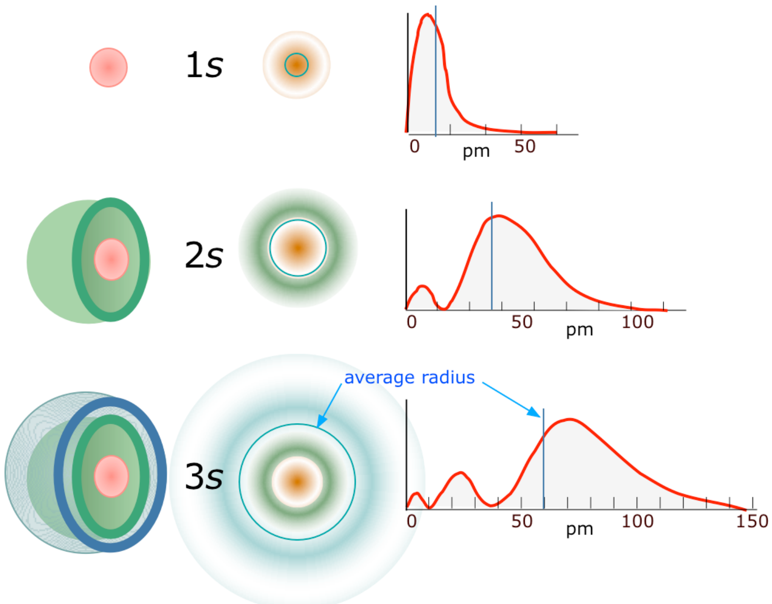
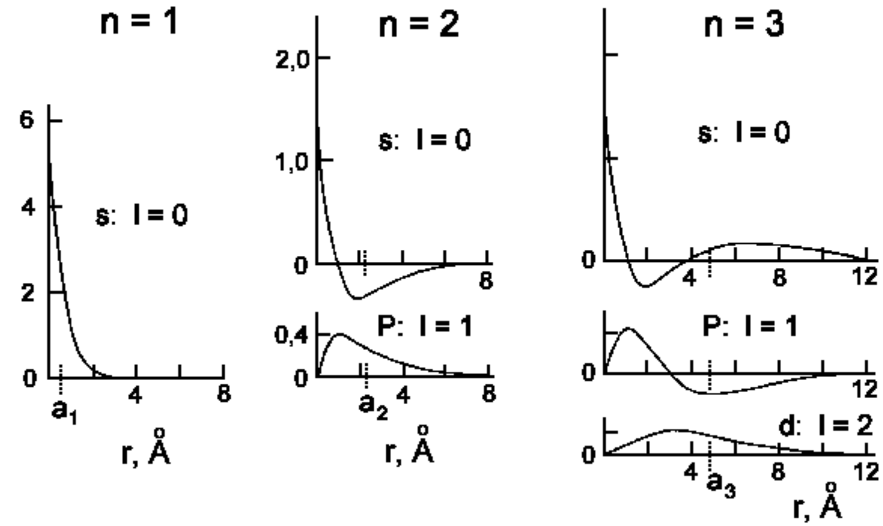
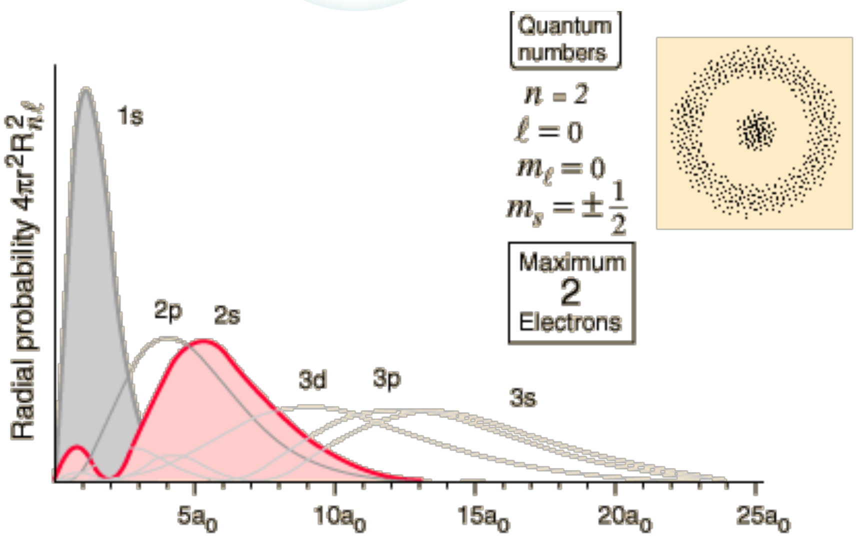
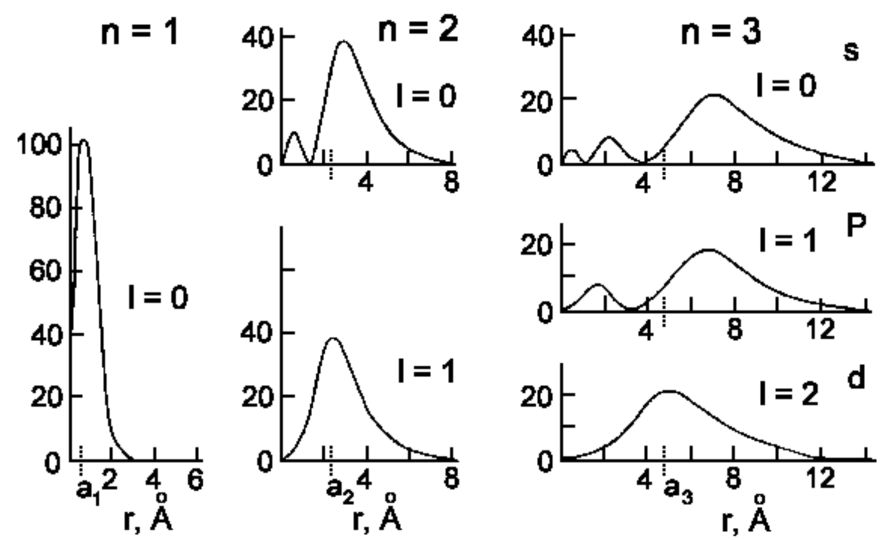
Wave functions

- Shells
- Orthogonality



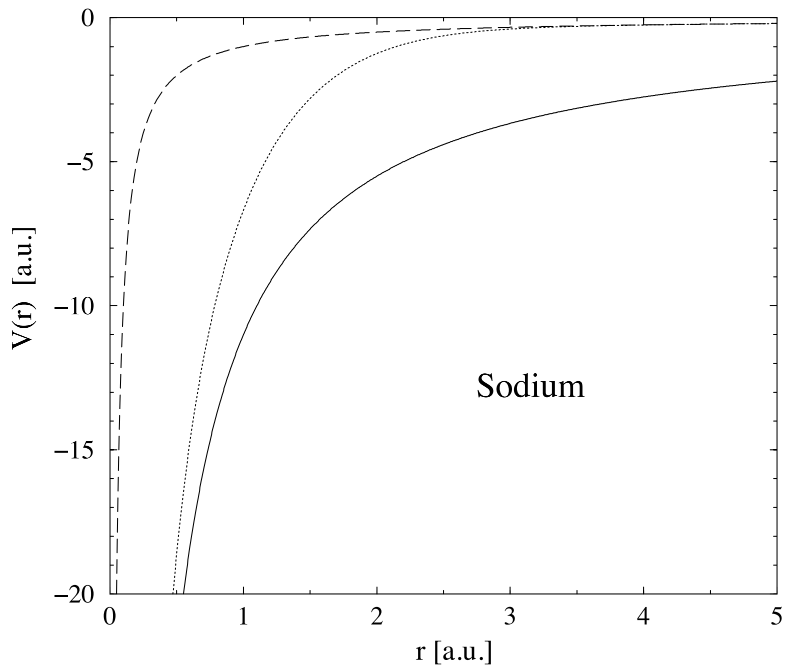






Effect of other electrons in neutral atoms

- Consider effect of electrons in closed shells for neutral Na
- large distances: nuclear charge screened to 1
- close to the nucleus: electron "sees" all 11 protons
- approximately:



- lifts H-like degeneracy: $\varepsilon_{2s} < \varepsilon_{2p}$

$$\varepsilon_{3s} < \varepsilon_{3p} < \varepsilon_{3d}$$

- "Far away" orbits: still hydrogen-like!

