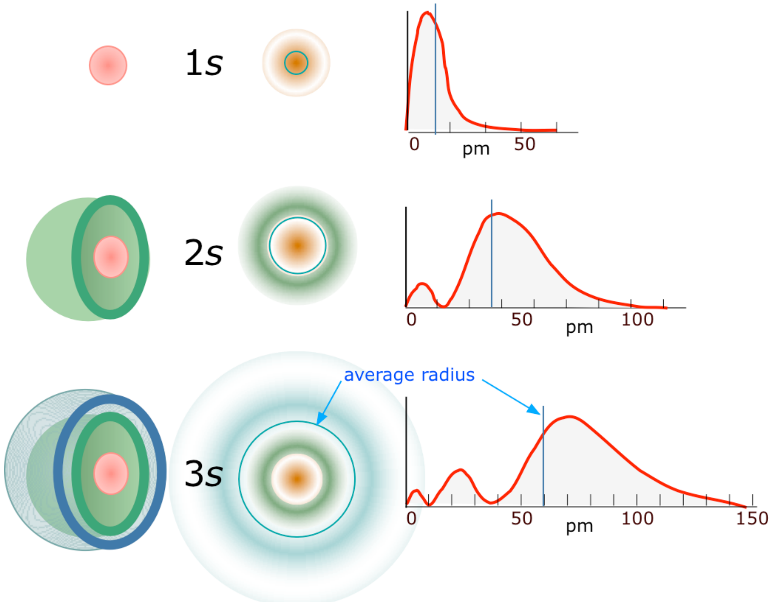
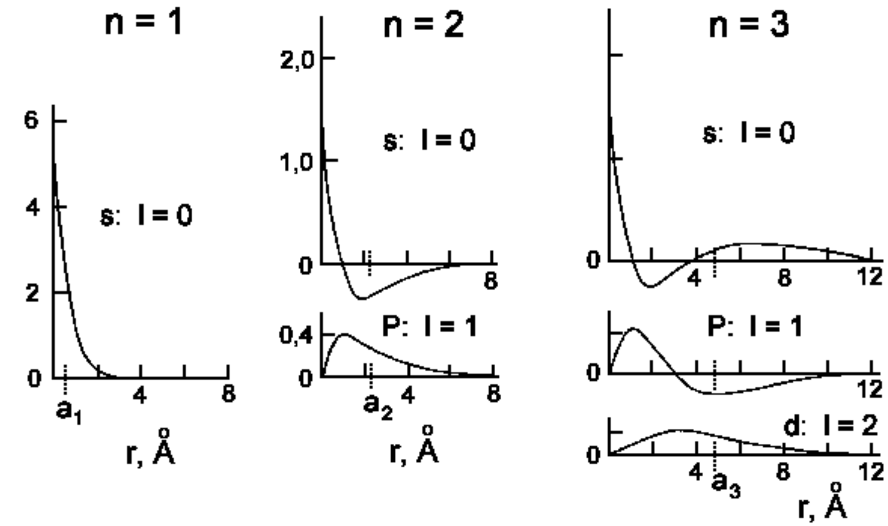
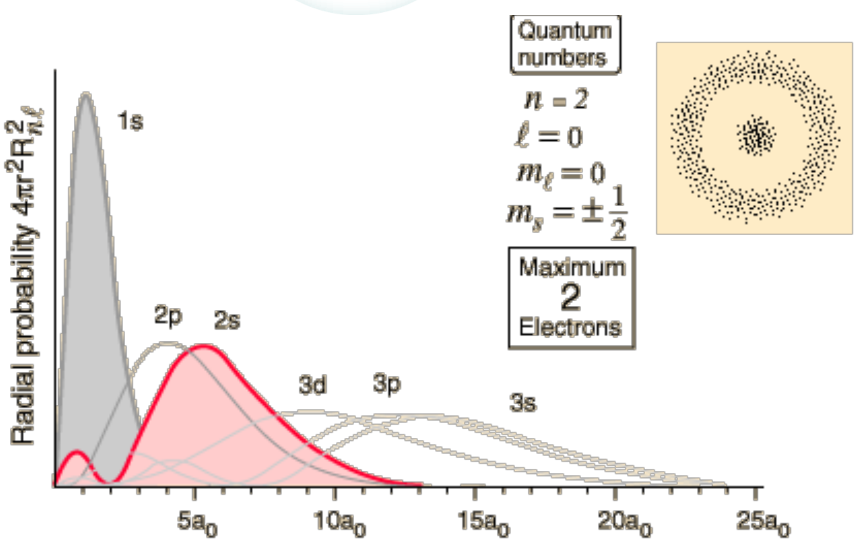
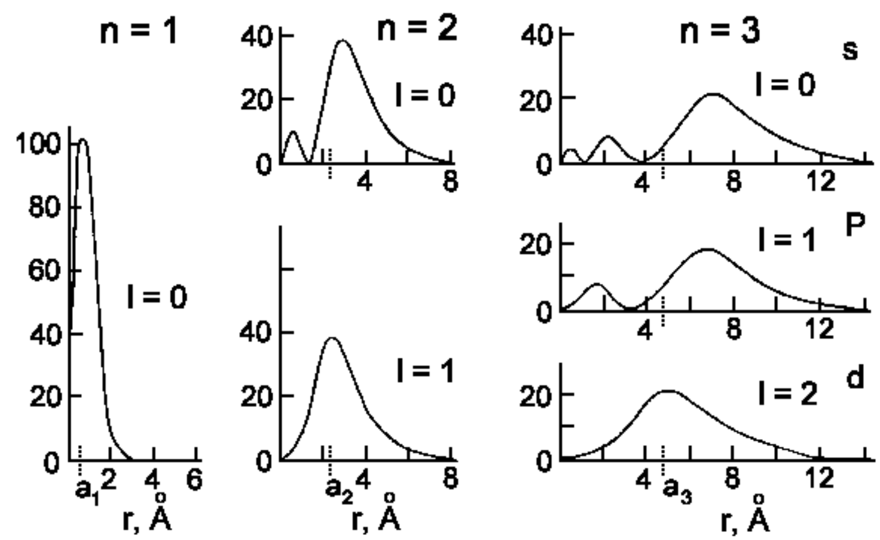
Wave functions

