Name:	
Student Number:	
Tutorial:	

Jan. 26th, 2023 Duration: 20 min

No.	Maximum	Marks
1-5	5	
6	10	
7	10	
Total:		/25

- 1. (5 pts) For the hydrogen atom, state whether the following statements are true or false.
- a) The state defined by n = 1 is the first excited state. __F___
- b) It takes more energy to ionize (remove) the electron from the n=2 of He⁺ than an H atom in its first excited state ____T
- c) The electron is farther from the proton (on average) of the hydrogen atom in the 2p state than in the 2s state. _____F_
- d) The 2s and 2p orbitals are 4-fold degenerate. ____T
- e) The energy required to ionize an H atom is higher for the n = 2, l = 0, m = 0, state than the n = 2, l = 1 m = 1 state in the presence of a 2 T magnetic field._____T__

(10 pts) What is the most probable radius for the 1s electron for Ni^{27+} ? Recall for hydrogen-like ions, the potential is $U=-Zke^2/r$. If you have trouble, please explain how you would find this value using the Radial 1s wavefunction solution $R_{nl}(r) = (2/(a_B)^{1/2})e^{-r/a_B}$.

8.51 • [old 9.45] Ni²⁷⁺ is a hydrogen-like ion with Z = 28. Its most probable radius (in the ground state) is $r_{\rm mp} = a_{\rm B}/Z = a_{\rm B}/28 = 1.89 \ {\rm pm}$; the corresponding energy is $E = -Z^2 E_R$, and the binding energy is $B = Z^2 E_R = 10.7 \ {\rm keV}$.

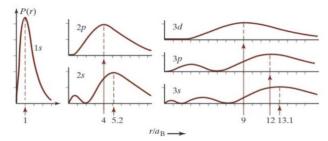
Full credit if they wrote down the radial probability density function for 1s with Z and show how to get the most probable position for the electron distribution.

I was thinking they could rationalize the reduction most probable position by knowing for Z=1 (Hydrogen) the most probable position is a_B, then given the potential attraction:

$$r_{mp} = a_B/Z$$
 or 1.89 x 10^{-12} m.

partial credits for writing down wavefunction (4 pts), indicating taking derivative to find maxima (4pts) ...2pts for correct answer a_B/Z

2. Following up on the above, <u>draw the 1s radial probability density for Ni²⁷⁺</u> and compare to the same orbital for hydrogen. <u>The plot does not have to be to scale</u>, just approximate - to clearly



show the basic trend as Z increases on the electron distribution relative to the nucleus.

The plot should be the left panel showing max for H, and overlayed the similar form for Ni²⁷⁺ but being significantly closer to the nucleus.

Credits...5pts for H 1s, 5pts showing significantly closer distribution for Ni²⁷⁺

Name:	
Student Number:	
Tutorial:	

Jan. 25rd, 2023 Duration: 20 min

No.	Maximum	Marks
1-5	5	
6	10	
7	10	
Total:		/25

- 1. Is the following statement True or False? The boundary conditions that the radial probability distribution goes to 0 as $r \to \infty$ leads to quantization of the hydrogen energy levels. T
- 2. The wavefunction for an electron in the 2Pz orbital contains a spherical harmonic $(Y_{l,m})$. Which of the following is the correct harmonic?
 - a) Y00
 - b) Y10
 - c) Y20
 - d) Y21

b)

- 3. True or False: The lowest energy state (the ground state) of a particle in a two-dimensional square well is not degenerate: T
- 4. True or False: An electron in a d orbital has a spherically symmetrical wavefunction. F
- 5. Hydrogen atom orbitals 3s, 3p and 3d have (choose the correct answer):
 - a) Same energy level
 - b) Same angular momentum
 - c) Same energy level and same angular momentum
 - d) Different energy level and different angular momentum.

a)

Table For Problem 6

The first few radial functions $R_{nl}(r)$ for the hydrogen atom. The variable ρ is an abbreviation for $\rho = r/a_{\rm B}$ and a stands for $a_{\rm B}$.

$$n = 1 n = 2 n = 3$$

$$l = 0 \frac{2}{\sqrt{a^3}}e^{-\rho} \frac{1}{\sqrt{2a^3}} \left(1 - \frac{1}{2}\rho\right)e^{-\rho/2} \frac{2}{\sqrt{27a^3}} \left(1 - \frac{2}{3}\rho + \frac{2}{27}\rho^2\right)e^{-\rho/3}$$

$$l = 1 \frac{1}{\sqrt{24a^3}}\rho e^{-\rho/2} \frac{8}{27\sqrt{6a^3}} \left(1 - \frac{1}{6}\rho\right)\rho e^{-\rho/3}$$

$$l = 2 \frac{4}{81\sqrt{30a^3}}\rho^2 e^{-\rho/3}$$

6. (10 pts) What is the probability that a 2p electron in hydrogen can be found in the region r>a_B? Use the above table to construct the proper radial probability density (distribution) for the 2p orbital. NOTE: You do not have to evaluate the integral, just write it down to show you know how to calculate the probability for a given electron distribution.

