HW 2

2.1

2.1.1

Ionization energy: $E_n = -\frac{Z^2}{n^2} R$ with $R = 13.6\,eV$

- for 2s electron in Li $Z_{eff} = +3 - 2 = +1$
  ($3 \cdot p^+$, $1s^2 e^-$)

- valence shell is 2s $\rightarrow n = 2$

$$\Rightarrow E_{1st}^{theo} = -\frac{Z_{eff}^2}{n^2} R = -\frac{1}{4} R = -3.4\,eV$$

$|E_{1st}^{theo}| < |E_{1st}^{exp}|$: 2s e^- does penetrate core region (screening not perfect)

2.1.2

$$E_{3rd} = -\frac{Z^2}{n^2} R = -\frac{3^2}{1^2} 13.6\,eV = 122.4\,eV$$

This value is <u>exact</u> as there are no e^- to shield nucleus.

2.2

2.2.1

Kr^{35+} : $Z = 36$, only one e^-

→ can be treated as H-like with $a_0^{Kr} = \frac{a_0^H}{36} = 1.47 \cdot 10^{-12}\,m$

Probability $P = \int_0^R |\psi_{1s}|^2 r^2 \, dr \, d\Omega$

assume ψ_{1s} is constant over very small core region

→ $\psi(0) = \psi(R) = -\frac{1}{\sqrt{\pi a_0^{Kr\,3}}}$

$$\Rightarrow P = \left(-\frac{1}{\sqrt{\pi\, a_0^{Kr\,3}}}\right)^2 V_{Sphere} = \frac{1}{\pi\, a_0^{Kr\,3}} \frac{4\pi}{3} R^3$$

$$= \frac{4\,(4.19 \cdot 10^{-15}\,m)^3}{3\,(1.47 \cdot 10^{-12}\,m)^3} = 3.1 \cdot 10^{-8}$$

very small but not zero

2.3

2.3.1

$$E_n = -\frac{z^2 R}{n^2} = -\frac{z^2 e^2}{8\pi\varepsilon_0 a_0 n^2}$$

for $n=1$, $z=1$ $\quad E_1 = -\dfrac{e^2}{8\pi\varepsilon_0 a_0}$

$E = T + V(r)$

$E < V(r)$ is classically forbidden

$$V(r) = -\frac{e^2}{4\pi\varepsilon_0 r}$$

$$\Rightarrow \quad -\frac{e^2}{8\pi\varepsilon_0 a_0} = -\frac{e^2}{4\pi\varepsilon_0 r} \quad \Leftrightarrow \quad \underline{r = 2a_0}$$

region of $r > 2a_0$ classically forbidden

2.3.2

ground state $\psi_{1s} = \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0}$

$$P = \int_{2a_0}^{\infty} \psi^* \psi \, 4\pi r^2 dr = \frac{4}{a_0^3} \underbrace{\int_{2a_0}^{\infty} r^2 e^{-\frac{2r}{a_0}} dr}_{\text{integr by parts}}$$

$$= \frac{4}{a_0^3} \left[r^2 \frac{e^{-2r/a_0}}{-2/a_0} \Bigg|_{2a_0}^{\infty} - 2r \frac{e^{-2r/a_0}}{(-\frac{2}{a_0})^2} \Bigg|_{2a_0}^{\infty} + 2 \frac{e^{-2r/a_0}}{(-\frac{2}{a_0})^3} \Bigg|_{2a_0}^{\infty} \right]$$

$$= \frac{4}{a_0^3} \left[0 - 2a_0^3 e^{-4} + a_0^3 e^{-4} + \frac{a_0^3}{4} e^{-4} \right]$$

$$= \frac{4}{a_0^3} \frac{13 a_0^3}{4} e^{-4} = 13 e^{-4} = 0.238 = \underline{\underline{23.8\%}}$$