Example: Na

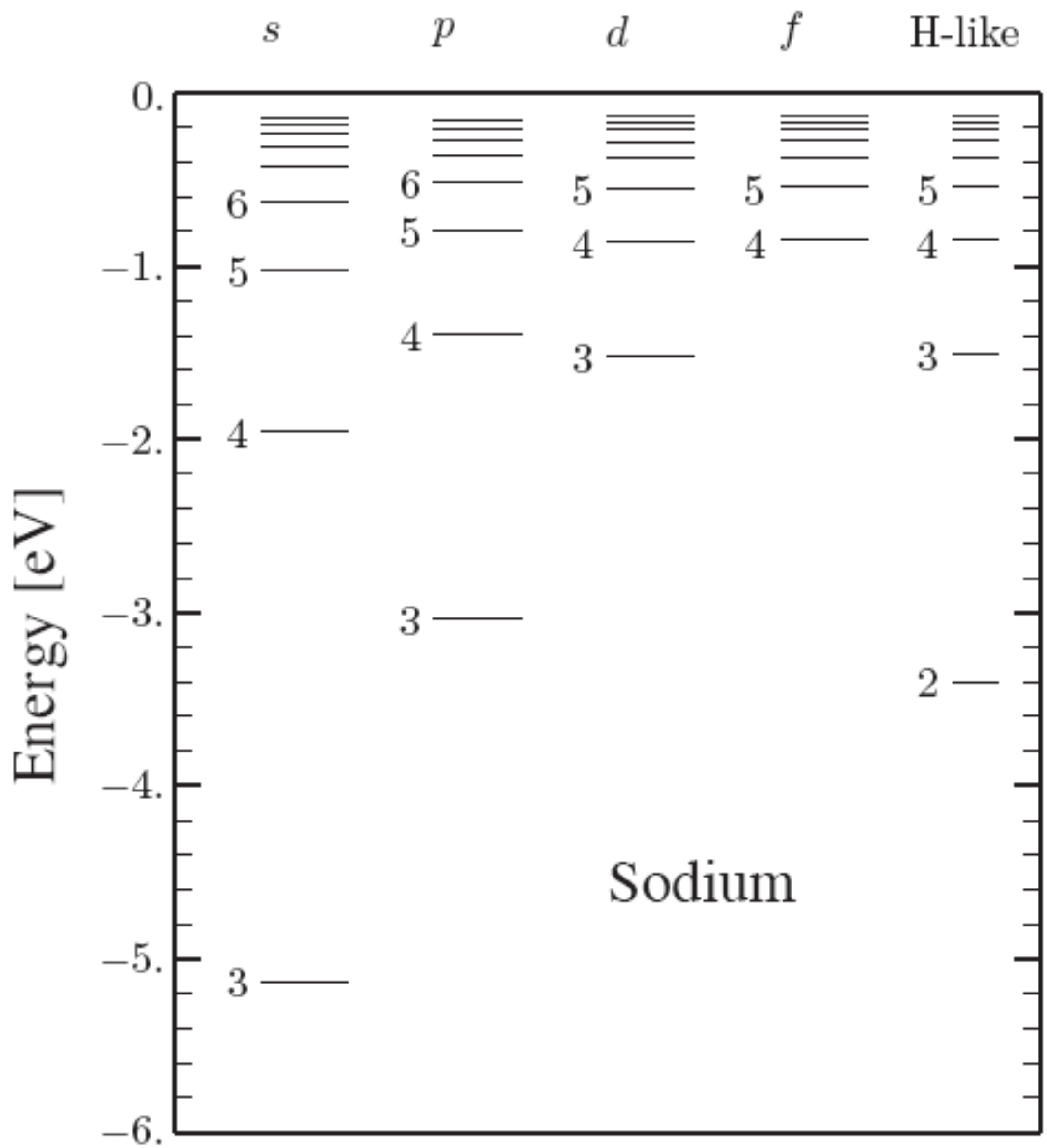
- Fill the lowest shells
- Use schematic potential

$$H_0 \left| n\ell m_\ell m_s \right\rangle = \varepsilon_{n\ell} \left| n\ell m_\ell m_s \right\rangle$$

- Ground state: fill lowest orbits according to Pauli

$$\left|300m_s, 211\tfrac{1}{2}, 211-\tfrac{1}{2}, ..., 100\tfrac{1}{2}, 100-\tfrac{1}{2}\right\rangle \equiv \left|\Phi_0(\mathrm{Na})\right\rangle$$

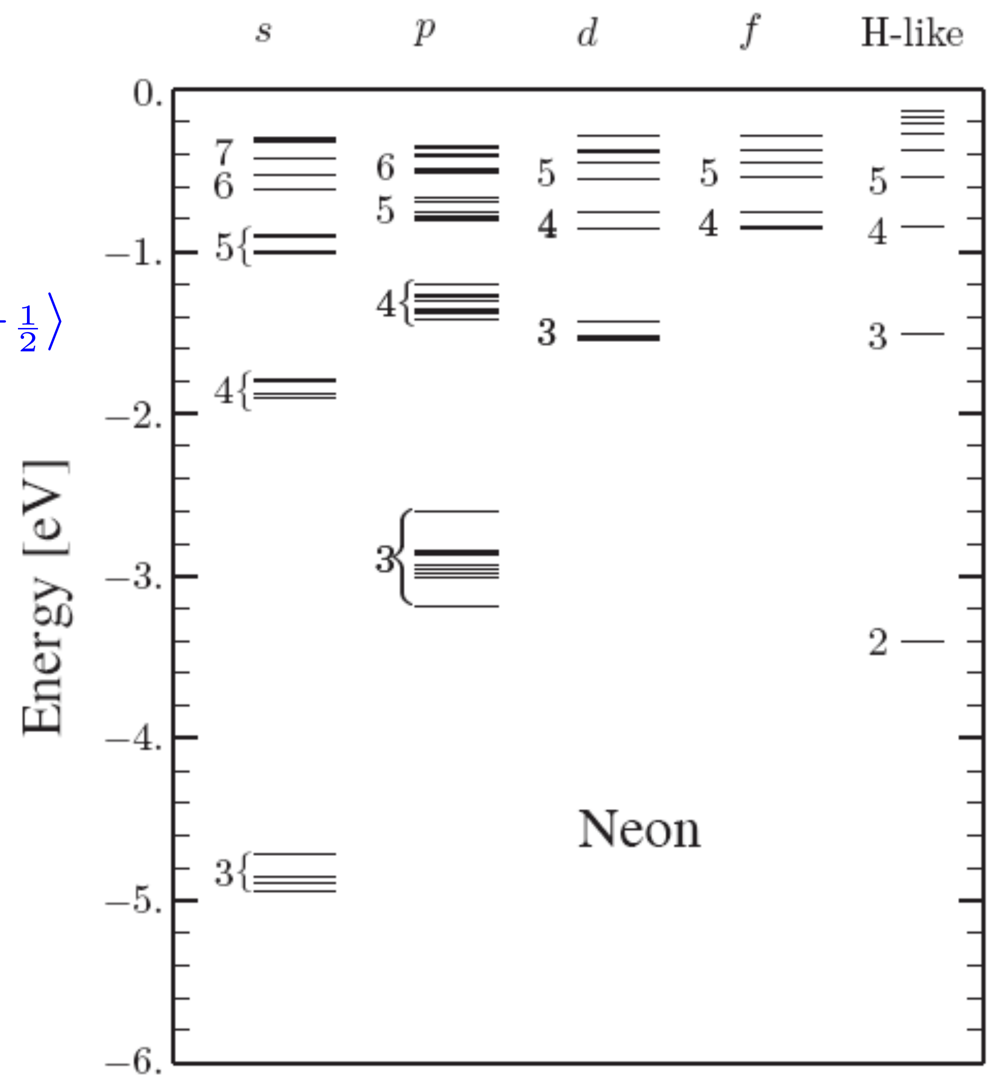
- Excited states?



Closed-shell atoms

- Neon
- Ground state

$$|\Phi_0(\mathrm{Ne})\rangle = |211\tfrac{1}{2}, 211-\tfrac{1}{2}, ..., 100\tfrac{1}{2}, 100-\tfrac{1}{2}\rangle$$

