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8 pts

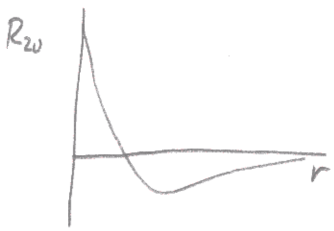
1. $R_{20} = \frac{1}{\sqrt{8}}\left(\frac{Z}{a_0}\right)^{3/2}(2-\rho)e^{-\rho/2}$

Node: $R_{20} = 0 \Rightarrow 2-\rho = 0 \Rightarrow \rho = 2 \Rightarrow \frac{2Z}{\cancel{n}a_0} r = 2$
$n=2$

(-2) node at $r=\infty$
(or other incorrect node)

$\Rightarrow \boxed{r = \frac{2a_0}{Z}} = \boxed{2a_0}$ for $Z=1$

From plot of R_{20} vs. r,



can see that antinode is at $r=0$.

Or we can establish location with derivative:

$$\frac{dR_{20}}{dr} = \frac{dR_{20}}{d\rho}\frac{d\rho}{dr} = 0 \qquad \text{where } \frac{d\rho}{dr} = \frac{2Z}{na_0}$$

and $$\frac{dR_{20}}{d\rho} = \frac{1}{\sqrt{8}}\left(\frac{Z}{a_0}\right)^{3/2}\left[(-1)e^{-\rho/2} + (2-\rho)\left(-\tfrac{1}{2}\right)e^{-\rho/2}\right] = 0$$

$$e^{-\rho/2}\left[-1-1+\frac{\rho}{2}\right] = 0$$

$$\Rightarrow e^{-\rho/2} = 0 \quad \text{or} \quad \frac{\rho}{2} - 2 = 0 \Rightarrow \rho = 4$$

$$\Rightarrow \rho = 0$$

When $\rho = 0$, $R_{20} = \frac{1}{\sqrt{8}}\left(\frac{Z}{a_0}\right)^{3/2} 2$

When $\rho = 4$, $R_{20} = \frac{1}{\sqrt{8}}\left(\frac{Z}{a_0}\right)^{3/2}(-2)e^{-2}$

$|R_{20}(\rho=0)| > R_{20}(\rho=4)$, so global extremum at $\rho = \boxed{r=0}$

-2 if this ignored

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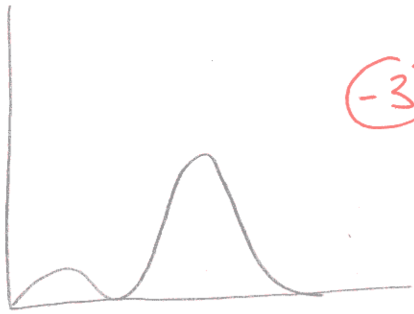
2. $\boxed{10 \text{ pts}}$

$r^2R_{20}^2$



r

(-3) no RDF

$$P(r) = r^2R_{20}^2 = r^2\left(\frac{1}{8}\right)\left(\frac{Z}{a_0}\right)^3\left(2-\frac{2Z}{na_0}r\right)^2 e^{-2Zr/na_0}$$

$n=2$ and $Z=1$,

$$\text{so } P(r) = \frac{1}{8a_0^3}r^2\left(2-\frac{1}{a_0}r\right)^2 e^{-r/a_0} = \frac{r^2}{8a_0^3}\left(4-\frac{4}{a_0}r+\frac{1}{a_0^2}r^2\right)e^{-r/a_0}$$

$$P(r) = \left(\frac{1}{2a_0^3}r^2 - \frac{1}{2a_0^4}r^3 + \frac{1}{8a_0^5}r^4\right)e^{-r/a_0}$$

$$\frac{dP(r)}{dr} = \left[\frac{1}{a_0^3}r - \frac{3}{2a_0^4}r^2 + \frac{1}{2a_0^5}r^3\right]e^{-r/a_0} - \frac{1}{a_0}\left[\frac{1}{2a_0^3}r^2 - \frac{1}{2a_0^4}r^3 + \frac{1}{8a_0^5}r^4\right] * e^{-r/a_0} = 0$$

