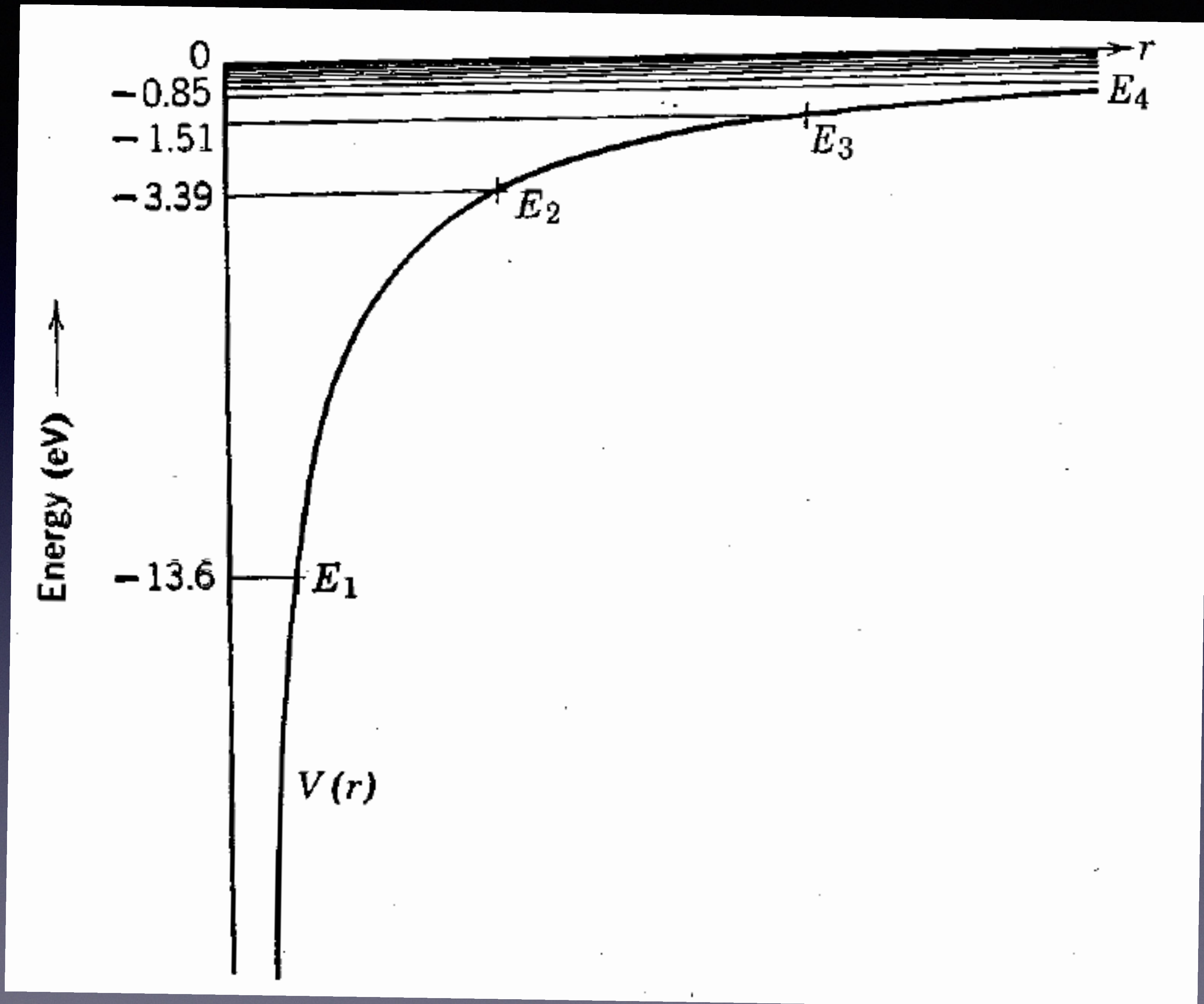


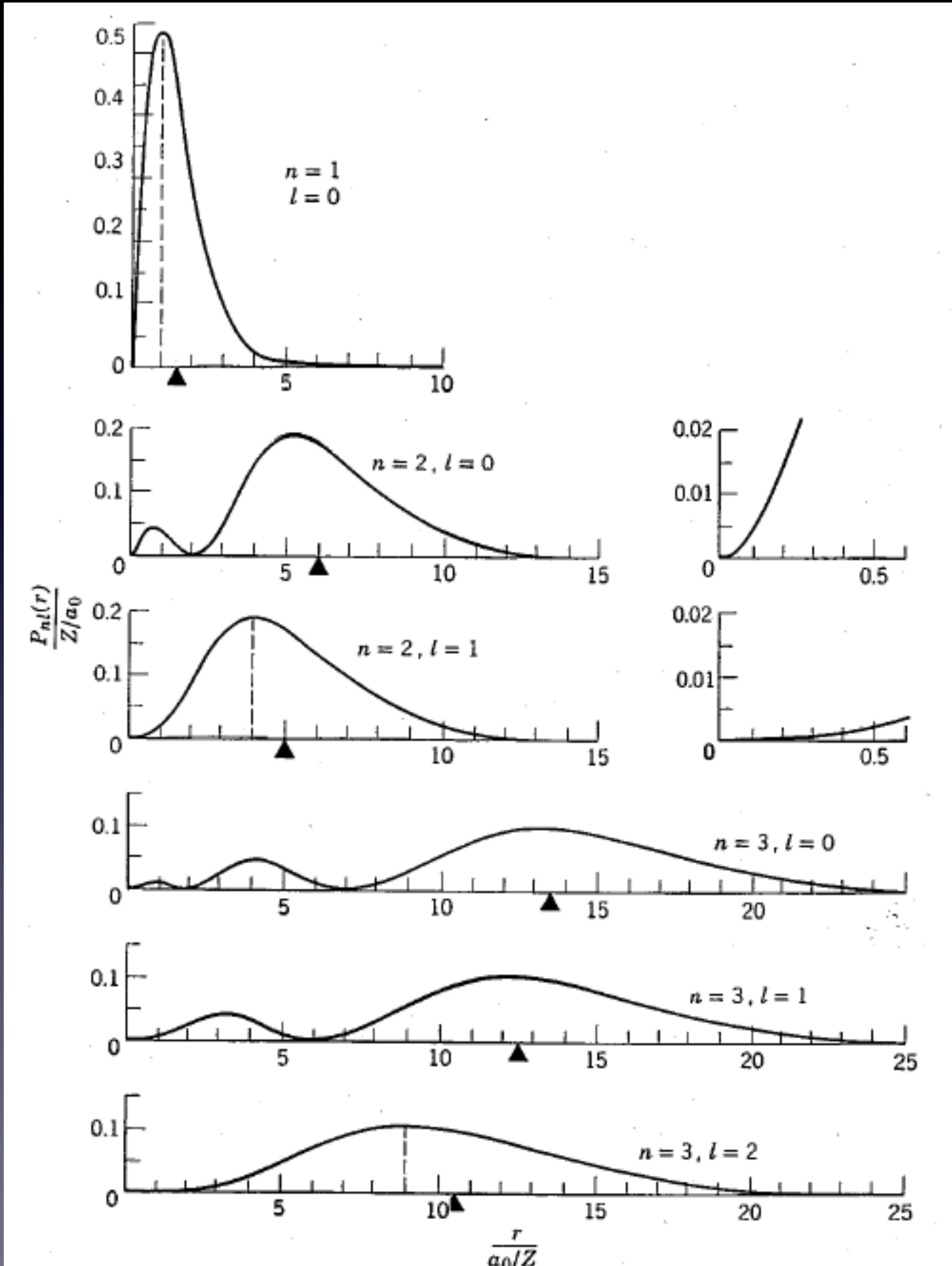
0
−0.85
−1.51
−3.39
−13.6
Energy (eV)
r
E4
E3
E2
E1
V(r)

Possible Values of l and m_l for $n = 1, 2, 3$

n	1	2		3		
l	0	0	1	0	1	2