- Shells
- Orthogonality









Hydrogen again

- Relevant references for factorization technique
  - Am J Phys 55, 913 (1987)
  - Am J Phys 46, 658 (1978)
- Factorization with the aim to go to momentum space!
- Consider $p = \sqrt{\boldsymbol{p} \cdot \boldsymbol{p}}$ before $r = \sqrt{\boldsymbol{r} \cdot \boldsymbol{r}}$

$$r_p = \frac{1}{2}\left(\frac{1}{p}\boldsymbol{p} \cdot \boldsymbol{r} + \boldsymbol{r} \cdot \boldsymbol{p}\frac{1}{p}\right) \qquad p_r = \frac{1}{2}\left(\frac{1}{r}\boldsymbol{r} \cdot \boldsymbol{p} + \boldsymbol{p} \cdot \boldsymbol{r}\frac{1}{r}\right)$$

- Hamiltonian $H = \dfrac{\boldsymbol{p}^2}{2m} - \dfrac{\hbar^2}{m a_0}\dfrac{1}{r}$

- It is also possible to write

$$\boldsymbol{\ell}^2 = \boldsymbol{p}^2\left(\boldsymbol{r}^2 - r_p^2\right) \quad \text{before} \quad \boldsymbol{\ell}^2 = \boldsymbol{r}^2\left(\boldsymbol{p}^2 - p_r^2\right)$$

Detour (artificial)

- Define "funny" operator

$$\Lambda = \boldsymbol{r}^2 \left(\boldsymbol{p}^2 - 2mE\right)^2 - 2i\hbar \boldsymbol{p} \cdot \boldsymbol{r} \left(\boldsymbol{p}^2 - 2mE\right) + 4\hbar^2 \left(\boldsymbol{p}^2 - 2mE\right)$$

- When acting on eigenstate of Hamiltonian $H\,|E\ell m\rangle = E\,|E\ell m\rangle$

  same effect as applying the operator $\boldsymbol{r}^2 \left(\boldsymbol{p}^2 - 2mH\right)^2$

- Proof requires to show that

$$\boldsymbol{r}^2 \left[H, \boldsymbol{p}^2\right] = \frac{2i\hbar^3}{ma_0} \left(\boldsymbol{p} \cdot \boldsymbol{r} + 2i\hbar\right) \frac{1}{r}$$

- Then it follows immediately that $\Lambda\,|E\ell m\rangle = \dfrac{4\hbar^4}{a_0^2}\,|E\ell m\rangle$
- Goal is now to factorize the "funny" operator

Development

- Works by defining

$$P_\ell^{\pm} = r_p\left(\boldsymbol{p}^2 - 2mE\right) \pm i\hbar\frac{\ell + \frac{1}{2} \pm \frac{1}{2}}{p}\left(\boldsymbol{p}^2 + 2mE\right)$$

