turn the `Mesh` to false and use a sufficient number for `PlotPoints` and appropriate ranges to make the plots look like the ones you've seen in freshman chemistry.)

10. Use MATHEMATICA to make a density plot of the $\left|\psi_{2p_x}\right|^2$ and $\left|\psi_{2p_y}\right|^2$. What do these plots tell us? (Hint: Define $\sigma = \sqrt{x^2 + y^2}$, $\phi = \arctan \frac{y}{x}$, $\theta = \pi$ (this puts us on the x-y plane) and plot versus x and y. Turn the `Mesh` to false and use a sufficient number for `PlotPoints` and appropriate ranges to make the plots look like the ones you've seen in freshman chemistry.)

11. Use MATHEMATICA to make a density plot of the $\left|\psi_{3d_{xy}}\right|^2$ and $\left|\psi_{3d_{x^2+y^2}}\right|^2$. What do these plots tell us? (Hint: Define $\sigma = \sqrt{x^2 + y^2}$, $\phi = \arctan \frac{y}{x}$, $\theta = \pi$ (this puts us on the x-y plane) and plot versus x and y. Turn the `Mesh` to false and use a sufficient number for `PlotPoints` and appropriate ranges to make the plots look like the ones you've seen in freshman chemistry.)

Reflective Exercises

12. A popular play called *Copenhagen* deals with a mysterious visit of Heisenberg to his mentor Bohr that occurred during World War II. At the time, Heisenberg was head of the German nuclear project and Bohr was in German occupied Denmark. Heisenberg claimed that the German nuclear project was focussed on creating nuclear power for use by Germany rather then focussed on the atomic bomb. Anyway, the question is raised as to whether or not it is ethical to work on nuclear power of any reason. Suppose that at some point in the future, your job required you to use your training to work on something that may be of tremendous benefit to society (such as nuclear power) but could potentially be very destructive (such as the atomic bomb). Also suppose that it was out of your control as to how your results would be used. How would you react to this situation?

13. Read the following excerpt from H. Brown's "*The Wisdom of Science: Its Relevance to Culture & Religion.*"

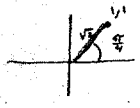
> ...there is little general appreciation of the cultural significance of science beyond its impact on technology. Although the dictionary tells us that science is another word for knowledge and that technology is concerned with the practical application of knowledge, this distinction is rarely made in public discussions, nor is it particularly useful because it is so hard to make in practice. An old joke says that if some venture is successful, such as a landing on the Moon, then the scientists will call is a 'triumph of science', and if is fails they will call it a 'failure of technology'. But this is not what actually happens. Nowadays almost every innovation from landing on the Moon to the invention of a better mouse trap, whether it is successful or not, is attributed to 'science'; the word technology is hardly ever used. Thus the popular image of science is inextricably confused with

technology and is therefore seen as being primarily an *instrument* for getting new things, new machines, new medicines, but not new understanding. Nowadays it is almost true to say that in most peoples's minds science is little more than a box of cleaver tricks which can produce the things which we want...

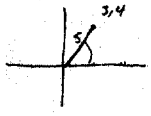
(a) Is the primary value of science to our culture it ability to produce amazing new things?

(b) Is there any way to justify spending taxpayer dollars to support basic science research (or science for science's sake) other than the fact that it might be useful from a practical standpoint some time in the future.

(c) The work I do has essentially no practical application. The same is true for the work Dr. Jensen did for his Ph.D. (his post-doctoral work was more practical however). Furthermore, if you took all the papers Dr. Jensen and myself have written and deleted them from the scientific literature the course of scientific history would be imperceptibly affected. Do we have any value at all from a science point of view? (Note: your answer will in no way affect your grade for the course.)