m_l	0	0	$-1, 0, +1$	0	$-1, 0, +1$	$-2, -1, 0, +1, +2$
Number of degenerate eigenfunctions for each l	1	1	3	1	3	5
Number of degenerate eigenfunctions for each n	1	4		9		

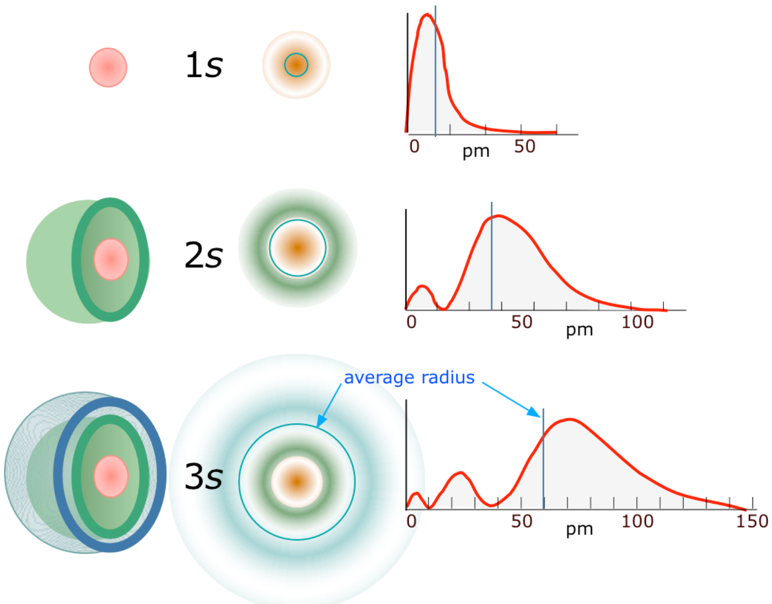
Some Eigenfunctions for the One-Electron Atom

