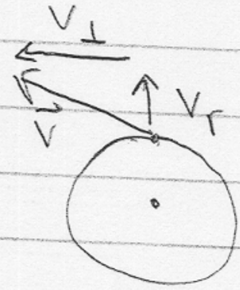
Last Time:



(see video)

Non-circular orbits

(1) $KE + PE = E \Rightarrow KE = E - V(r)$

(2) $L = r\,p_\perp$ ← angular momentum is constant

$L = m r v_\perp$ ↙ r and $v_\perp$ change

$KE = \frac{1}{2} m v_r^2 + \frac{1}{2} m v_\perp^2$

(note also $\omega = \frac{d\theta}{dt} = \frac{v_\perp}{r}$

$L = m r^2 \omega$)

$$KE = \underbrace{\frac{1}{2} m v_r^2}_{\text{radial}} + \underbrace{\frac{L^2}{2mr^2}}_{\text{angular}}$$

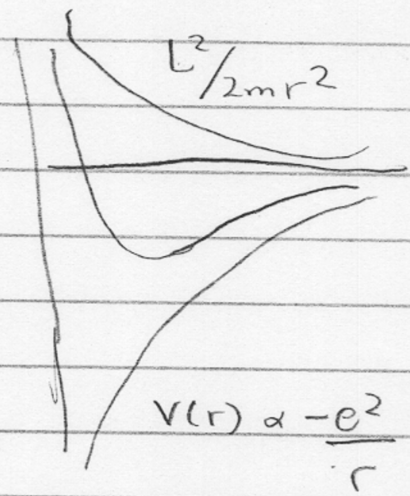
So

$$\frac{1}{2} m v_r^2 + \underbrace{\frac{L^2}{2mr^2} + V(r)}_{V_{eff}(r)} = E$$

$$\underbrace{\frac{1}{2} m v_r^2}_{\text{radial KE}} = E - V_{eff}(r)$$

Quantum mechanically: $L^2 = \overset{\text{discrete}}{\ell(\ell+1)} \hbar^2$

$$V^{\ell}_{eff}(r) = V(r) + \underbrace{\frac{\ell(\ell+1)\hbar^2}{2mr^2}}_{\text{centrifugal potential}}$$



Now we studied the Schrödinger equation

$$\left[\frac{-\hbar^2}{2m}\left(\underbrace{\frac{\partial^2}{\partial x^2}}_{\text{X-KE}} + \underbrace{\frac{\partial^2}{\partial y^2}}_{\text{Y-KE}} + \frac{\partial^2}{\partial z^2}\right) + V(r)\right]\psi = E\psi$$

In spherical coords;

angular momentum squared $\vec{L} = r \times \vec{P}$

$$\left[\underbrace{\frac{-\hbar^2}{2m}\left(\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}\right)}_{\text{radial KE}} + \underbrace{\frac{1}{2mr^2}\overbrace{-\hbar^2\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right)}^{\equiv \mathbb{L}^2}}_{\text{angular KE}}\right.$$

$$\left. + V(r)\right]\psi = E$$

So

$$\left[\underbrace{\frac{-\hbar^2}{2m}\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}}_{\text{radial}} + \underbrace{\frac{\mathbb{L}^2}{2mr^2}}_{\text{angular KE}} + V(r)\right]\psi = E\psi$$

Now try separation of Vars

$$\psi = R_{n\ell}(r)\, Y_{\ell m}(\theta, \phi)$$

Find Homework

$$\left[\frac{-\hbar^2}{2m}\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} + \overbrace{\frac{l(l+1)\hbar^2}{2mr^2} + V(r)}^{V^{l}_{eff}(r)}\right] R = E R$$

where

$$\underbrace{\left(\frac{\mathbb{L}^2}{2mr^2}\right)}_{\text{angular KE op}} \underbrace{Y(\theta,\phi)}_{\text{wave fcn on spher}} = \underbrace{\frac{l(l+1)\hbar^2}{2mr^2}}_{\text{angular KE}} Y \qquad l=0,1,2,3,\ldots$$

