Phys514 Fall 2013: Homework 1 Solution

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1 Foot 2.4 (25 pts)

The probability is given by

$$\begin{aligned}
\int_0^{r_b} 4\pi r^2 \left|\psi(r)\right|^2 \, dr &= \frac{4}{a_0^3}\int_0^{r_b} r^2 e^{-2r/a_0} \, dr \\
&= 4\int_0^{r_b/a_0} x^2 e^{-2x} \, dx \\
&= 4\int_0^{r_b/a_0} x^2(1-2x+\dots) \, dx \\
&= \boxed{\frac{4}{3}\left(\frac{r_b}{a_0}\right)^3 + \mathcal{O}\left(\frac{r_b}{a_0}\right)^4}
\end{aligned}$$

The electronic charge density is

$$\begin{aligned}
\rho_e(r) &= -e\left|\psi(r)\right|^2 \\
&= -\frac{e}{\pi a_0^3} e^{-2r/a_0} \\
&= \boxed{-\frac{e}{\pi a_0^3}\left(1-\frac{2r}{a_0}\right) + \mathcal{O}\left(\frac{r}{a_0}\right)^2}
\end{aligned}$$

2 Foot 4.3 (25 pts)

Given the binding energies in sodium, we can calculate $n^* = \sqrt{13.6\mathrm{eV}/E}$ and $\delta = n - n^*$

Configuration	E[eV]	n^*	δ_s
3s	5.14	1.63	1.37
4s	1.92	2.66	1.34
5s	1.01	3.67	1.33
6s	0.63	4.65	1.35

We observe that the quantum defect varies slightly with n

The binding energy for 8s in sodium is[1] E $= 13.6\mathrm{eV}/(8-1.35)^2 = \boxed{0.31\text{ eV}}$; and in hydrogen is E $= 13.6\mathrm{eV}/8^2 = \boxed{0.21\text{ eV}}$. The valence electron in sodium is more tightly bound to the core than in hydrogen.

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[1] $\delta_s = 1.35$ for $n > 5$ (Foot), but taking the average is also fine.

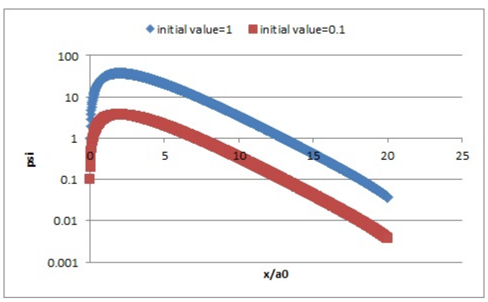
3 Foot 4.6 (25 pts)

The given transitions are necessarily from $4s$ to np, since $\Delta l = \pm 1$ in electric dipole transitions. The following table shows the binding energy $E = IE - hc/\lambda$, the effective principal number $n^* = \sqrt{13.6\text{eV}/E}$ and the quantum defect $\delta = n - n^*$ for the transitions, all starting from $4s_{1/2}$

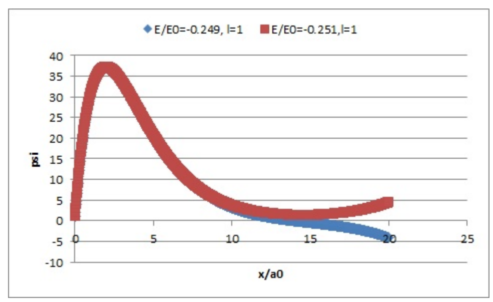
λ[nm]	Final state	E [eV]	n^*	δ_p
769.9	$4p_{1/2}$	2.729	2.23	1.77
766.5	$4p_{3/2}$	2.722	2.24	1.78
404.7	$5p_{1/2}$	1.276	3.26	1.74
404.4	$5p_{3/2}$	1.274	3.27	1.73
344.7	$6p_{1/2}$	0.743	4.28	1.72
344.6	$6p_{3/2}$	0.742	4.28	1.72

The next doublet is $4s_{1/2} \to 7p_{1/2}, 7p_{3/2}$. To find the corresponding wavelength, we calculate the average quantum defect $\delta_p = 1.74$, then the binding energy $E = 13.6\text{eV}/(7-1.74)^2 = 0.491\text{eV}$ and finally $\lambda = hc/(4.34 - 0.491)\text{eV} = \boxed{322.1\text{nm}}$. We estimate the splitting from the formula $\Delta E_{FS} = \frac{Z_i^2 Z_o^2}{(n^*)^3 l(l+1)} \alpha^2 hcR_\infty \propto 1/(n^*)^3$, where the splitting for $6p$ can be used as a reference. We obtain $\Delta E_{FS} \approx \left(\frac{4.28}{5.26}\right)^3 0.001\text{eV} = \boxed{0.5\text{meV}}$ and the splitting in wavelength is therefore $\Delta\lambda_{FS} \approx |d\lambda/dE|\Delta E = hc/(3.85\text{eV})^2\ 0.5\text{meV} \approx \boxed{0.04\text{nm}}$

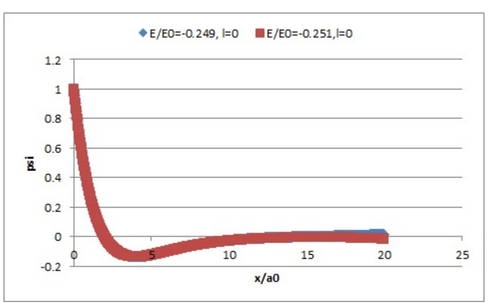
4 Foot 4.10 (25 pts)



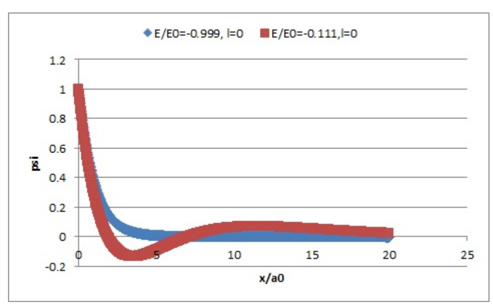
(a) Part (5.i): Psi for two different initial values, with $E/E_0 = -0.25$, l=1 and step=0.02. The shape is the same (note the log scale)



(b) Part (5.ii): Psi for two trial energies, with l=1 and step=0.02



(c) Part (5.iii): Psi for two trial energies, with l=0 and step=0.02



(d) Part (6): Psi for two different eigenenergies, with l=0 and step=0.02. The results are consistent with $E/E_0 = -1/n^2$