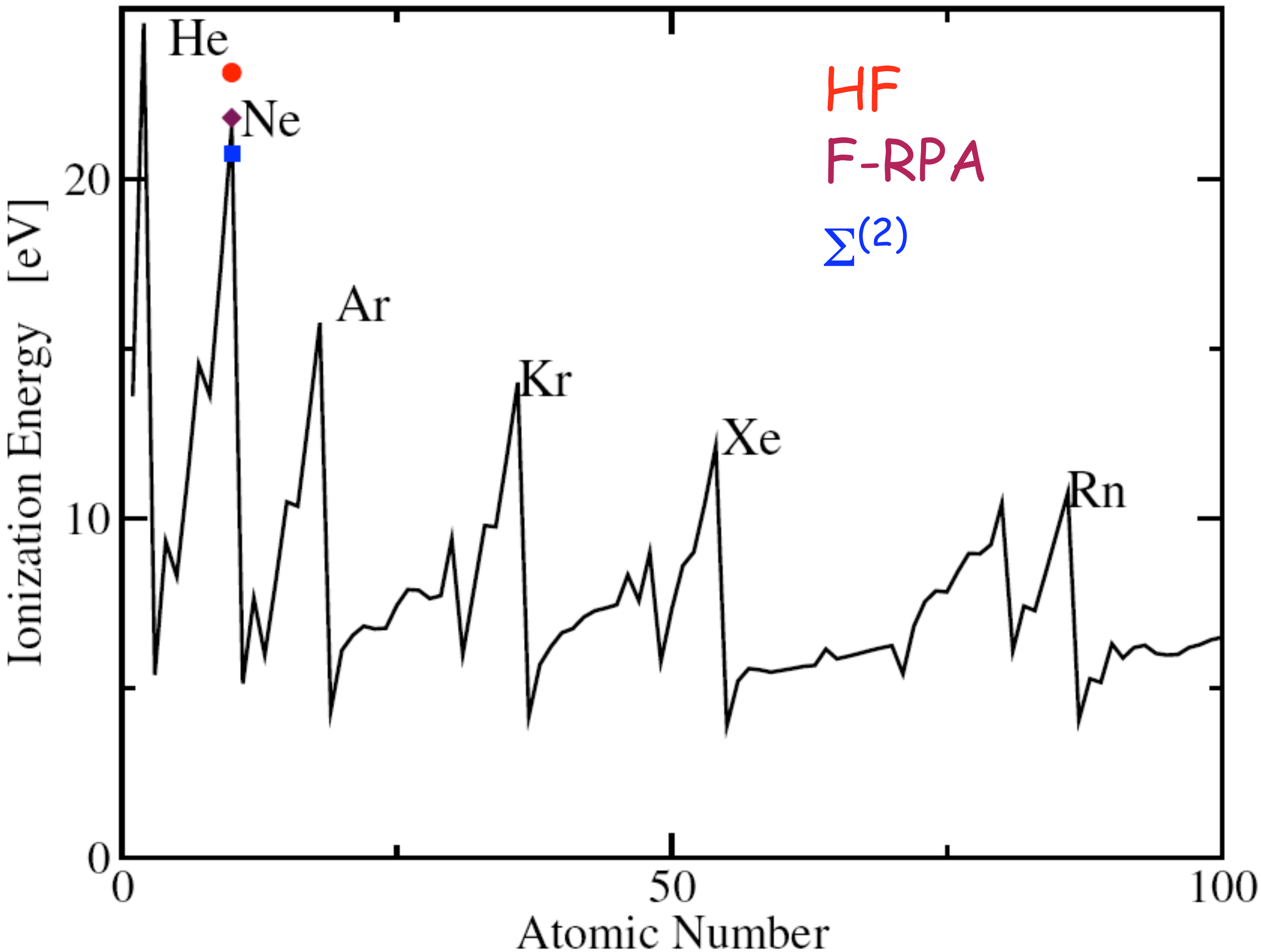


- Excited states

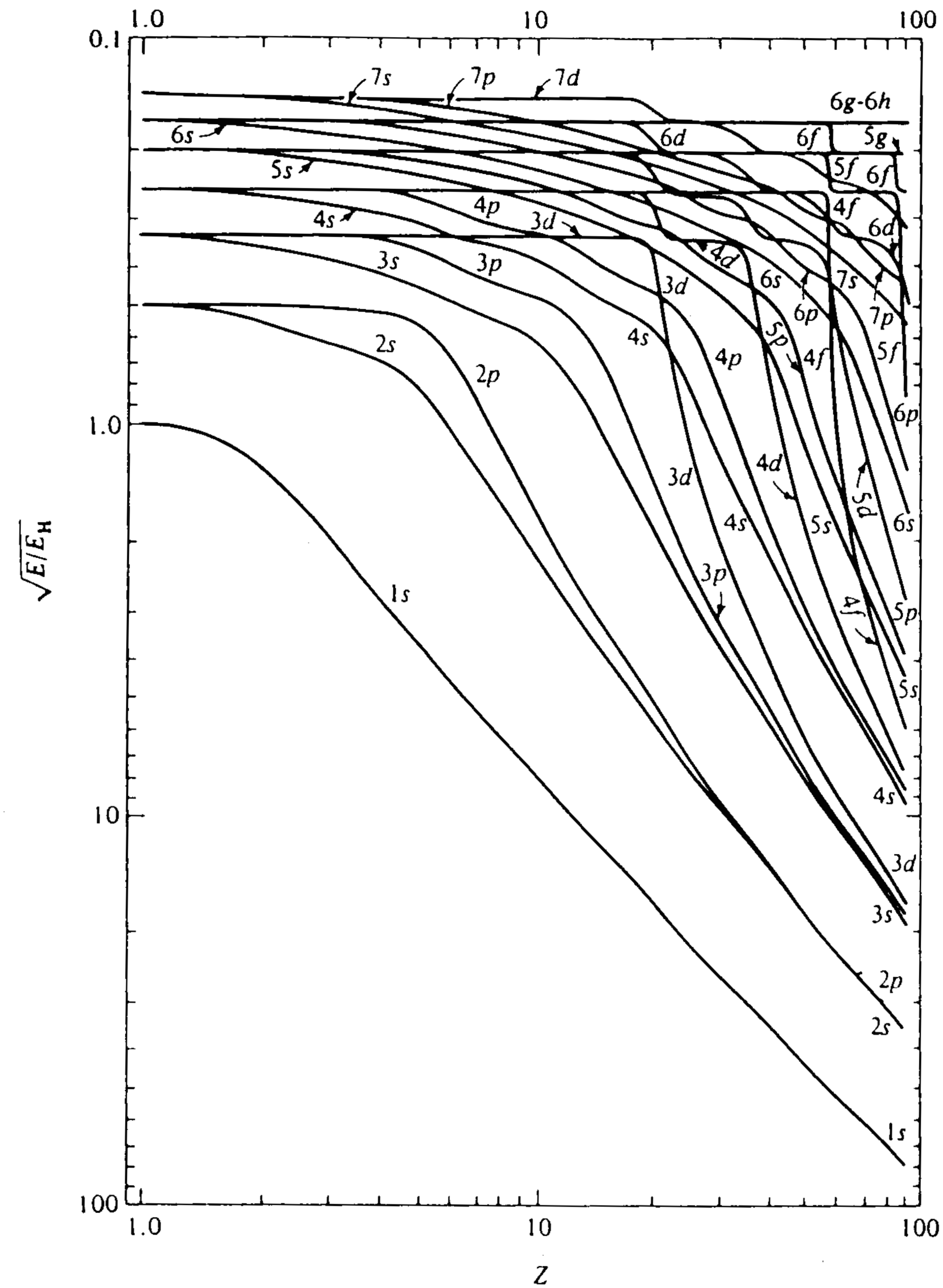
$$|n\ell\ (2p)^{-1}\rangle = a^\dagger_{n\ell} a_{2p}\, |\Phi_0(\mathrm{Ne})\rangle$$

- operators: see later
- Note the H-like states
- Splitting?
- Basic shell structure of atoms understood ⇒ IPM

Periodic table



Level sequence (approximately)



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 $\quad p = \sqrt{\boldsymbol{p} \cdot \boldsymbol{p}} \quad$ before $\quad r = \sqrt{\boldsymbol{r} \cdot \boldsymbol{r}}$

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

- Hamiltonian $\quad H = \dfrac{\boldsymbol{p}^2}{2m} - \dfrac{\hbar^2}{ma_0}\dfrac{1}{r}$

- 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 $H\left|E\ell m\right\rangle = E\left|E\ell m\right\rangle$

  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 $\Lambda\left|E\ell m\right\rangle = \dfrac{4\hbar^4}{a_0^2}\left|E\ell m\right\rangle$
- 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 $\Lambda_\ell = P_{\ell\pm 1}^\mp P_\ell^\pm - 4\hbar^2\left(\ell + \frac{1}{2} \pm \frac{1}{2}\right)^2 2mE$
- 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

$$P_\ell^\pm\left|E\ell\right\rangle = p_{E\ell}^\pm\left|E\ell\pm1\right\rangle$$

More development

- Normalization

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

- For bound states factor must break off for

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

- 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 $P^{\pm}_{\ell}\left|E\ell\right\rangle = p^{\pm}_{E\ell}\left|E\ell\pm 1\right\rangle$

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

- insert E and note phase choice!

Differential equation in momentum space

- Final result

$$\left(p^2+\frac{\hbar^2}{a_0^2n^2}\right)\frac{d}{dp}\langle p|n\ell\rangle+\left\{\left[\pm\left(\ell+\frac{1}{2}\pm\frac{1}{2}\right)+3\right]p+\frac{\hbar^2}{a_0^2n^2}\frac{1}{p}\left[1\mp\left(\ell+\frac{1}{2}\pm\frac{1}{2}\right)\right]\right\}\langle p|n\ell\rangle=$$
$$\frac{2\hbar}{a_0}\left[1-\frac{\left(\ell+\frac{1}{2}\pm\frac{1}{2}\right)^2}{n^2}\right]^{1/2}\langle p|n\ell\pm1\rangle$$