$$P(r \ge a) = \frac{4}{a^3} \int_a^{\infty} r^2 e^{-2r/a} dr = \frac{1}{2} \int_2^{\infty} s^2 e^{-s} ds.$$

(In the last expression we have made the substitution 2r/a = s.) Two successive integrations by parts (in which the end-point terms do not all vanish) give

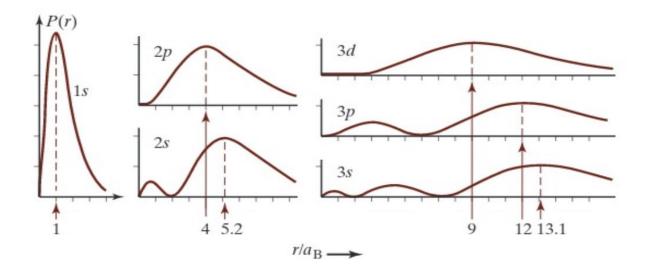
$$P(r \ge a) = 2e^{-2} + 2e^{-2} + e^{-2} = 5e^{-2} = 0.68.$$

That is, 68% of the electron probability distribution is outside the Bohr radius, and 32% is inside.

The above is for $ls...so\ P(r) = 4\pi r^2 | \frac{1}{\sqrt{24a^3}} pe^{-r/2} |^2$ integrated as above.

Partial credit if they construct the right orbital..R(2p) (5pts), integration limits (3pt), quadratic (2pts)

7. (10 pts). Following up on the above, sketch the radial probability density for the 2p orbital and compare to the radial distribution density for the 2s orbital of hydrogen. Shade in the area corresponding to question above.



The plots should be something close to the second panel with shading from $r/a_B = 1$ to full extent of plot. It should show higher probability for 2s electrons to be below a_B .

³ pts for generally correct distribution/shape for 2s

³ pts for 2p

⁴ pts for showing correctly the limits to the probability distribution in shading the appropriate area.

Name:	
Student Number:	
Tutorial:	

Jan. 24rd, 2023 Duration: <u>20 min</u>

No.	Maximum	Marks
1-5	5	
6	10	
7	10	
Total:		/25

1.	The 3p orbital in the Hydrogen atom describes the state with the following quantum number: a) m=3, l=2 b) n=3, l=1 c) n=3, l=2 d) l=3, n=2 e) l=3, m=1 b)
2.	Two states of the Hydrogen atom are degenerate if they correspond to the same (circle all that apply): a) Energy level b) Angular momentum c) Quantum number n d) Quantum number l e) Quantum number m
3.	A Hydrogen atom with principal quantum number n has degeneracy of (choose the correct answer): a) n b) $n-1$ c) n^2 d) \sqrt{n}
4.	 Hydrogen atom orbitals 3s, 3p and 3d have (choose the correct answer): a) Same energy level b) Same angular momentum c) Same energy level and same angular momentum d) Different energy level and different angular momentum
5.	Choose the correct statement: if the quantum number of an orbital is I=0, the corresponding wave function would be: a) Constant with respect to R b) Constant with respect to θ and ϕ c) Varies as θ varies d) Varies as ϕ varies

a)

b)

The first few radial functions $R_{nl}(r)$ for the hydrogen atom. The variable ρ is an abbreviation for $\rho = r/a_{\rm B}$ and a stands for $a_{\rm B}$.

	n = 1	n = 2	n = 3
<i>l</i> = 0	$\frac{2}{\sqrt{a^3}}e^{-\rho}$	$\frac{1}{\sqrt{2a^3}}\bigg(1-\frac{1}{2}\rho\bigg)e^{-\rho/2}$	$\frac{2}{\sqrt{27a^3}} \left(1 - \frac{2}{3}\rho + \frac{2}{27}\rho^2\right) e^{-\rho/3}$
<i>l</i> = 1		$\frac{1}{\sqrt{24a^3}}\rho e^{-\rho/2}$	$\frac{8}{27\sqrt{6a^3}} \bigg(1 - \frac{1}{6}\rho \bigg) \rho e^{-\rho/3}$
<i>l</i> = 2			$\frac{4}{81\sqrt{30a^3}}\rho^2 e^{-\rho/3}$

6. a) (10 pts) The average value or expectation value <r> for any state (re: assigned home work) is given by <r>= $\int r P(r)dr$ (recall $P(r) = 4\pi r^2 |R(r)|^2$) Show how you would calculate <r> for the 1s state of hydrogen. You don't need to evaluate the integral. The hydrogenic wavefunctions are listed in the table below.