Find only (for) certain values of ang KE (discrete)

does angular wave fcn fits on sphere

Finally define

$$u_{nl} = \sqrt{4\pi r^2}\, R_{nl}$$

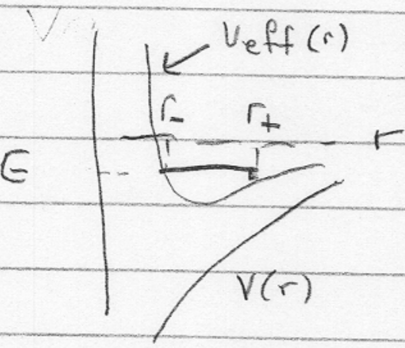
radial wave fcn

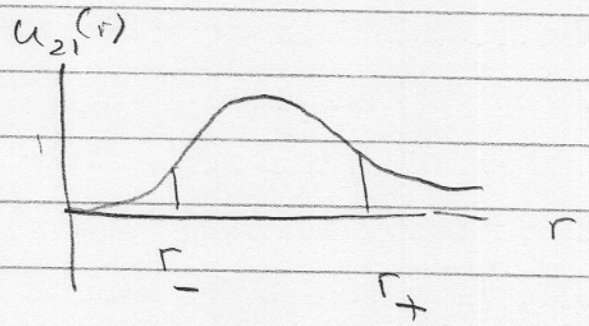
and show

$$\underbrace{\left[\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial r^2} + V^{l}_{eff}(r)\right] u_{nl}(r) = E_{nl}(r)}_{\text{1D Schrödinger Eq in the eff pot}}$$

Example - Sketch the $n=2$ $l=1$ radial wave-fcn determine the inflection points

Sol $n=2$ $l=1$ has $(n-1)-l=0$ radial excitations. It is therefore the ground state of $l=1$ eff potential





Then, $$V_{eff}^{(r)} = -\frac{e^2}{4\pi r} + \frac{\overbrace{2\hbar^2}^{l(l+1)\hbar^2}}{2mr^2}$$

We have

$$\frac{d^2u}{dr^2} = -\frac{2m}{\hbar^2}\left(E - V_{eff}(r)\right)u$$

$(u''=0)$

So inflection points are when $E - V_{eff} = 0$

$$E_2 = \frac{-\hbar^2}{2ma_0}\frac{1}{2^2} = \frac{-13.6}{2^2}$$

So

$$E = V_{eff}(r)$$

$$\frac{-\hbar^2}{2ma_0^2}\,\frac{1}{2^2} = \frac{-e^2}{4\pi\varepsilon_0 r} + \frac{2\hbar^2}{2mr^2}$$

Solve for r: (Homework) - gives quadratic eqn

$$\boxed{r = a_0\,(4 \pm 2\sqrt{2})}$$

$$= (1.17 \text{ and } 6.82)\,a_0$$

Explicitly (Skipped in class)

First switch to $\bar{r} = \frac{r}{a_0}$

$$\frac{-\hbar^2}{2ma_0^2}\,\frac{1}{2^2} = \frac{-e^2}{4\pi\varepsilon_0 a_0}\,\frac{1}{\bar{r}} + \frac{\hbar^2}{2ma_0^2}\,\frac{2}{\bar{r}^2}$$

using:

$$\frac{\hbar^2}{2ma_0^2} = \frac{1}{2}\,\frac{e^2}{4\pi\varepsilon_0 a_0} = 13.6\,\text{eV}$$

We have (dividing by $\hbar^2/2ma_0^2$)

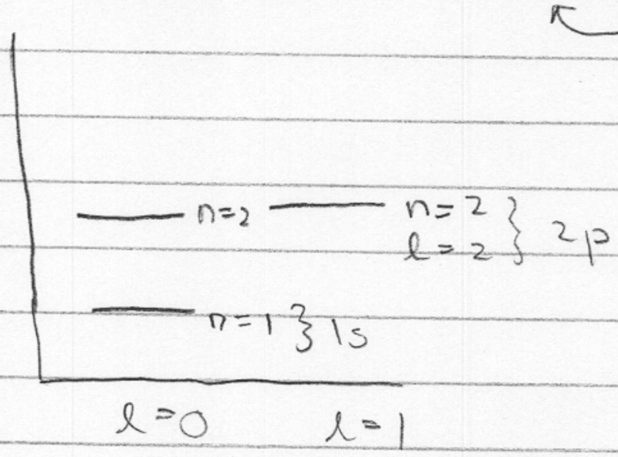
$$-\frac{1}{2^2} = -\frac{2}{\bar{r}} + \frac{2}{\bar{r}^2}$$

$$\bar{r}^2 = 8\bar{r} + 8 \Rightarrow \boxed{\bar{r} = 4 \pm 2\sqrt{2}}$$

The periodic table

- No two electrons can Occupy the same state (Pauli-Principle
- Electrons fill Hydrogen orbitals one by one
- But can be spin up or spin down

I'm not going to try to explain this



$[H] = \underbrace{[\uparrow]}_{1s^1}$

$l = 0, 1, 2, 3, 4$
or
s, p, d, f, g

$[He] = \underbrace{[\uparrow\downarrow]}_{1s^2}$

$[Li] = \underbrace{[He]}_{1s^2}\ \underbrace{[\uparrow\quad]}_{2s^1}$

Why fill up 2s before 2p?