- Use $\boldsymbol{\ell}^2 = \boldsymbol{p}^2\left(\boldsymbol{r}^2 - r_p^2\right)$ to replace $\boldsymbol{r}^2$ in Λ and use $\boldsymbol{p}\cdot\boldsymbol{r} = r_p p - 2i\hbar$
- Inserting and replacing the square of the orbital angular momentum by its eigenvalue, one finds

$$\Lambda_\ell = r_p^2\left(\boldsymbol{p}^2 - 2mE\right)^2 + \frac{\hbar^2\ell(\ell+1)}{p^2}\left(\boldsymbol{p}^2 - 2mE\right)^2 - 2i\hbar r_p p\left(\boldsymbol{p}^2 - 2mE\right)$$

- Check that $\Lambda_\ell = P_{\ell\pm1}^{\mp}P_\ell^{\pm} - 4\hbar^2\left(\ell + \frac{1}{2} \pm \frac{1}{2}\right)^2 2mE$
- Note $\Lambda_\ell\left|E\ell\right\rangle = \frac{4\hbar^4}{a_0^2}\left|E\ell\right\rangle$
- As before $\Lambda_{\ell\pm1}\left(P_\ell^{\pm}\left|E\ell\right\rangle\right) = \frac{4\hbar^4}{a_0^2}\left(P_\ell^{\pm}\left|E\ell\right\rangle\right)$ implies that the energy doesn't change

$$P_\ell^{\pm}\left|E\ell\right\rangle = p_{E\ell}^{\pm}\left|E\ell \pm 1\right\rangle$$

More development

- Normalization

$$\left|p_{E\ell}^{\pm}\right|^2 = \frac{4\hbar^4}{a_0^2}\left[1 + \left(\ell + \frac{1}{2} \pm \frac{1}{2}\right)^2 \frac{2ma_0^2}{\hbar^2}E\right]$$

- For bound states factor must break off for

$$1 + (\ell_{max} + 1)^2 \frac{2ma_0^2}{\hbar^2}E = 0$$

- With the usual solutions $E_n = -\frac{\hbar^2}{2ma_0^2}\frac{1}{n^2}$ with $n = \ell_{max} + 1$

- Go to momentum representation with $r_p = i\hbar\left(\frac{\partial}{\partial p} + \frac{1}{p}\right)$

- apply to $P_\ell^{\pm}\left|E\ell\right\rangle = p_{E\ell}^{\pm}\left|E\ell \pm 1\right\rangle$

$$\langle p|\, r_p \left(p^2 - 2mE\right) \pm i\hbar\frac{\ell + \frac{1}{2} \pm \frac{1}{2}}{p}\left(p^2 + 2mE\right)|n\ell\rangle = \frac{2\hbar^2}{a_0} i \left[1 - \frac{(\ell + \frac{1}{2} \pm \frac{1}{2})^2}{n^2}\right]^{1/2}\langle p|n\ell \pm 1\rangle$$

- insert E and note phase choice!

Differential equation in momentum space

- Final result

$$\left(p^2+\frac{\hbar^2}{a_0^2n^2}\right)\frac{d}{dp}\langle p|n\ell\rangle+\left\{\left[\pm\left(\ell+\frac{1}{2}\pm\frac{1}{2}\right)+3\right]p+\frac{\hbar^2}{a_0^2n^2}\frac{1}{p}\left[1\mp\left(\ell+\frac{1}{2}\pm\frac{1}{2}\right)\right]\right\}\langle p|n\ell\rangle=$$

$$\frac{2\hbar}{a_0}\left[1-\frac{\left(\ell+\frac{1}{2}\pm\frac{1}{2}\right)^2}{n^2}\right]^{1/2}\langle p|n\ell\pm 1\rangle$$

- For $\ell=\ell_{max}$ use upper result (rhs --> 0)

$$\left[\left(p^2+\frac{\hbar^2}{a_0^2n^2}\right)\frac{d}{dp}+(n+3)\,p+\frac{\hbar^2}{a_0^2n^2}\frac{1}{p}\,(1-n)\right]\langle p|n\ell=n-1\rangle=0$$

- Solution

$$\langle p|n\ell=n-1\rangle=\phi_{n\ell=n-1}(p)=N\frac{p^{n-1}}{\left(p^2+\frac{\hbar^2}{a_0^2n^2}\right)^{n+1}}$$