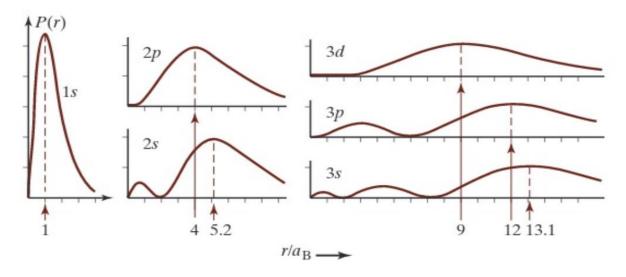
 $P(r) = (4/a^3)r^2e^{-2r/a}$, where a denotes the Bohr radius. Therefore

$$\langle r \rangle = \int r P(r) dr = (4/a^3) \int r^3 e^{-2r/a} dr.$$

Main point is recognize that R(r) in table ..l=0, n=1 function must be squared and multiplied by r^2 to give the prob. density and expectation value then involves r^3 .

I would give 6-7/10 depending on how presented if they wrote the right function R(r) but did not square it and use proper integration over a volume element $(x4\pi r^2)$

7. (10 pts) Following up on the above question, sketch the Radial Probability Density for the 1s orbital and explicitly indicate the maximum probability and expectation <r>, average position of the electron relative to the nucleus. The plot only needs to be approximate to clearly show the distinction. Explain the difference between the average and most probable radii.



They should show there is a maximum probability away from the nucleus as per P(r) 1s above followed by an exponential decay. They should know the maximum is at a_B but fine to show a max..and the <r> should be further from the nucleus than most prob..or words to the effect that one is the average value over the whole atomic volume. Same n have same <r>related to the binding energy.

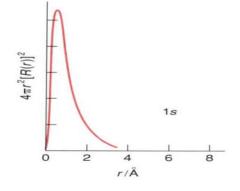
Name:	
Student Number:	
Tutorial:	

Jan. 23rd, 2023 Duration: 20 min

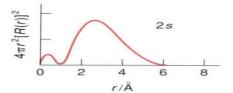
No.	Maximum	Marks
1.	5	
2.	10	
3.	10	
Total:		/25

- 1. (5 pts) For the hydrogen atom, state whether the following statements are true or false.
- a) The state defined by n = 2 is the first excited state. ___T__
- b) It takes more energy to ionize (remove) the electron from the n=2 state than from the ground state. __F__
- c) The electron is farther from the nucleus (on average) in the n=4 state than in the n=2 state.____T___
- d) The wavelength of light emitted when the electron drops from n=5 to the n = 3 in hydrogen is longer than from n= 4 to n= 2 (See equation for energies of the hydrogen atom; E \propto 1/n²).__T___
- e) The energy required to ionize an H atom is higher for the n = 2, l = 0, m = 0, state than the n = 2, l = 1 m = 1 state in the presence of a 2 T magnetic field._____T ..+ve sign convention.
- 2. (10 pts) The relative radial probability densities (i.e. $4\pi r^2[R(r)]^2$) for the 1s, 2s and 2p orbitals are shown below. On the figure showing the 1s probability distribution, sketch the corresponding orbital for 3s. On the figure for 2s, sketch the 3p orbital probability distribution. On the 2p plot, sketch the corresponding radial probability density for 3d orbitals as indicated. Show the nodes and trend for the maxima in probability distribution as a function of r as n and 1 increases.

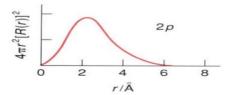
Plot radial prob. density for **3s overlayed on 1s** in this figure.

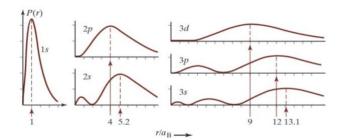


Plot radial prob. for **3p overlayed on 2s** in this figure.



Plot radial prob. for **3d overlayed on 2p** in this figure.





- -3s compared to 1s should show prob. density to have a higher <r> than for 1s and should show 2 nodes. Specific details are not important..qualitative dependence of 1s relative to 3s
- 3p should should show a node with density further from nucleus than 2s
- 3d should not have a node and probability distribution displaced further from nucleus

Be generous here..qualitative is okay. As guideline...6 pts for qualitatively correct, 2 for correct number of nodes, 2 pts for <r> increasing with n

3. (10 pts) The <u>radial wavefunctions</u> for the hydrogen atom for the cases l = n - 1 (maximum value for l) is given by:

$$R(r) = Ar^{n-1}e^{-r/na_{B}}$$

a) (5pts) Write down the radial density function.

$$P(r) = 4\pi r^2 [R(r)]^2 = Kr^{2n}e^{-2r/na}$$

...need to show they realize they need to use the wavefunction squared for probability/intensity and integrate over a volume element viz multiply R(r) by $4\pi r^2$. I would give 3/5 if they forget to use r^2 .

b) (5pts) Find the most probable radius for the electron distribution for l = n - 1 (using above). (If you have problems in constructing the radial density function, explain how you would do this calculation for partial credit.)

3

$$dP/dr = 2K(n - r/na)r^{2n-1}e^{-2r/na}$$

Min. at r=0 and max. at n²a_B

I would give partial credit if they explain in words if they don't do the math...again 3/5