- 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

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

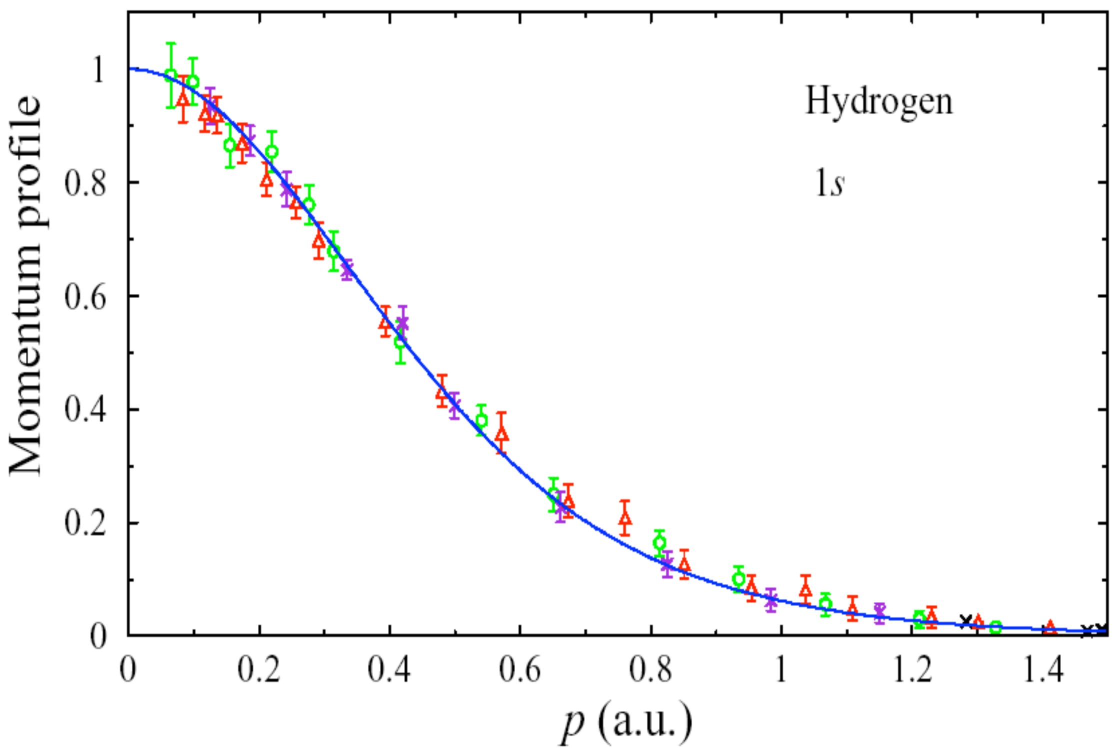
Direct knockout reactions

- 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

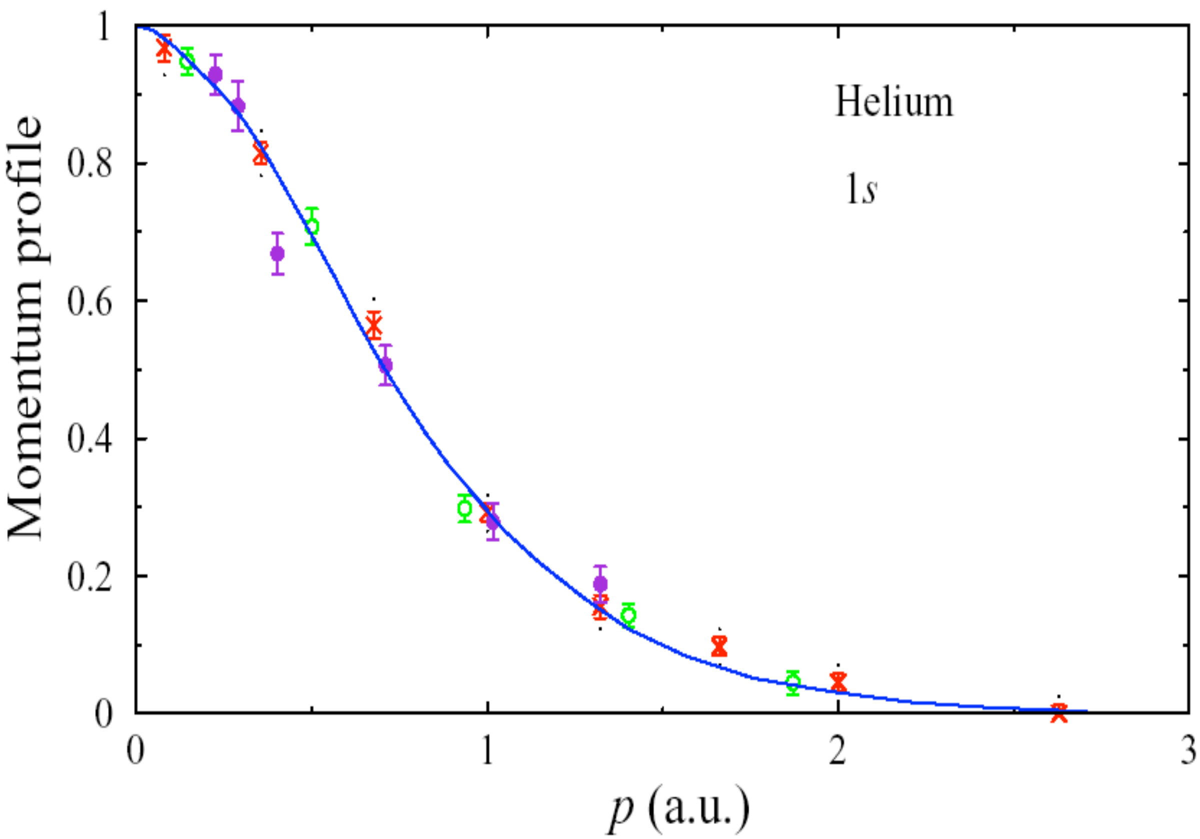
$$\langle 0 | \, a_{\boldsymbol{p}} \, | n=1, \ell=0 \rangle = \langle \boldsymbol{p} \, | n=1, \ell=0 \rangle = \phi_{1s}(\boldsymbol{p})$$



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

Helium

- IPM description is very successful
- Closed-shell configuration $1s^2$
- Reaction more complicated than for Hydrogen
- DWIA (distorted wave impulse approximation)



$$S = \int d\boldsymbol{p} \, \left| \langle \Psi_n^{N-1} | \, a_{\boldsymbol{p}} \, | \Psi_0^N \rangle \right|^2$$

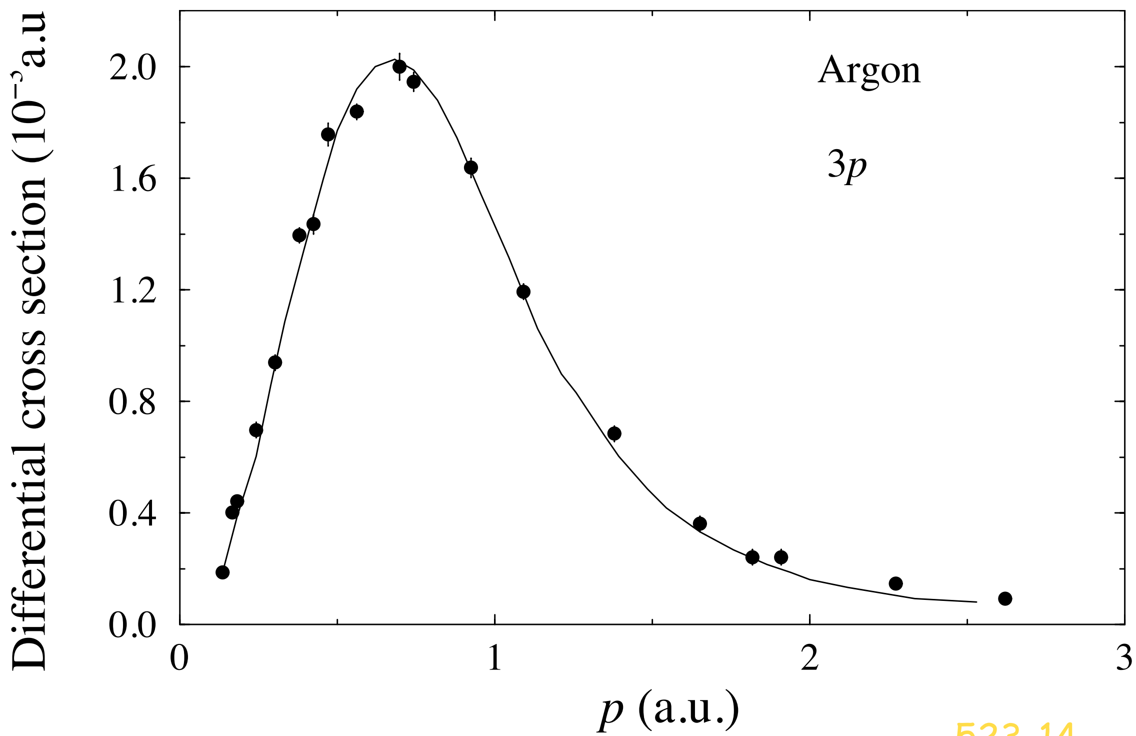
agreement with IPM!

$\rightarrow 1$

Phys. Rev. A8, 2494 (1973)

Other closed-shell atoms

- Spectroscopic factor becomes less than 1
- Neon $2p$ removal: S = 0.92 with two fragments each 0.04
- IPM not the whole story: fragmentation of sp strength
- Summed strength: like IPM
- IPM wave functions still excellent
- Example: Argon $3p$ S = 0.95
- Rest in 3 small fragments



Fragmentation in atoms

- ~All the strength remains below (above) the Fermi energy in closed-shell atoms
- Fragmentation can be interpreted in terms of mixing between