$$= e^{-r/a_0}\left[\frac{r}{a_0^3} - \frac{3}{2a_0^4}r^2 + \frac{1}{2a_0^5}r^3 - \frac{1}{2a_0^4}r^2 + \frac{1}{2a_0^5}r^3 - \frac{1}{8a_0^6}r^4\right] = 0$$

$$\Rightarrow r - \frac{3}{2a_0}r^2 + \frac{1}{2a_0^2}r^3 - \frac{1}{2a_0}r^2 + \frac{1}{2a_0^2}r^3 - \frac{1}{8a_0^3}r^4 = 0$$

$$-r\left[-1+\frac{2}{a_0}r - \frac{1}{a_0^2}r^2 + \frac{1}{8a_0^3}r^3\right] = 0$$

$r=0$ (min) or $r^3 - 8a_0r^2 + 16a_0^2r - 8a_0^3 = 0 = f(r)$

Plot $f(r)$ vs. r in Excel:

- Have r be a multiple of a_0 $(0.01a_0, 0.02a_0, \ldots)$
- Set $a_0 = 1$
- The zeroes of the function will have units of a_0

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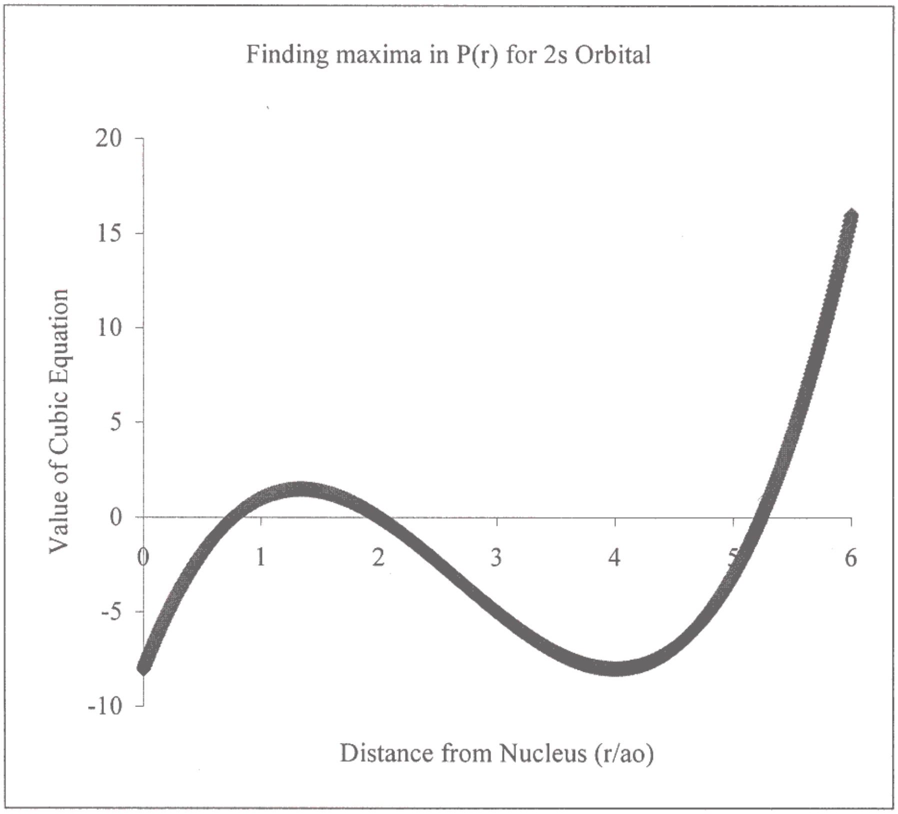
Experiment 2: Exploring Atomic Orbitals
Question 2