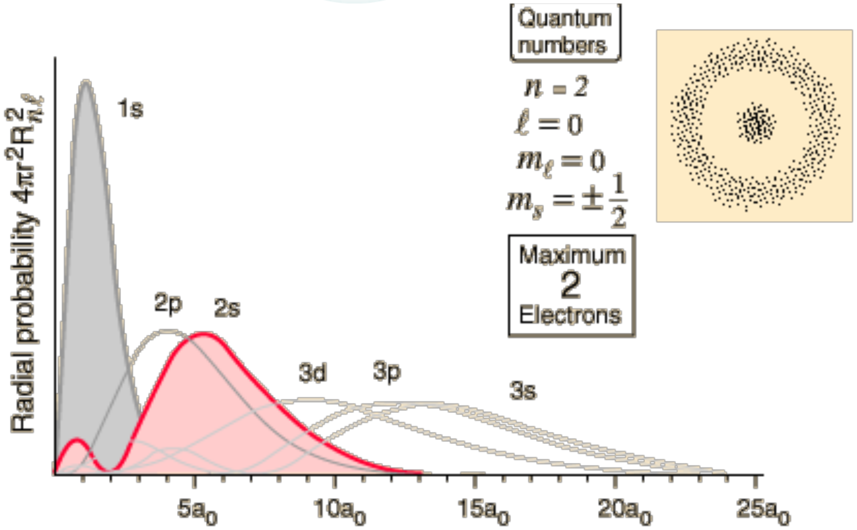
Quantum Numbers n	l	m_l	Eigenfunctions
1	0	0	$\psi_{100} = \frac{1}{\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2} e^{-Zr/a_0} = \underbrace{\left(\frac{Z}{a_0}\right)^{3/2} 2 e^{-Zr/a_0}}_{R_{10}} \underbrace{\frac{1}{\sqrt{4\pi}}}_{Y_{00}}$
2	0	0	$\psi_{200} = \frac{1}{4\sqrt{2\pi}}\left(\frac{Z}{a_0}\right)^{3/2}\left(2-\frac{Zr}{a_0}\right) e^{-Zr/2a_0} = \underbrace{\left(\frac{Z}{2a_0}\right)^{3/2}\left(2-\frac{Zr}{a_0}\right)e^{-Zr/2a_0}}_{R_{20}} \frac{1}{\sqrt{4\pi}}$
2	1	0	$\psi_{210} = \frac{1}{4\sqrt{2\pi}}\left(\frac{Z}{a_0}\right)^{3/2}\frac{Zr}{a_0} e^{-Zr/2a_0}\cos\theta = \underbrace{\left(\frac{Z}{2a_0}\right)^{3/2}\frac{Zr}{\sqrt{3}\,a_0} e^{-Zr/2a_0}}_{R_{21}} Y_{10}$
2	1	± 1	$\psi_{21\pm1} = \frac{1}{8\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2}\frac{Zr}{a_0} e^{-Zr/2a_0}\sin\theta\, e^{\pm i\varphi}$ ⋮
3	0	0	$\psi_{300} = \frac{1}{81\sqrt{3\pi}}\left(\frac{Z}{a_0}\right)^{3/2}\left(27-18\frac{Zr}{a_0}+2\frac{Z^2r^2}{a_0^2}\right) e^{-Zr/3a_0}$
3	1	0	$\psi_{310} = \frac{\sqrt{2}}{81\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2}\left(6-\frac{Zr}{a_0}\right)\frac{Zr}{a_0} e^{-Zr/3a_0}\cos\theta$
3	1	± 1	$\psi_{31\pm1} = \frac{1}{81\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2}\left(6-\frac{Zr}{a_0}\right)\frac{Zr}{a_0} e^{-Zr/3a_0}\sin\theta\, e^{\pm i\varphi}$
3	2	0	$\psi_{320} = \frac{1}{81\sqrt{6\pi}}\left(\frac{Z}{a_0}\right)^{3/2}\frac{Z^2r^2}{a_0^2} e^{-Zr/3a_0}(3\cos^2\theta - 1)$
3	2	± 1	$\psi_{32\pm1} = \frac{1}{81\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2}\frac{Z^2r^2}{a_0^2} e^{-Zr/3a_0}\sin\theta\cos\theta\, e^{\pm i\varphi}$
3	2	± 2	$\psi_{32\pm2} = \frac{1}{162\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2}\frac{Z^2r^2}{a_0^2} e^{-Zr/3a_0}\sin^2\theta\, e^{\pm 2i\varphi}$