① (a) 

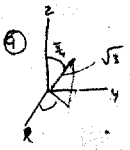
$(1,1) \rightarrow (\sqrt{2}, \frac{\pi}{4})$

(b) 

$r = \sqrt{3^2+4^2} = 5$

$\phi = \arctan 4/3 = 0.413$

$(3,4) \rightarrow (5, 0.413)$

② (a) 

$(1,1,1) \rightarrow (\sqrt{3}, \frac{\pi}{4}, \frac{\pi}{4})$

(b) 

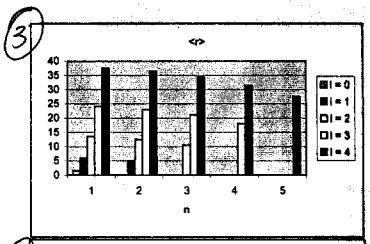
$(1,1,0) \rightarrow (\sqrt{2}, \frac{\pi}{4}, \frac{\pi}{2})$

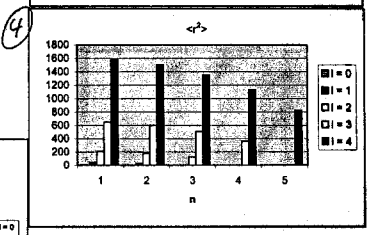
③, ④, ⑤ together on next page

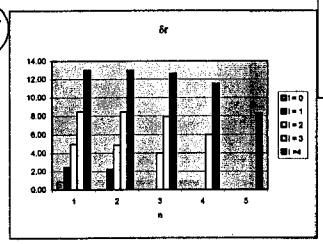
n	0	1	2	3	4
1	1.5				
2	6	5			
3	13.5	12.5	10.5		
4	24	23	21	18	
5	37.5	36.5	34.5	31.5	27.5

1	3				
2	42	30			
3	207	180	126		
4	648	600	504	360	
5	1575	1500	1350	1125	825

1	0.87				
2	2.45	2.24			
3	4.97	4.87	3.97		
4	8.49	8.43	7.94	6.00	
5	12.99	12.95	12.64	11.52	8.29

③ 

④ 

⑤ 

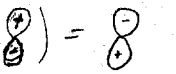
⑥ $\psi_{3dxy} = \frac{1}{81\sqrt{\pi}}\left(\frac{1}{a_0}\right)^{3/2} r^2 e^{-\frac{r}{3}} \sin^2\theta \cos 2\phi$, $\psi_{3dx^2-y^2} = \frac{1}{81\sqrt{\pi}}\left(\frac{1}{a_0}\right)^{3/2} r^2 e^{-\frac{r}{3}} \sin^2\theta \sin 2\phi$

From Euler Identities

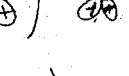
$\psi_{3dxy} = \frac{1}{2}(e^{2i\phi} + e^{-2i\phi})$ $\quad \psi_{3dx^2-y^2} = \frac{1}{2i}(e^{2i\phi} - e^{2i\phi})$

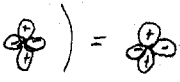
$\psi_{3d_2} \propto \psi_{3dxy} + i\psi_{3dx^2-y^2} = \Lambda e^{2i\phi}$ ✓

$\psi_{3d_{-2}} \propto \psi_{3dxy} - i\psi_{3dx^2-y^2} = \Lambda e^{-2i\phi}$ ✓

⑦ (a) $\hat{\pi}$  so $\hat{\pi}\psi_{1s} = \psi_{1s}$

(b) $\hat{\pi}$  so $\hat{\pi}\psi_{2p_z} = -\psi_{2p_z}$

(c) $\hat{\pi}$  so $\hat{\pi}\psi_{3dxy} = -\psi_{3dxy}$

(d) $\hat{\pi}$  so $\hat{\pi}\psi_{3dx^2-y^2} = \psi_{3dx^2-y^2}$

⑧ We quantize two dimensions, so 2 quantum numbers. The periodic table would be different since the period of the table is determined by the quantum numbers.

⑨, ⑩, ⑪ see last years solutions

⑫ your words

⑬ your words.