r (ao)	nasty cubic
0	-8
0.01	-7.840799
0.02	-7.683192
0.03	-7.527173
0.04	-7.372736
0.05	-7.219875
0.06	-7.068584
0.07	-6.918857
0.08	-6.770688
0.09	-6.624071
0.1	-6.479
0.11	-6.335469
0.12	-6.193472
0.13	-6.053003
0.14	-5.914056
0.15	-5.776625
0.16	-5.640704
0.17	-5.506287
0.18	-5.373368
0.19	-5.241941
0.2	-5.112
0.21	-4.983539
0.22	-4.856552
0.23	-4.731033
0.24	-4.606976
0.25	-4.484375
0.26	-4.363224
0.27	-4.243517
0.28	-4.125248
0.29	-4.008411
0.3	-3.893
0.31	-3.779009
0.32	-3.666432
0.33	-3.555263
0.34	-3.445496
0.35	-3.337125
0.36	-3.230144
0.37	-3.124547
0.38	-3.020328
0.39	-2.917481
0.4	-2.816
0.41	-2.715879



Zoom in on values where the cubic equation changes sign:

r (ao)	nasty cubic
0.7	-0.377
0.71	-0.314889
0.72	-0.253952
0.73	-0.194183
0.74	-0.135576
0.75	-0.078125
0.76	**-0.021824**
0.77	**0.033333**
0.78	0.087352
0.79	0.140239
0.8	0.192

r (ao)	nasty cubic
5.2	-0.512
5.21	-0.372039
5.22	-0.230552
5.23	**-0.087533**
5.24	**0.057024**
5.25	0.203125
5.26	0.350776
5.27	0.499983
5.28	0.650752
5.29	0.803089
5.3	0.957

So maxima in radial probability density at **0.76ao** and **5.24ao**
(the zero at 2.0ao corresponds to the radial node)

(in Mathematica, $(3-\sqrt{5})a_0 \cong 0.76a_0$ and $(3+\sqrt{5})a_0 \cong 5.24a_0$

$\boxed{+8}$ 2 right answers
$\boxed{+4}$ 1 " answer
$\boxed{+2}$ some effort

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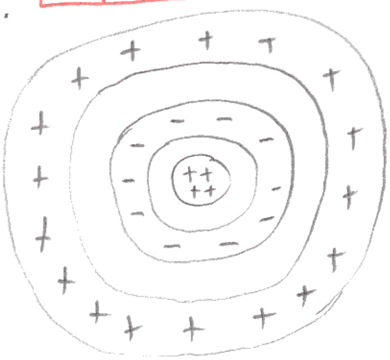
3. $\boxed{4\ pts}$