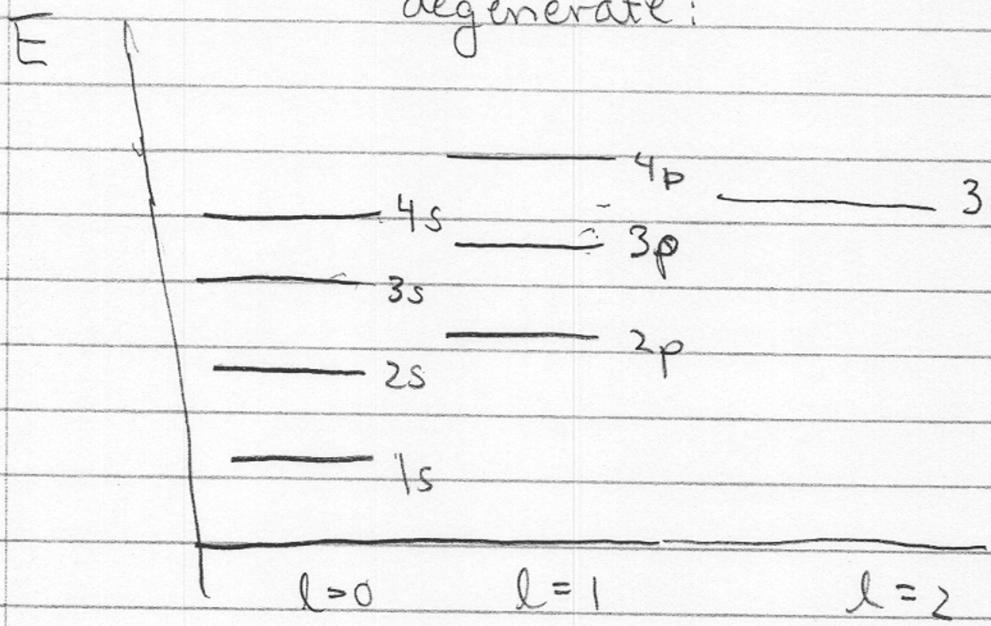
Electron Configurations in the Perodic Table

1 H 1s																	2 He 1s
3 Li 2s	4 Be											5 B	6 C	7 N 2p	8 O	9 F	10 Ne
11 Na 3s	12 Mg											13 Al	14 Si	15 P 3p	16 S	17 Cl	18 Ar
19 K 4s	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn 3d	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As 4p	34 Se	35 Br	36 Kr
37 Rb 5s	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc 4d	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb 5p	52 Te	53 I	54 Xe
55 Cs 6s	56 Ba	57 La	72 Hf	73 Ta	74 W	75 Re 5d	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi 6p	84 Po	85 At	86 Rn
87 Fr 7s	88 Ra	89 Ac	104 Rf	105 Db	106 Sg	107 Bh 6d	108 Hs	109 Mt	110	111	112	113	114				

58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd 4f	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm 5f	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr

by: Sarah Faizi

Answer: only for the strict $\frac{-1}{r}$ (Coulomb) potential are 2s and 2p degenerate:



So it's energetically favorable to fill 2s orbitals before 2p

Be: [He] $\underbrace{[\uparrow\downarrow]}_{2s^2}$

B: (He)($1s^2$) $\underbrace{[\uparrow]}_{2p^1}$

C: (He)($1s^2$) $\underbrace{[\uparrow\uparrow]}_{2p^2}$ p - waves can have $m = -1, 0, 1$

N: (He)($1s^2$) $\underbrace{[\uparrow\uparrow\uparrow]}_{2p^3}$ x 2 for spin

O: (He)($1s^2$) $\underbrace{[\uparrow\uparrow\uparrow\ \downarrow]}_{2p^4}$

F: (He)($1s^2$) $\underbrace{[\uparrow\uparrow\uparrow\ \downarrow\downarrow]}_{2p^5}$

Ne: (He)($1s^2$) $\underbrace{[\uparrow\uparrow\uparrow\downarrow\downarrow\downarrow]}_{2p^6}$

Hunds Rule: Within a shell fill up orbitals before changing the spin, Spins want to be aligne