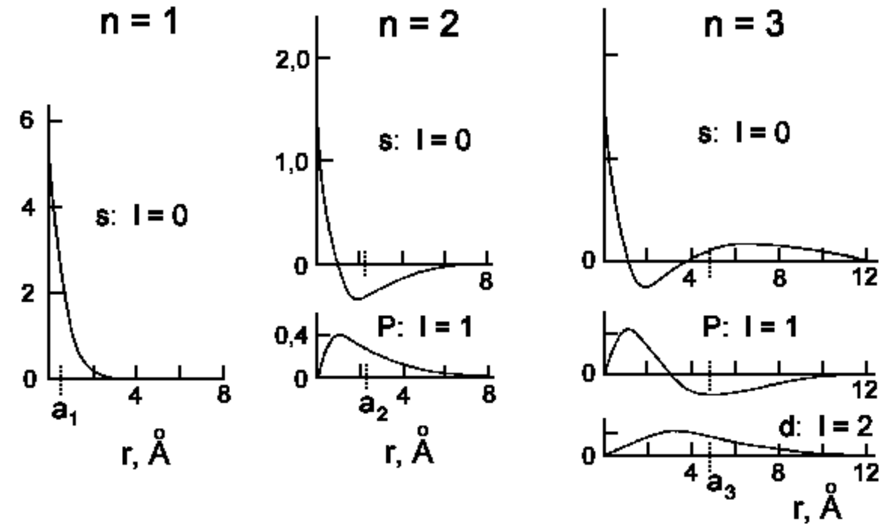

n = 1
l = 0
n = 2, l = 0
n = 2, l = 1
n = 3, l = 0
n = 3, l = 1
n = 3, l = 2
$\frac{P_{nl}(r)}{Z/a_0}$
$\frac{r}{a_0/Z}$