$$a_\alpha \left|\Phi_0^N\right\rangle$$

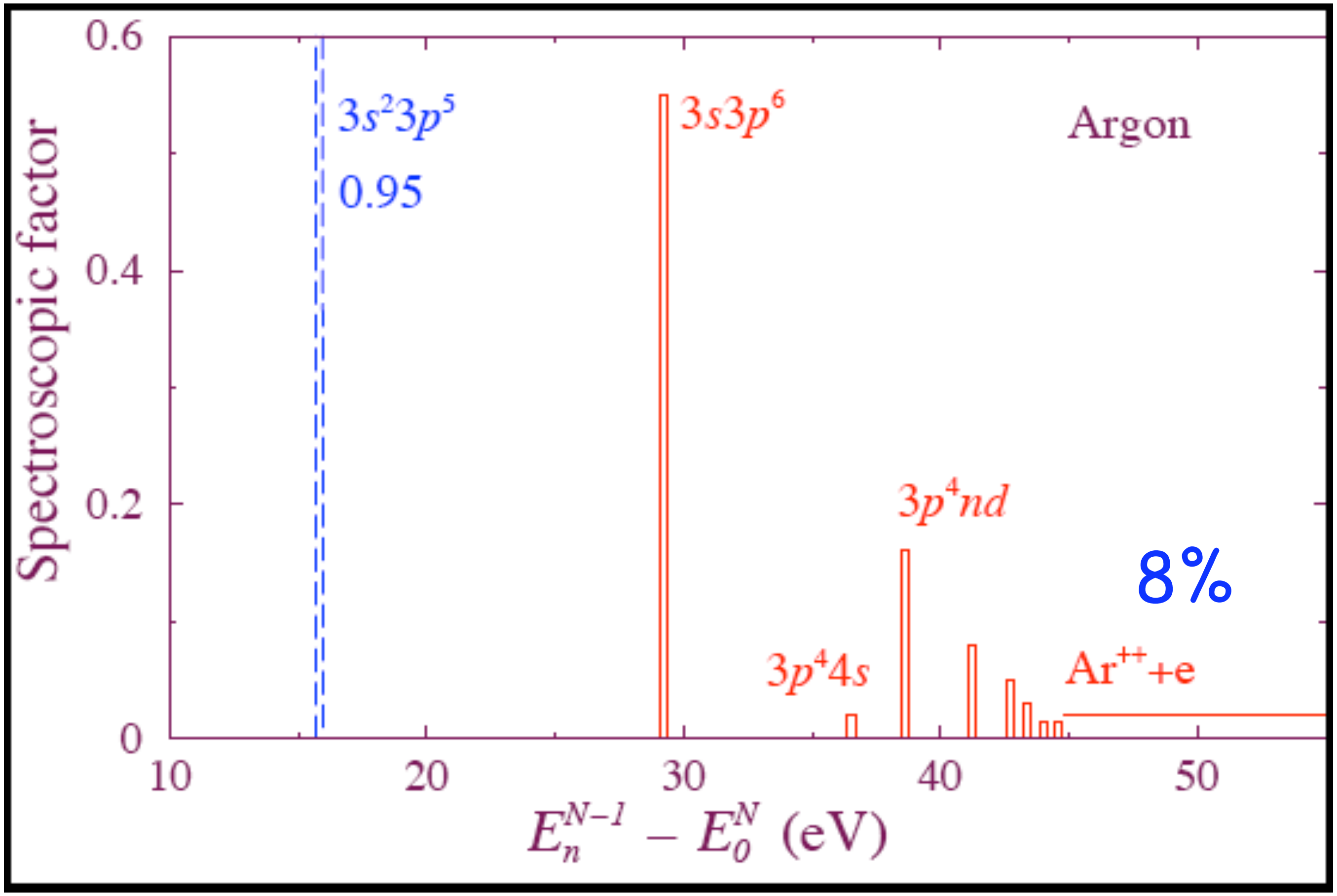
- and

$$a_\beta a_\gamma a_\delta^\dagger \left|\Phi_0^N\right\rangle$$

- with the same "global" quantum numbers
- Example: Argon ground state $\left|\Phi_0^N\right\rangle = \left|(3s)^2(3p)^6(2s)^2(2p)^6(1s)^2\right\rangle$
- Ar$^+$ ground state $\left|(3p)^{-1}\right\rangle = a_{3p}\left|\Phi_0^N\right\rangle = \left|(3s)^2(3p)^5(2s)^2(2p)^6(1s)^2\right\rangle$
- excited state $\left|(3s)^{-1}\right\rangle = a_{3s}\left|\Phi_0^N\right\rangle = \left|(3s)^1(3p)^6(2s)^2(2p)^6(1s)^2\right\rangle$
- also $\left|(3p)^{-2}4s\right\rangle = a_{3p}a_{3p}a_{4s}^\dagger\left|\Phi_0^N\right\rangle = \left|(4s)^1(3s)^2(3p)^4(2s)^2(2p)^6(1s)^2\right\rangle$
- and $\left|(3p)^{-2}nd\right\rangle = a_{3p}a_{3p}a_{nd}^\dagger\left|\Phi_0^N\right\rangle = \left|(nd)^1(3s)^2(3p)^4(2s)^2(2p)^6(1s)^2\right\rangle$

Argon spectroscopic factors

- s strength also in the continuum: $Ar^{++} + e$
- note vertical scale
- red bars: 3s fragments exhibit substantial fragmentation



(e,e′p) data for nuclei

- Requires DWIA
- Distorted waves required to describe elastic proton scattering at the energy of the ejected proton
- Consistent description requires that cross section at different energy for the outgoing proton is changed accordingly
- Requires substantial beam energy and momentum transfer
- Initiated at Saclay and perfected at NIKHEF, Amsterdam
- Also done at Mainz and currently at Jefferson Lab, VA
- Momentum dependence of cross section dominated by the corresponding sp wave function of the nucleon before it is removed

Inclusion of SO potential and magic numbers

- Sign of SO?

$$V_{\ell s}\left(\frac{\boldsymbol{\ell}\cdot\boldsymbol{s}}{\hbar^2}\right)r_0^2\frac{1}{r}\frac{d}{dr}f(r)$$