Ground state

- Normalization

$$|N|^2 = \frac{2^{4n+2}(n!)^2}{\pi(2n)!}\left(\frac{\hbar}{a_0 n}\right)^{2n+3}$$

- Other wave functions: use lowering operator
- Ground state wave function

$$\phi_{10} = 4\sqrt{\frac{2}{\pi}}\left(\frac{\hbar}{a_0}\right)^{5/2}\frac{1}{\left(p^2 + \frac{\hbar^2}{a_0^2}\right)^2}$$

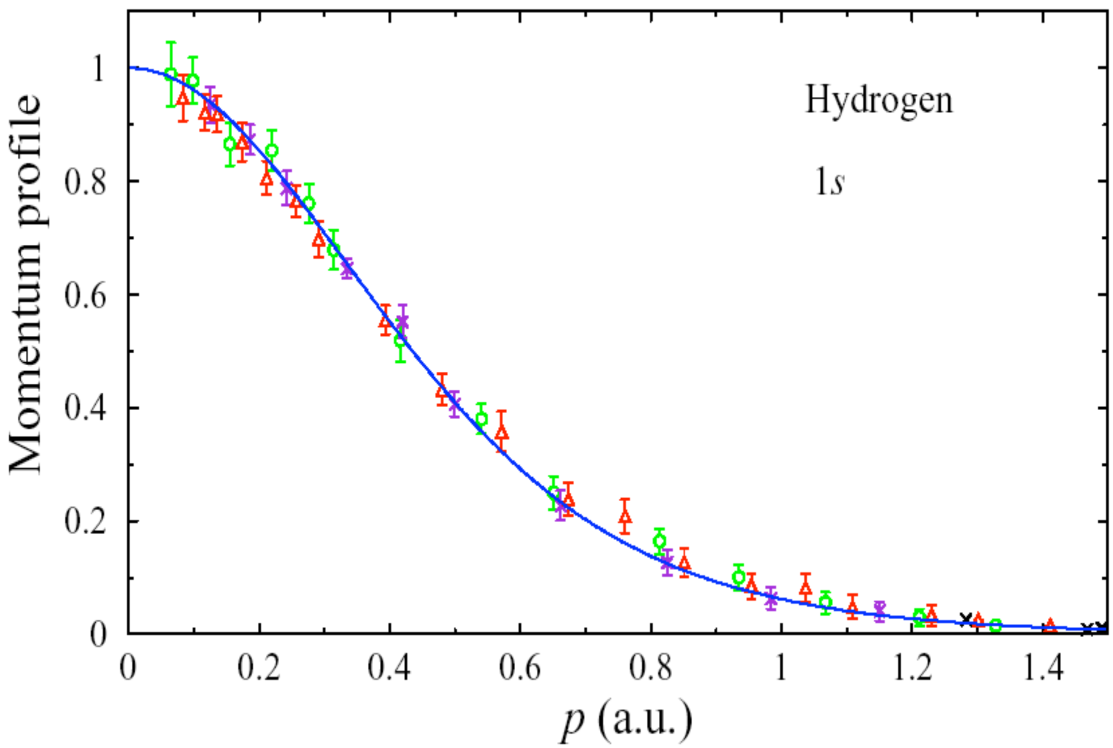
Direct knockout reactions

- Atoms: (e,2e) reaction
- Nuclei: (e,e′p) reaction [and others like (p,2p), (d,^{3}He), (p,d), etc.]
- Physics: transfer large amount of momentum and energy to a bound particle; detect ejected particle together with scattered projectile → construct spectral function
- Impulse approximation: struck particle is ejected
- Other assumption: final state ~ plane wave on top of N-1 particle eigenstate (more serious in practical experiments) but good approximation if ejectile momentum large enough
- If relative momentum large enough, final state interaction can be neglected as well
- -> PWIA = plane wave impulse approximation
- Cross section proportional to spectral function

(e,2e) data for atoms

- Start with Hydrogen
- Ground state wave function $\phi_{1s}(\boldsymbol{p}) = \frac{2^{3/2}}{\pi} \frac{1}{(1+p^2)^2}$
- (e,2e) removal amplitude

$$\langle 0|\, a_{\boldsymbol{p}}\, |n=1, \ell=0\rangle = \langle \boldsymbol{p}\, |n=1, \ell=0\rangle = \phi_{1s}(\boldsymbol{p})$$



Hydrogen 1s wave function "seen" experimentally
Phys. Lett. 86A, 139 (1981)