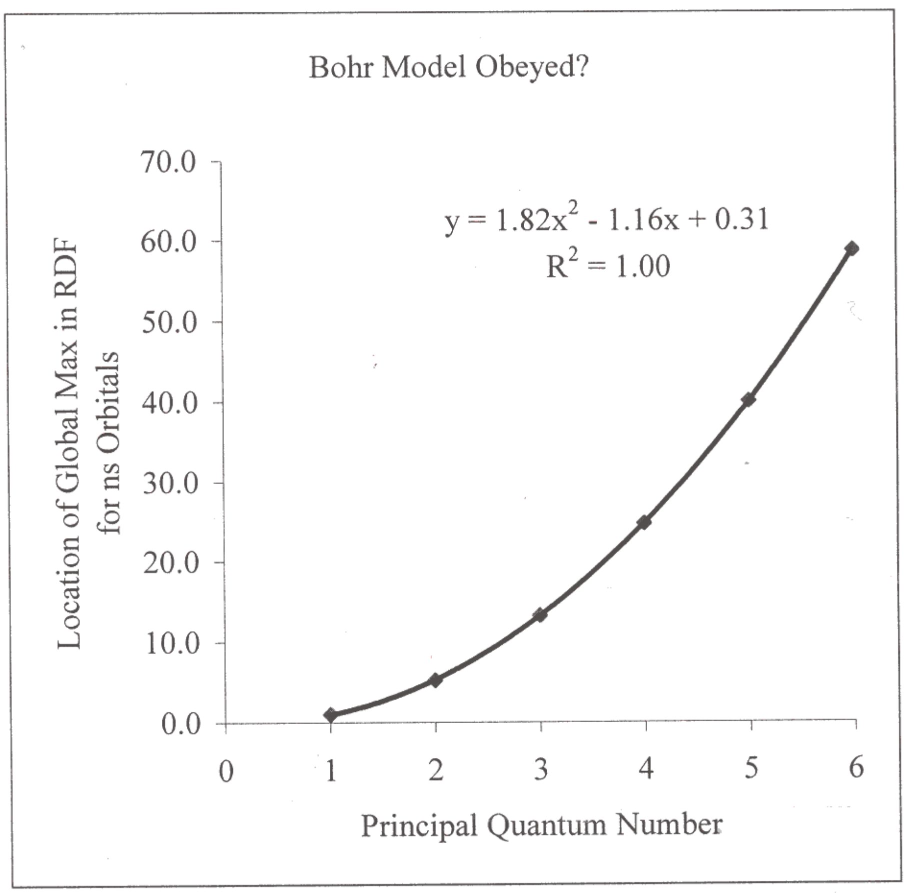


(-2) Wrong signs
(-3) missing layer of prob density

Experiment 2: Exploring Atomic Orbitals
Question 4

$\boxed{8\ pts}$

n	location of global max in RDF (ao)
1	1.0
2	5.2
3	13.2
4	24.7
5	40.0
6	58.7



5. YES; a quadratic fit of the location of the RDF's global max vs. n is perfectly precise.

$\boxed{4pts}$

(-2) Bohr is consistent with QM

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10 pts

6. $R_{21} = \frac{1}{\sqrt{24}}\left(\frac{Z}{a_0}\right)^{3/2} \rho e^{-\rho/2}$

$$\frac{dR_{21}}{d\rho} = \frac{1}{\sqrt{24}}\left(\frac{Z}{a_0}\right)^{3/2}\left[\rho\left(-\tfrac{1}{2}\right)e^{-\rho/2} + e^{-\rho/2}\right] = 0$$

$$e^{-\rho/2}\left[1 - \frac{\rho}{2}\right] = 0 \Rightarrow \rho = \frac{2Z}{na_0}r = 2$$

$$\Rightarrow r = \frac{na_0}{Z} = \boxed{2a_0} \quad (n=2, Z=1)$$

(-3) max amp at $r = \infty$

(-3) wrong finite value (found max in RDF)

The R_{21} orbital experiences a centrifugal barrier which pushes it away from the nucleus. R_{20} has no orbital angular momentum, and ∴ no such barrier

(-2) just discusses node

7. 4 pts

(-2) funny extraneous contours

8. 4 pts The lobes in Q7 enclose less than 100% of the prob density. $\psi^*\psi$ is very low (although not zero) in the immediate vicinity of the planar angular node.

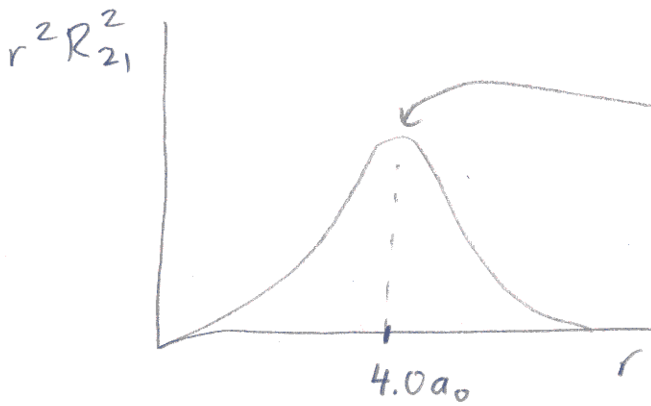
(-2) vague (-4) doesn't answer question

9. 2 pts

NOT A P ORBITAL!!