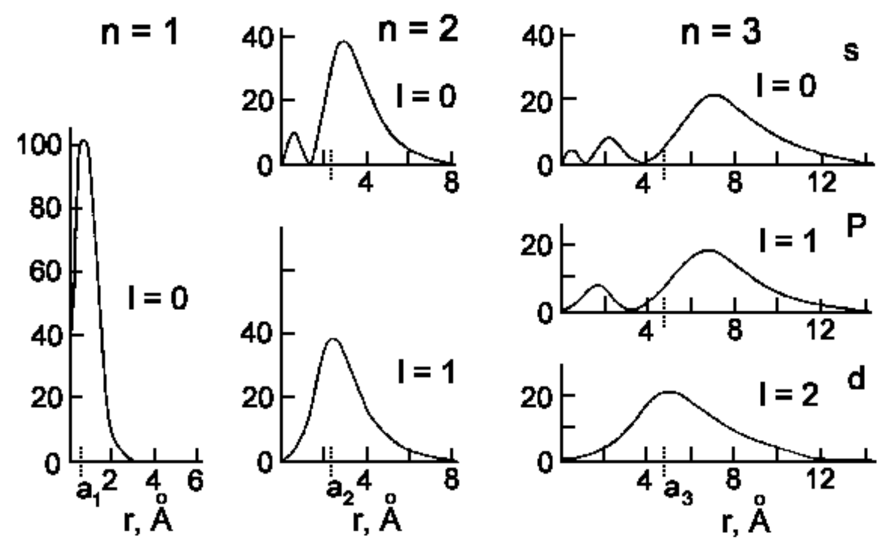
Wave functions

- Shells
- Orthogonality



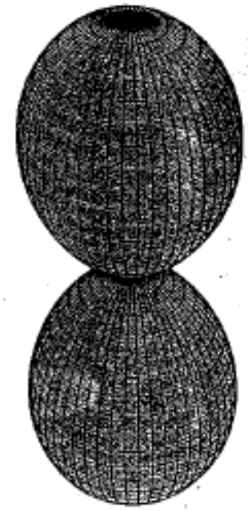






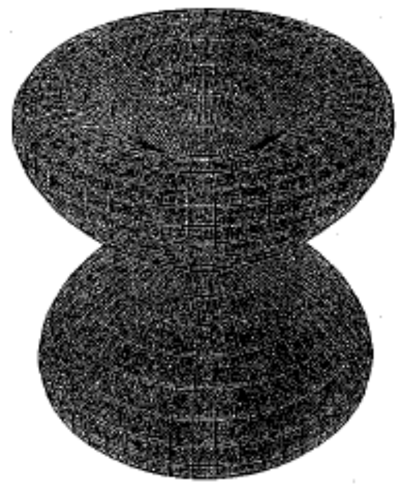
(a) $\ell = 0, m = 0$

(b1) $\ell = 1, m = \pm 1$



(b2) $\ell = 1, m = 0$

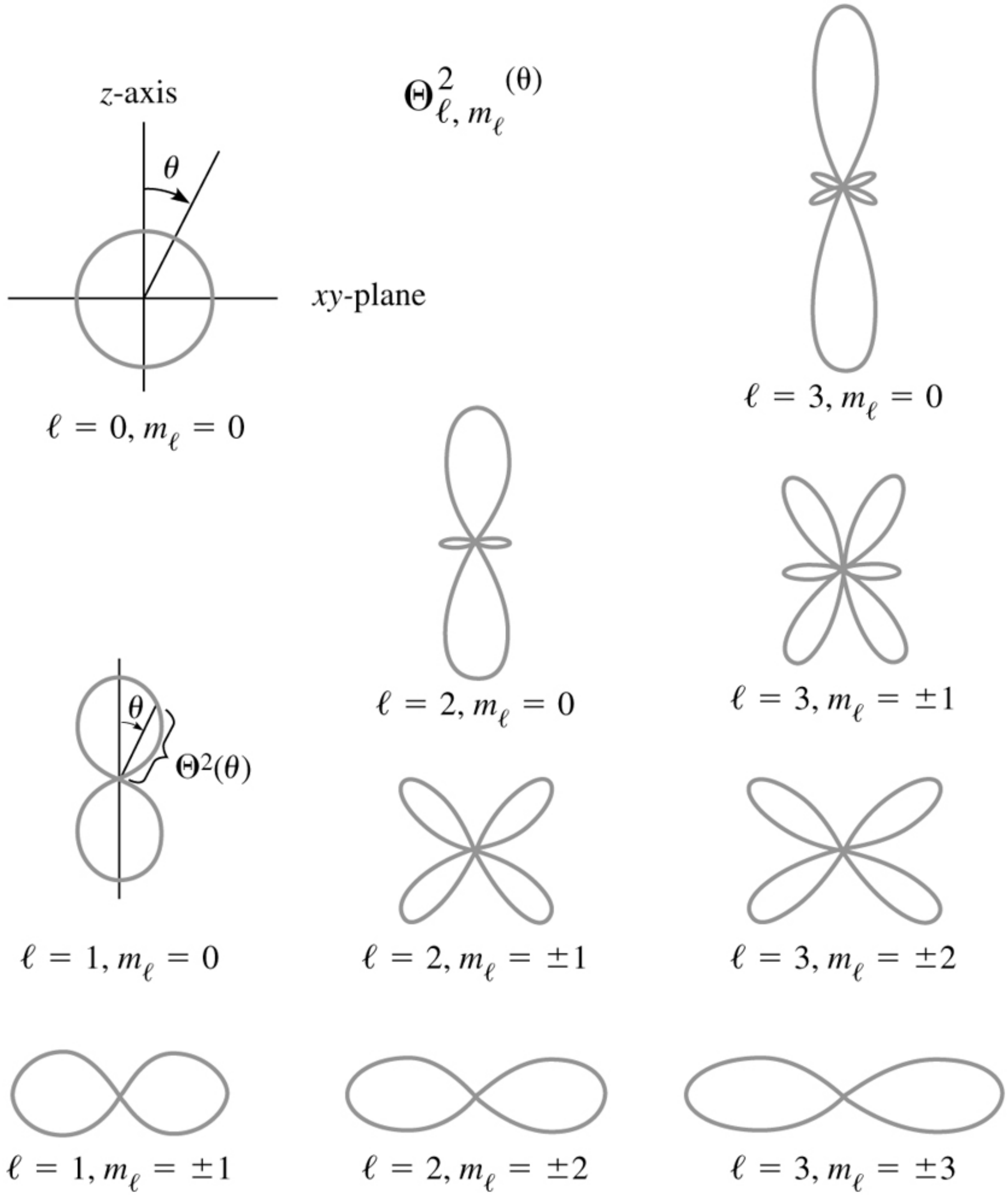