$$V_{\ell s} = -0.44V$$

- Consequence for

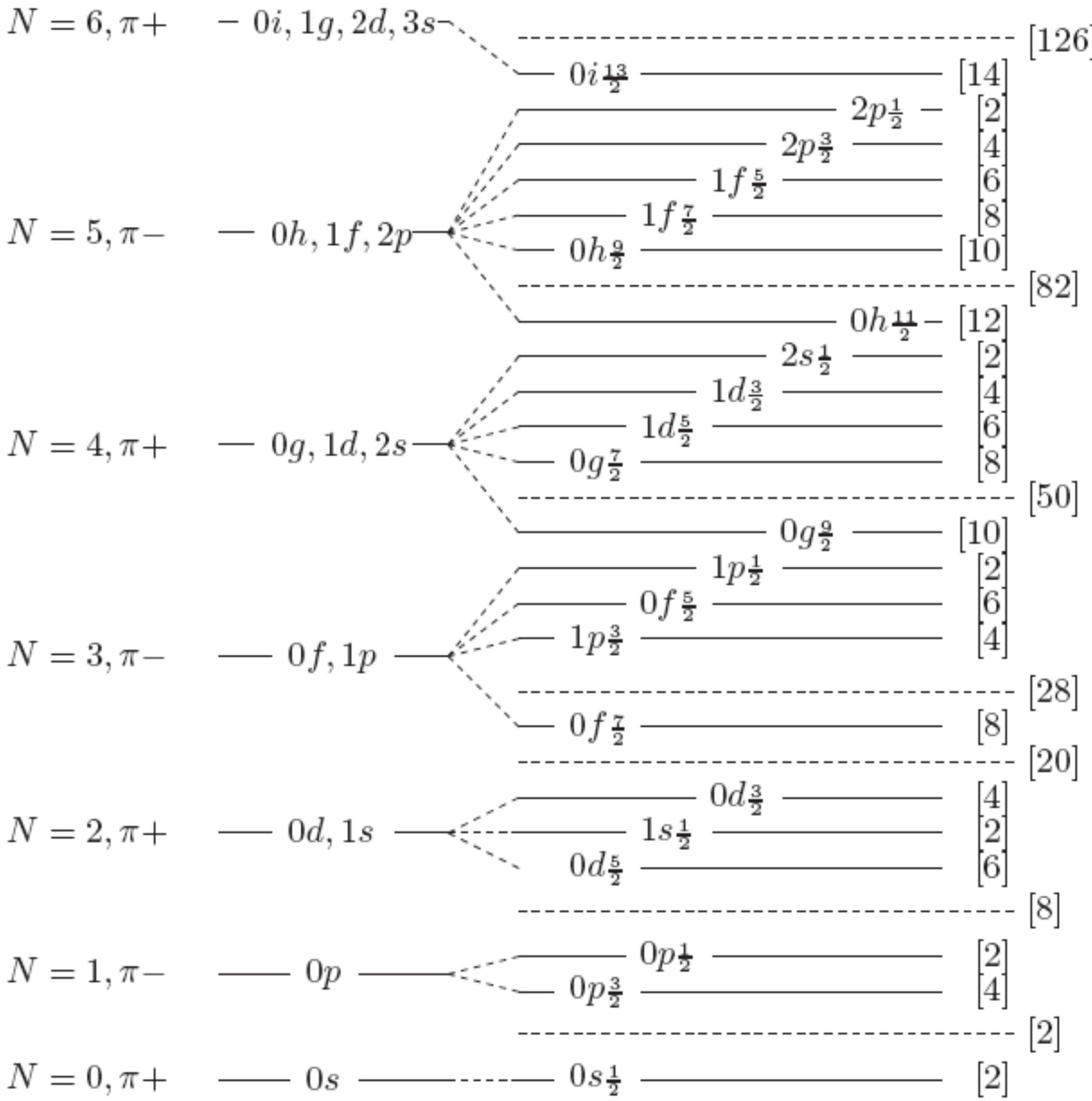
$$0f\tfrac{7}{2}$$

$$0g\tfrac{9}{2}$$

$$0h\tfrac{11}{2}$$

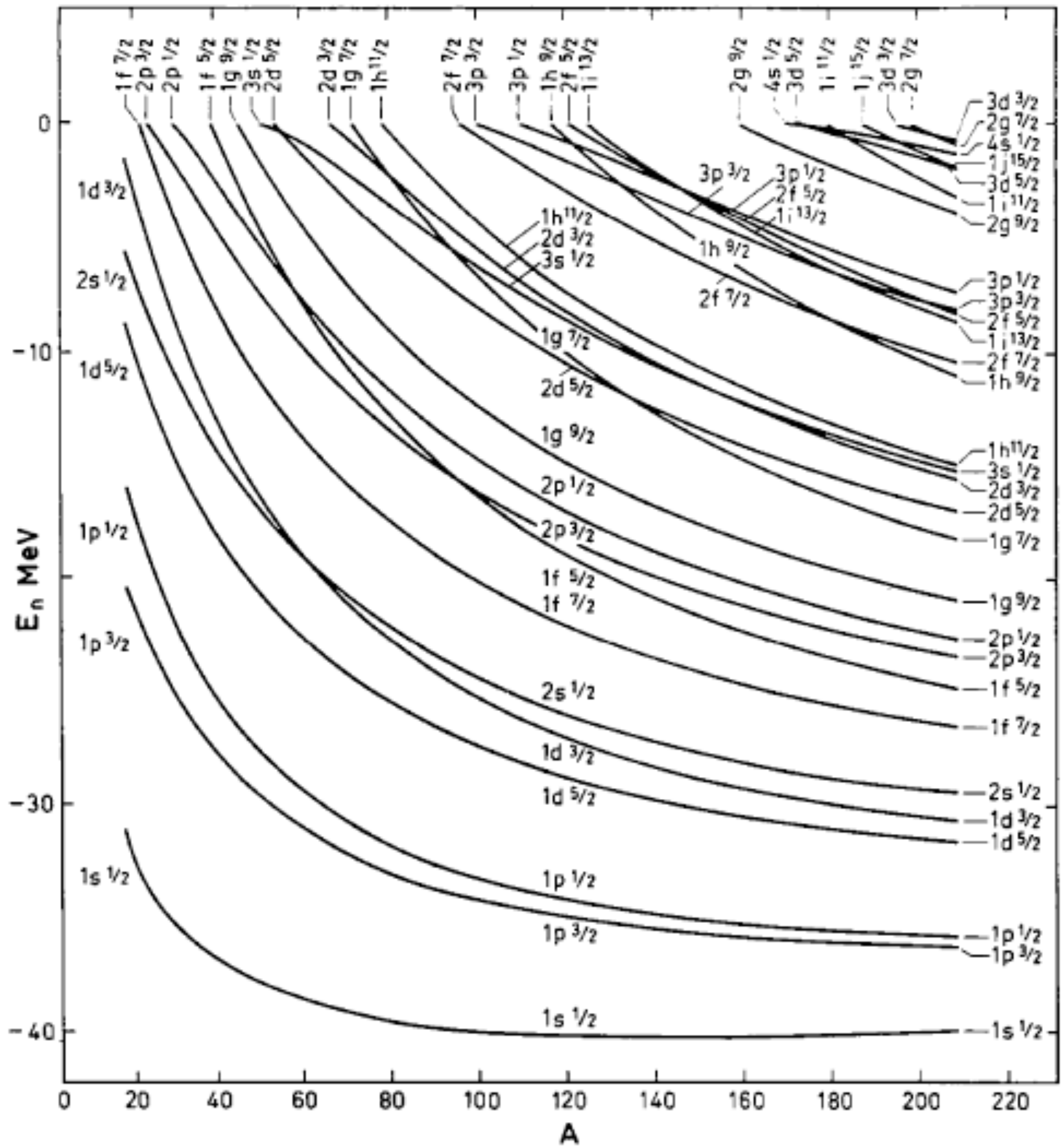
$$0i\tfrac{13}{2}$$

- Noticeably shifted
- Correct magic numbers!



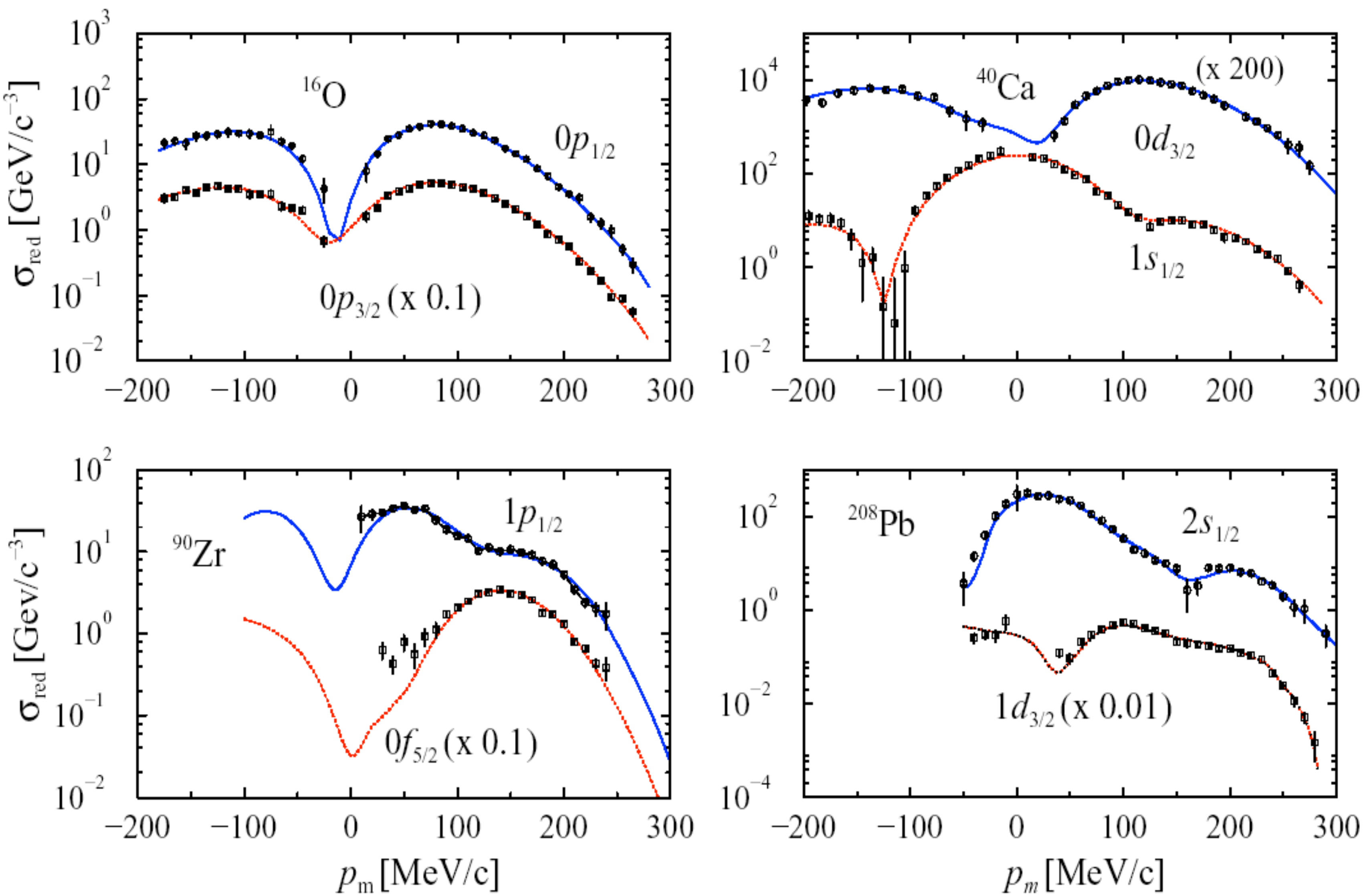
Neutron levels as a function of A

- Phenomenological!
- Calculated from Woods-Saxon plus spin-orbit



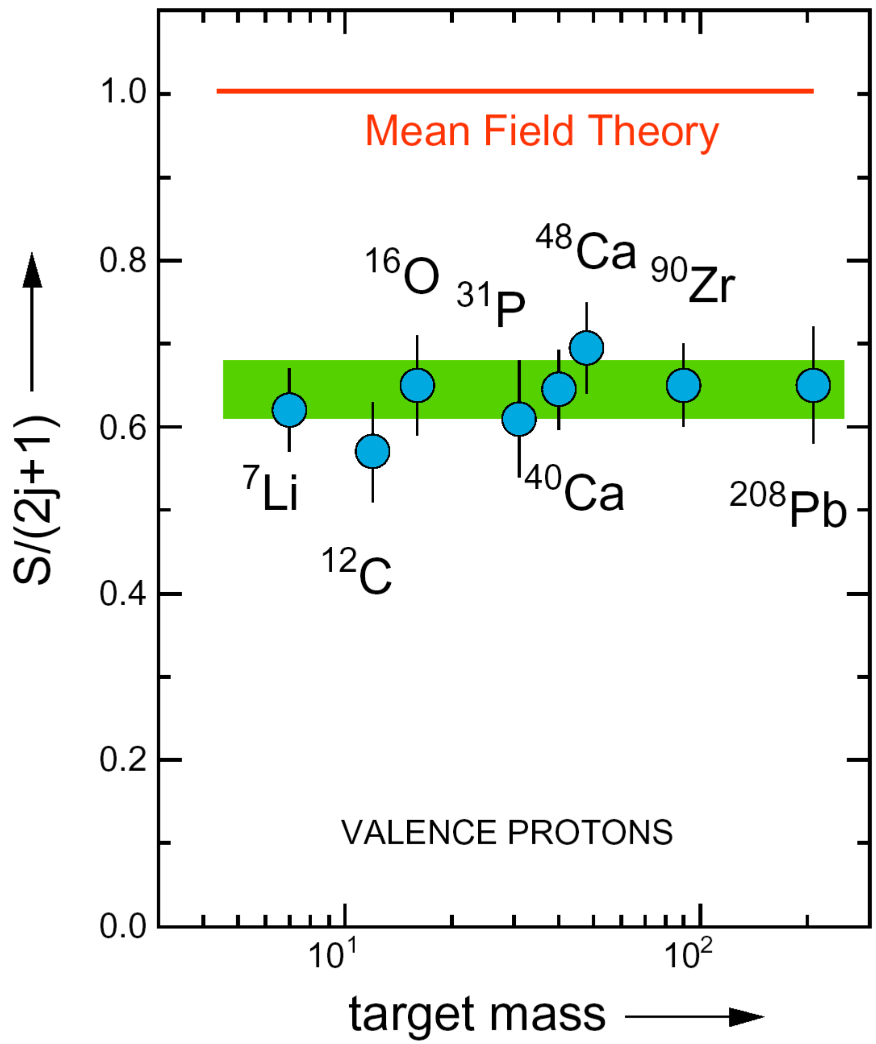
Momentum profiles for nucleon removal

- Closed-shell nuclei
- NIKHEF data, L. Lapikás, Nucl. Phys. A553, 297c (1993)