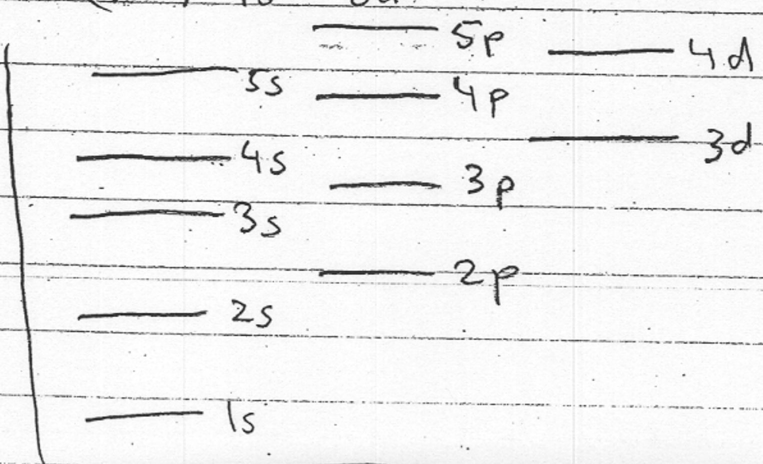
⋮ Continue
⋮

K: (Ar) $4s^1$

Ca: (Ar) $4s^2$

Then a change:

Sc: (Ar) $4s^2\ 3d^1$ ← Why?   Look at Picture:



Its energetically favorable to fill up 3d before 4p

Chemical Nature of Elements

1. Atoms w completely closed shells are exceptionally stable inert noble gasses

2. Look at table of ionization energies (Energy to rip off an electron)

   For those atoms w closed shells It costs more?

Why !!

Its due the angular wave fcns $Y_{\ell m}$

Shell structure in the periodic table

Ionization Energy = Energy to rip off electron

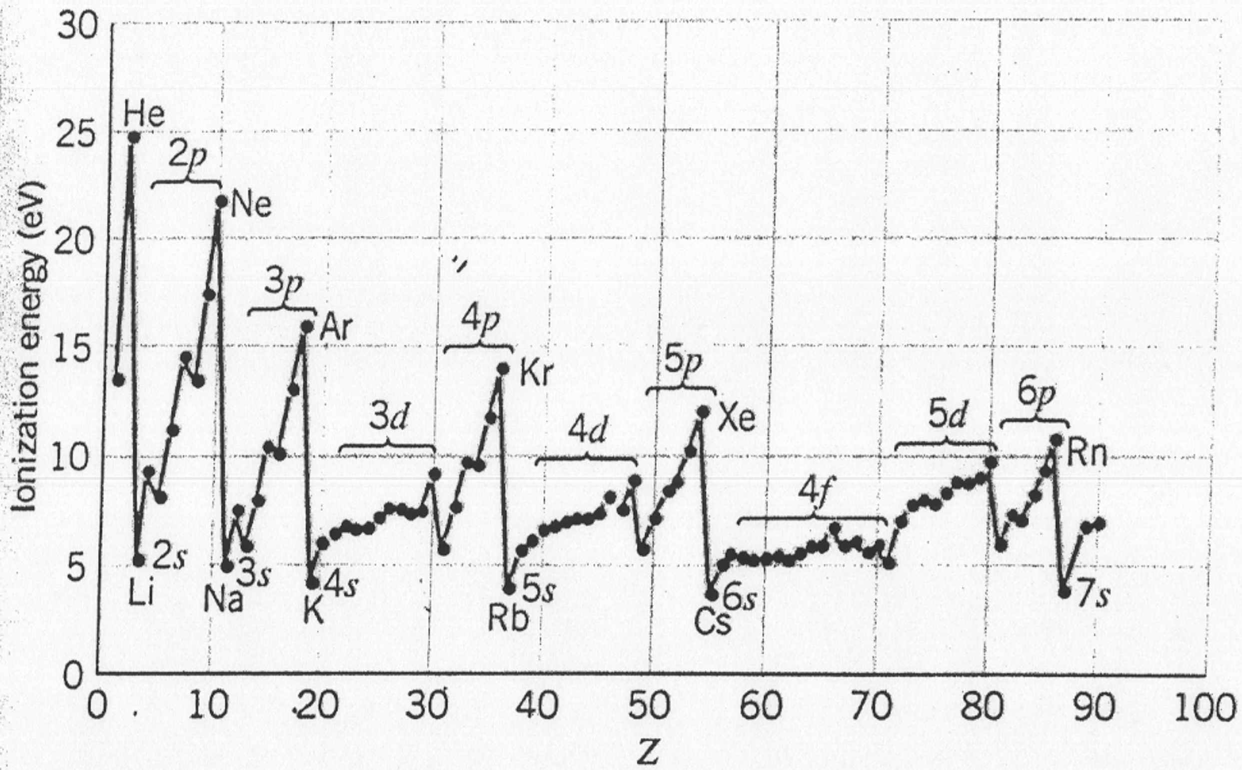


FIGURE 8.4 Ionization energies of neutral atoms of the elements.