(c1) $\ell = 2, m = \pm 2$



(c2) $\ell = 2, m = \pm 1$

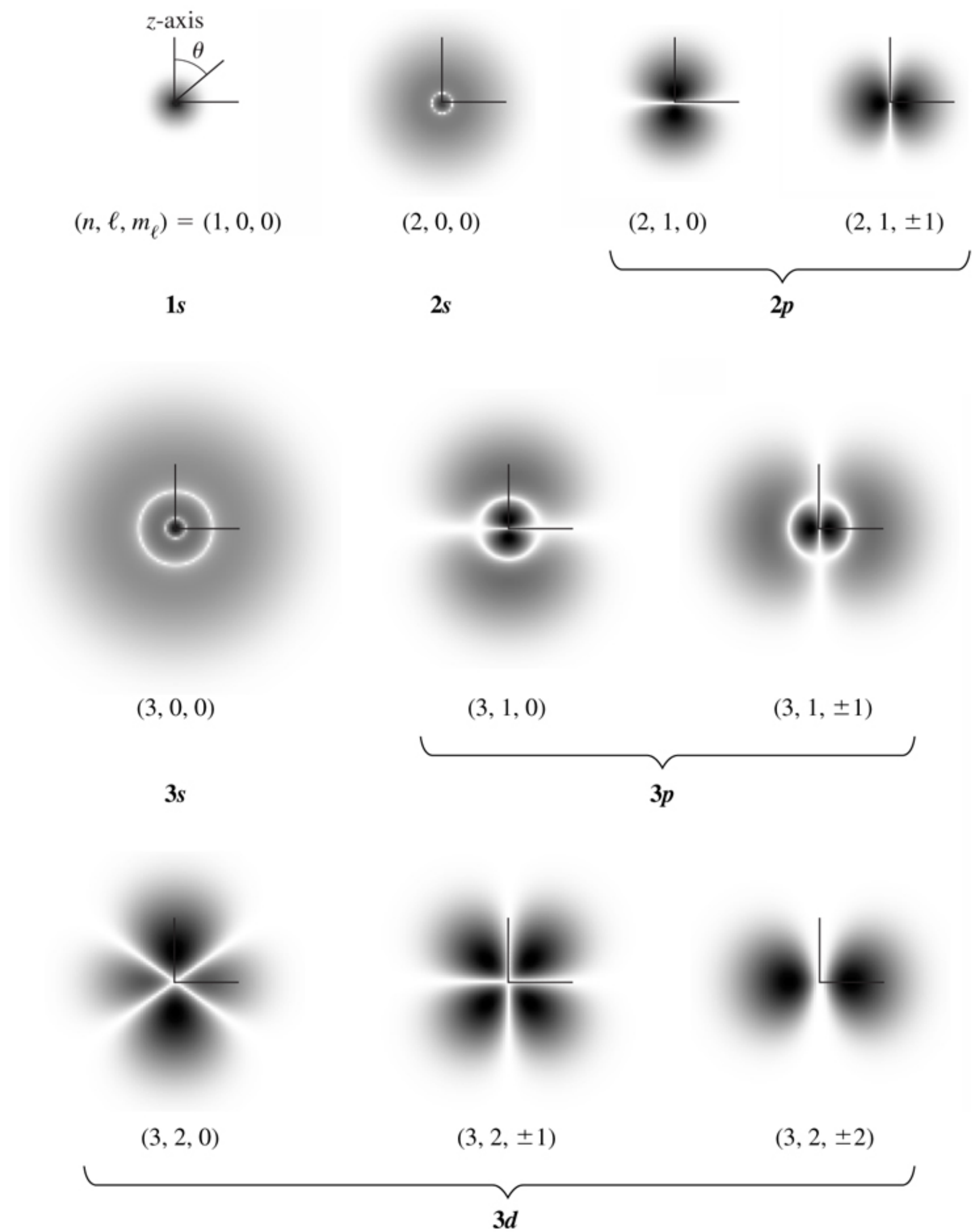
(c3) $\ell = 2, m = 0$

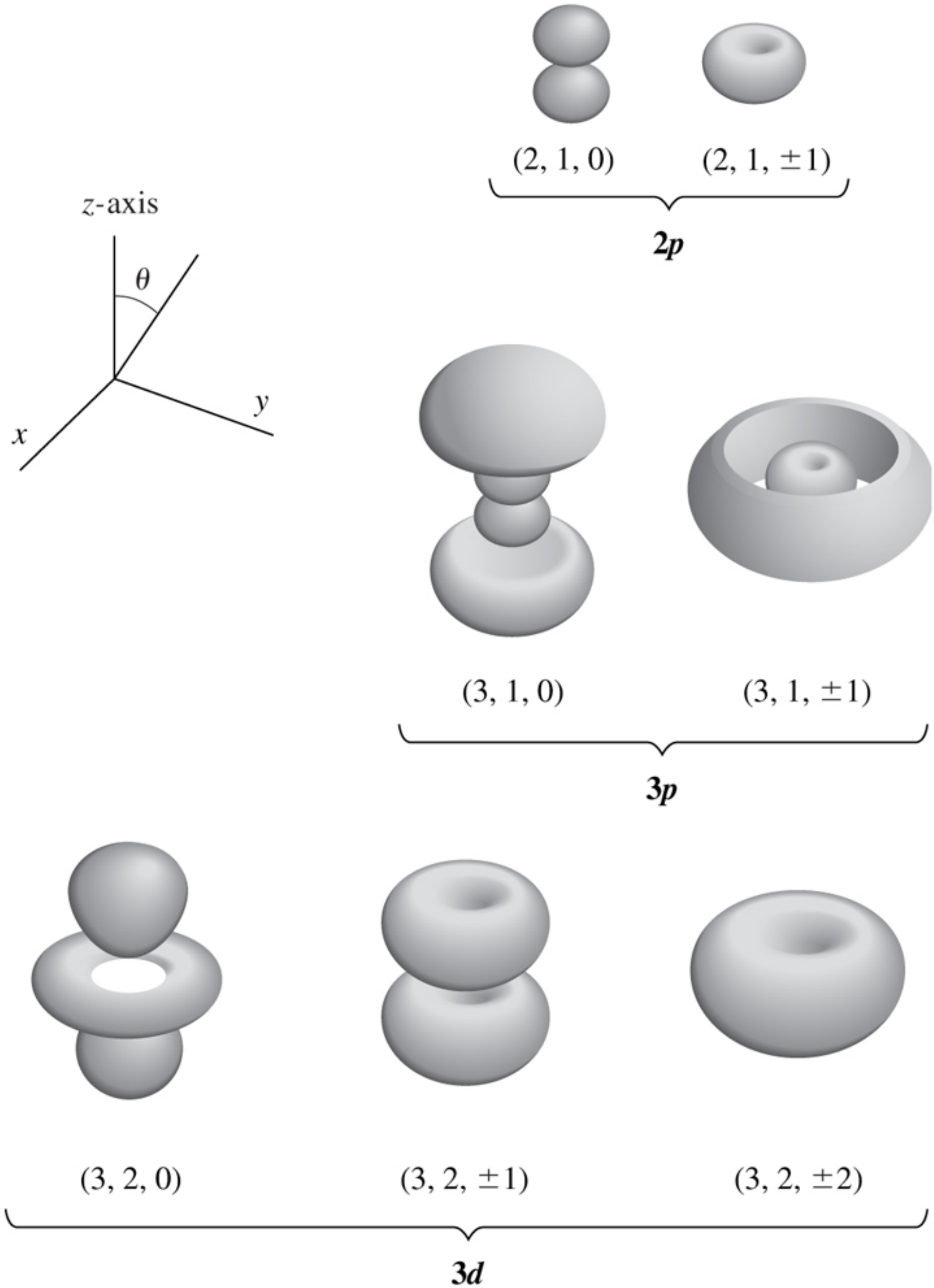
(c4) $\ell = 5, m = 0$

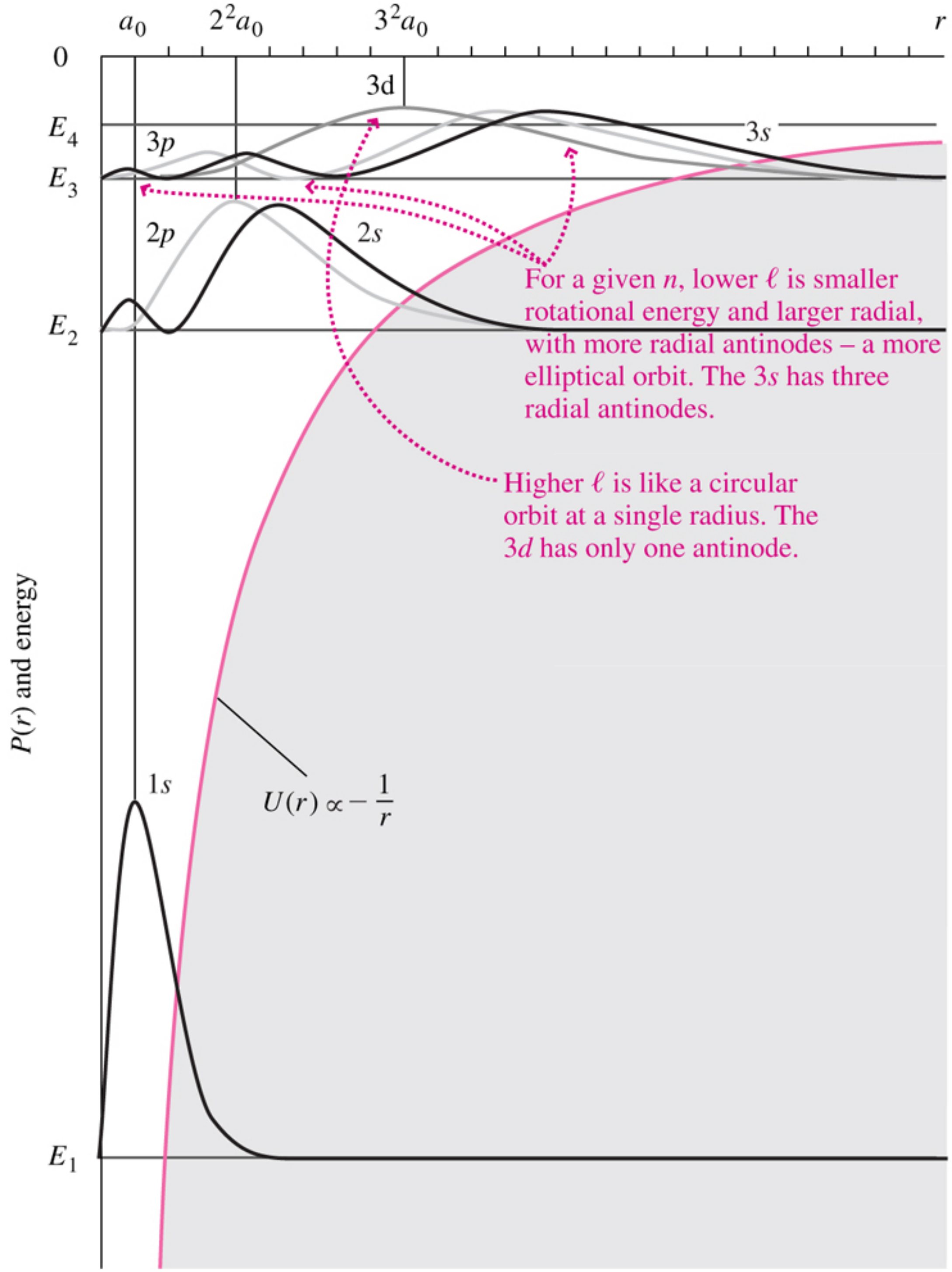


z-axis
θ
xy-plane
$\Theta^2_{\ell, m_\ell}(\theta)$
$\ell = 0, m_\ell = 0$
$\ell = 3, m_\ell = 0$
$\ell = 2, m_\ell = 0$
$\ell = 3, m_\ell = \pm 1$
θ
$\Theta^2(\theta)$
$\ell = 1, m_\ell = 0$
$\ell = 2, m_\ell = \pm 1$
$\ell = 3, m_\ell = \pm 2$
$\ell = 1, m_\ell = \pm 1$
$\ell = 2, m_\ell = \pm 2$
$\ell = 3, m_\ell = \pm 3$