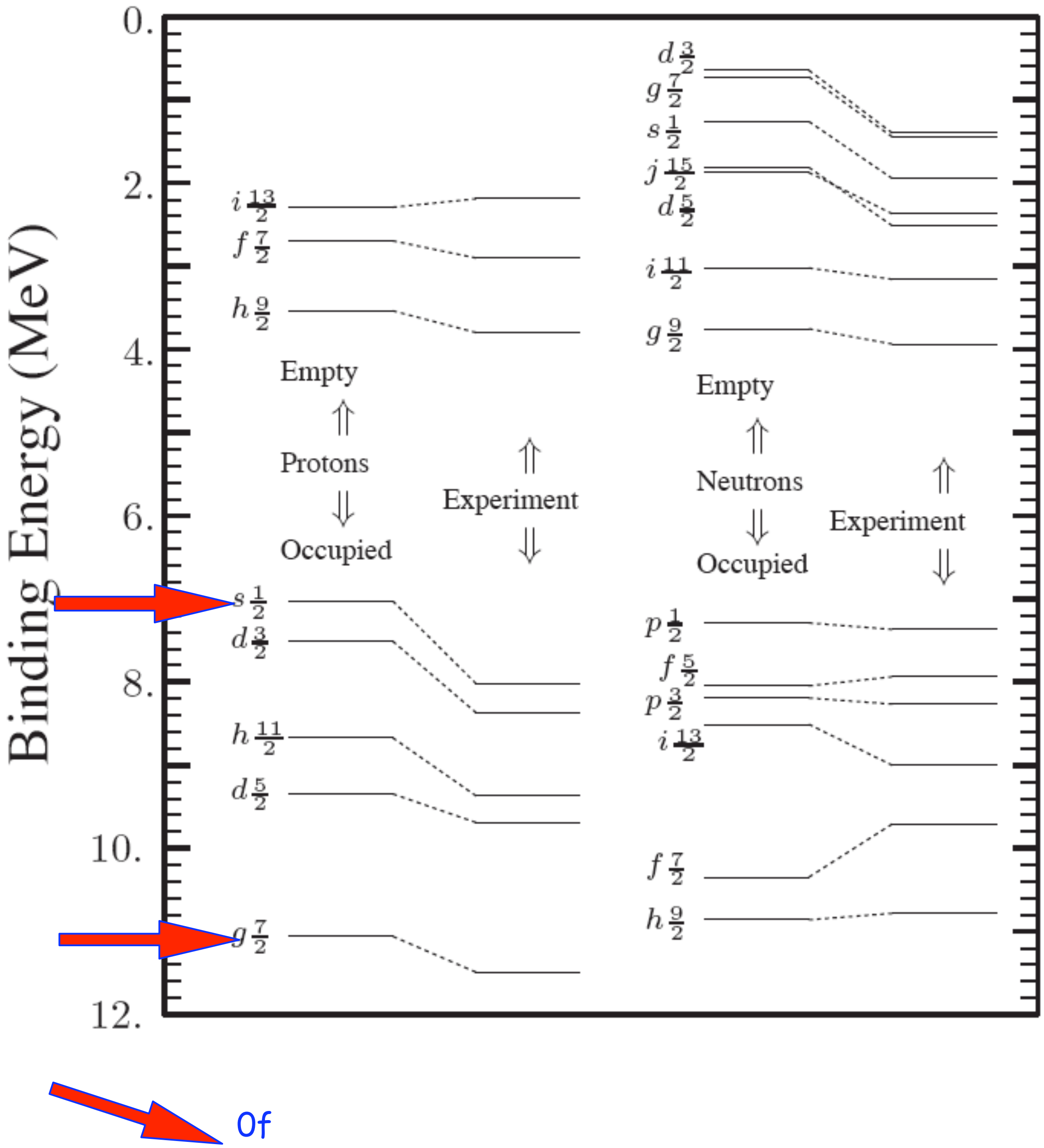
But...