(-1) lobes don't touch at nucleus

10. $\boxed{10\ pts}$



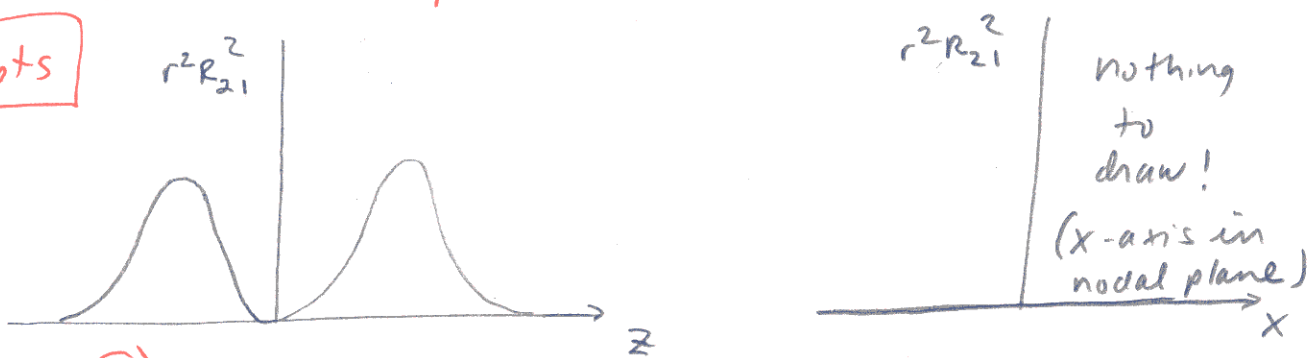
Compared to RDF of 2s

- 1 fewer maximum
- This max is closer than the max in $r^2R^2_{20}$
- No radial node

(2 for full credit)

(-3) only one comparison

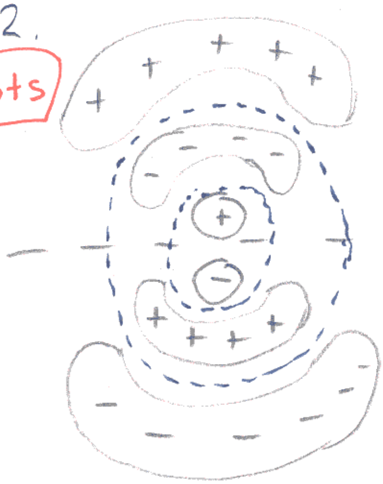
11. $\boxed{8\ pts}$



nothing to draw! (x-axis in nodal plane)

(-3) no lump for -z axis

12. $\boxed{8\ pts}$

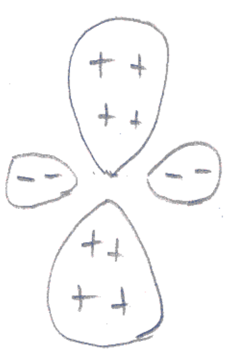


$4 - 1 - 1 = 2$ radial nodes (blue circles)

$l = 1 \Rightarrow 1$ angular node

(-3) no specific discussion of # of nodes

13. $\boxed{4\ pts}$



(-2) no signs

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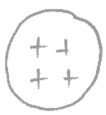
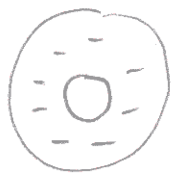
14. (a) 

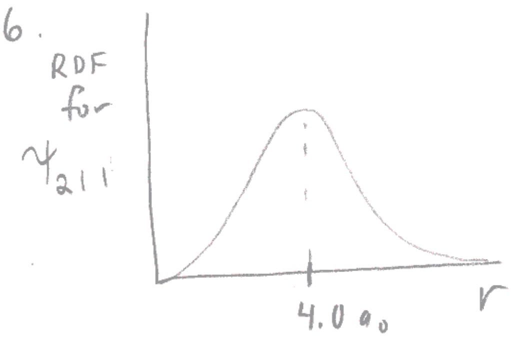
(b) 

(c) 

(for (a) and (c), some of the central doughnut can be depicted)

-3 one bad Xsect

15. Nothing required

16. 

identical to RDF for ψ_{210}, since orientation has no effect on RDF (and that is the only difference between ψ_{210} and ψ_{211})

-4 no explanation why