- Spectroscopic factors substantially smaller than simple IPM



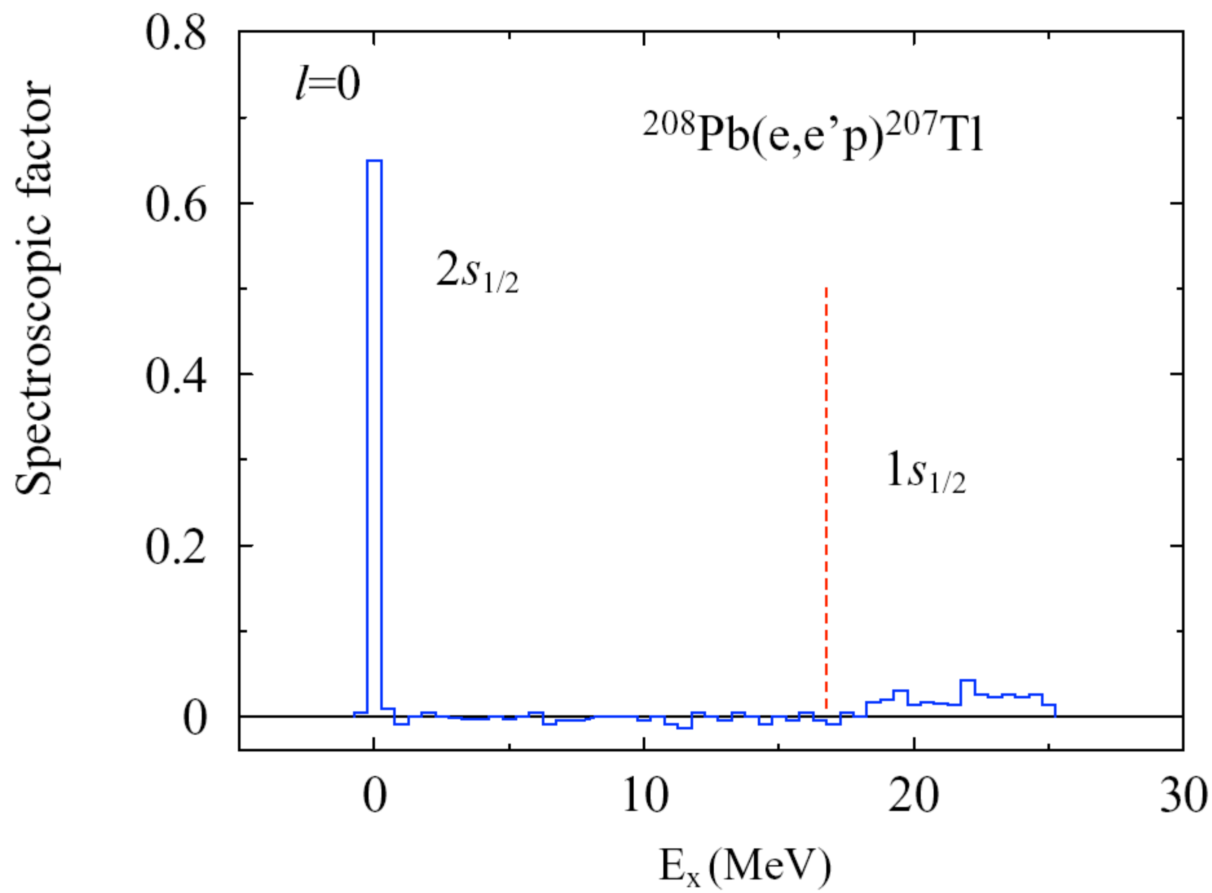
Remember

- ^{208}Pb sp levels



Fragmentation patterns

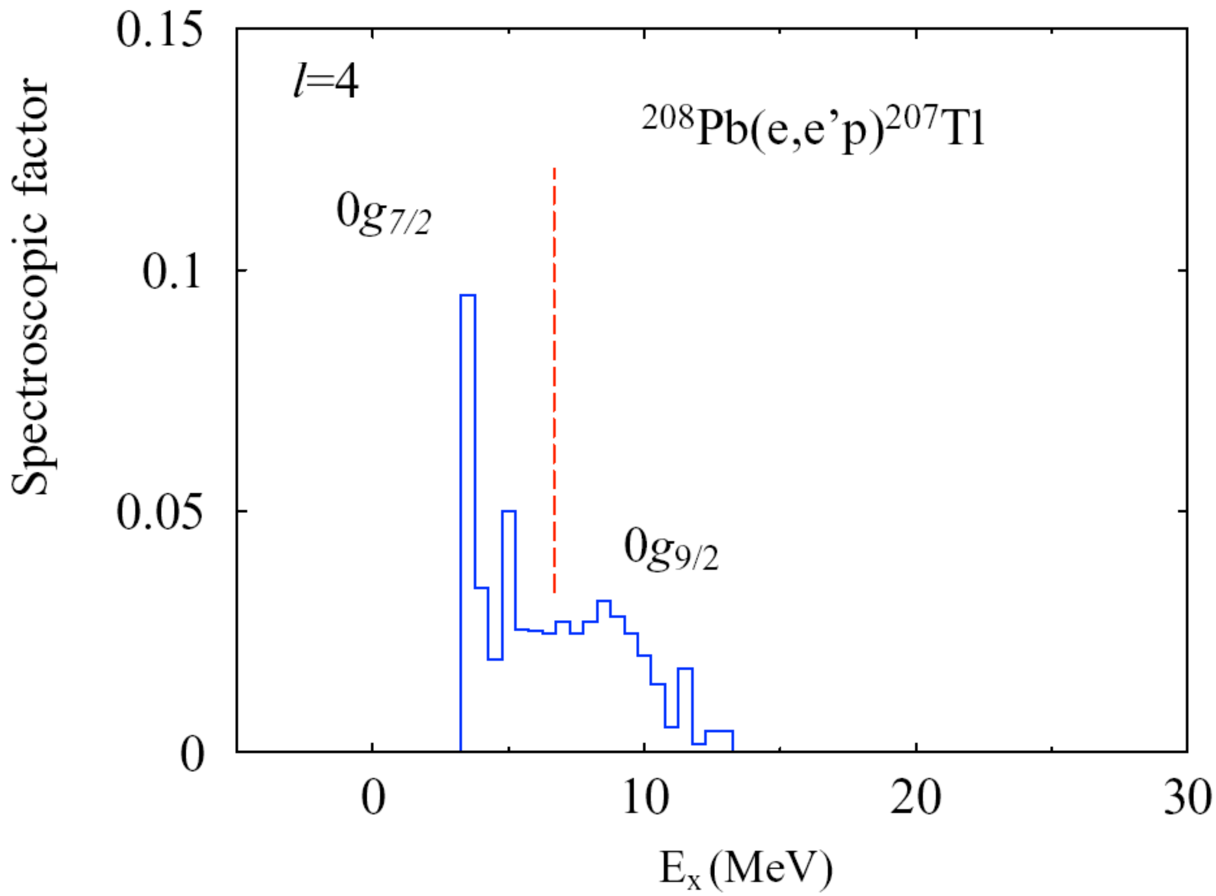
- ^{208}Pb(e,e′p) NIKHEF data: Quint thesis
- $S(2s_{1/2})=0.65$
- other data:
- $n(2s_{1/2})=0.75$



- very different from atoms

Fragmentation patterns

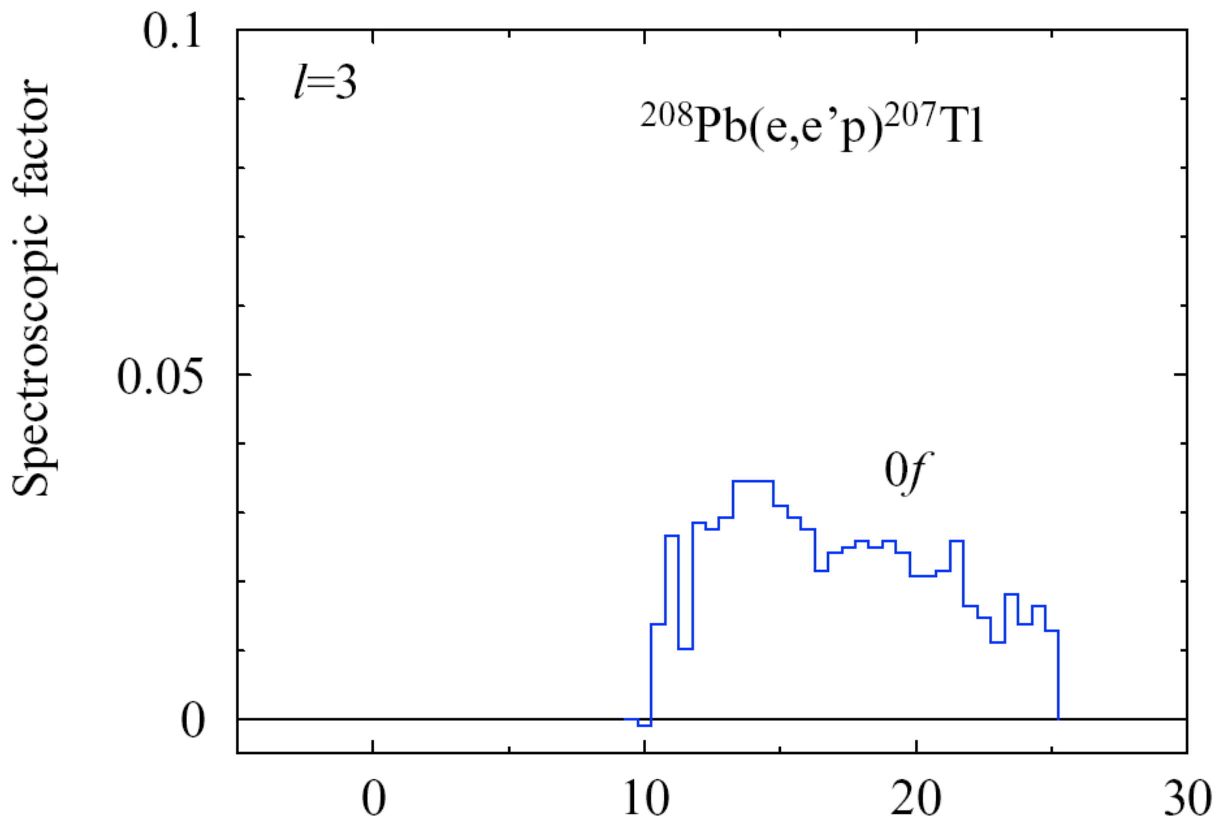
- ^{208}Pb(e,e′p) NIKHEF data: Quint thesis



- start of strong fragmentation
- also very different from atoms

Fragmentation patterns

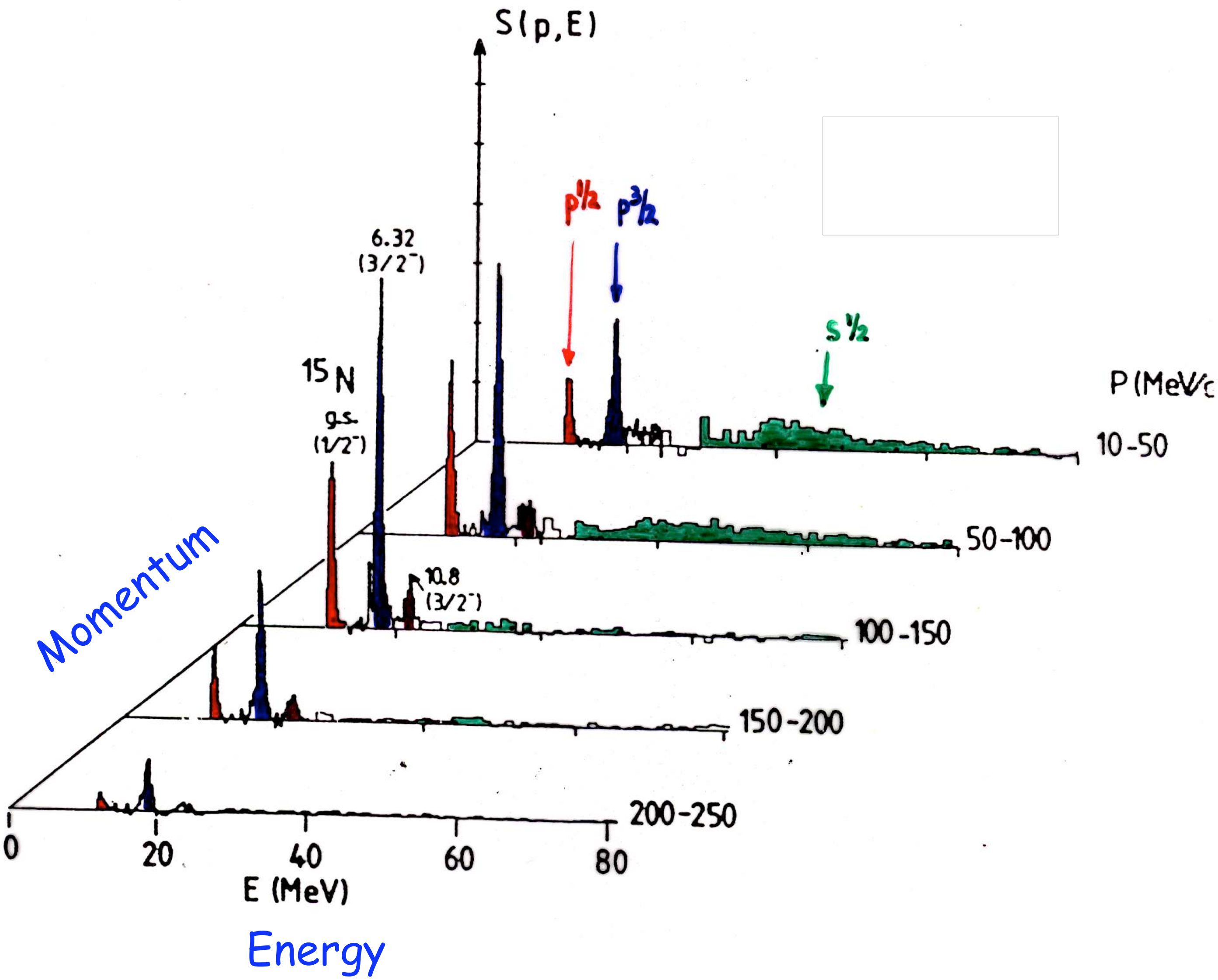
- ^{208}Pb(e,e′p) NIKHEF data: Quint thesis



- deeply bound states: strong fragmentation
- again different from atoms

^{16}O data from Saclay

- Simple interpretation!
- Mougey et al., Nucl. Phys. A335, 35 (1980)



Recent Pb experiment

- 100 MeV missing energy
- 270 MeV/c missing momentum
- complete IPM domain