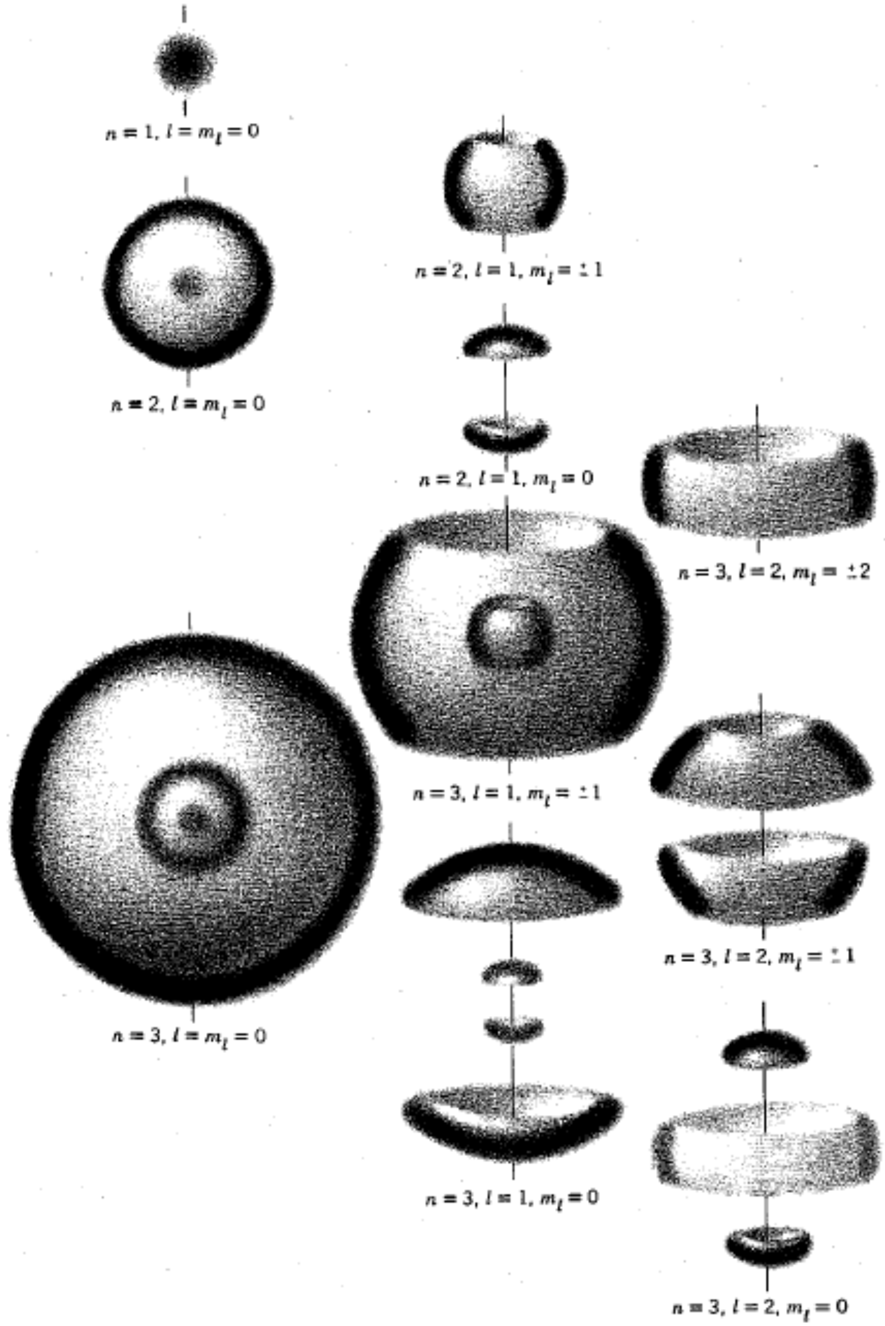
$$|\psi(r,\theta,\phi)|^2 = R^2(r)\,\Theta^2(\theta)$$




z-axis
θ
x
y
(2, 1, 0)
(2, 1, ±1)
2p
(3, 1, 0)
(3, 1, ±1)
3p
(3, 2, 0)
(3, 2, ±1)
(3, 2, ±2)
3d



a_0
2^2a_0
3^2a_0
r
0
3d
E_4
$3p$
$3s$
E_3
$2p$
$2s$
For a given n, lower ℓ is smaller rotational energy and larger radial, with more radial antinodes – a more elliptical orbit. The 3s has three radial antinodes.
E_2
Higher ℓ is like a circular orbit at a single radius. The 3d has only one antinode.
$P(r)$ and energy
$1s$
$U(r) \propto -\frac{1}{r}$
E_1



n = 1, l = m_l = 0
n = 2, l = m_l = 0
n = 2, l = 1, m_l = ±1
n = 2, l = 1, m_l = 0
n = 3, l = 2, m_l = ±2
n = 3, l = 1, m_l = ±1
n = 3, l = m_l = 0
n = 3, l = 2, m_l = ±1
n = 3, l = 1, m_l = 0
n = 3, l = 2, m_l = 0

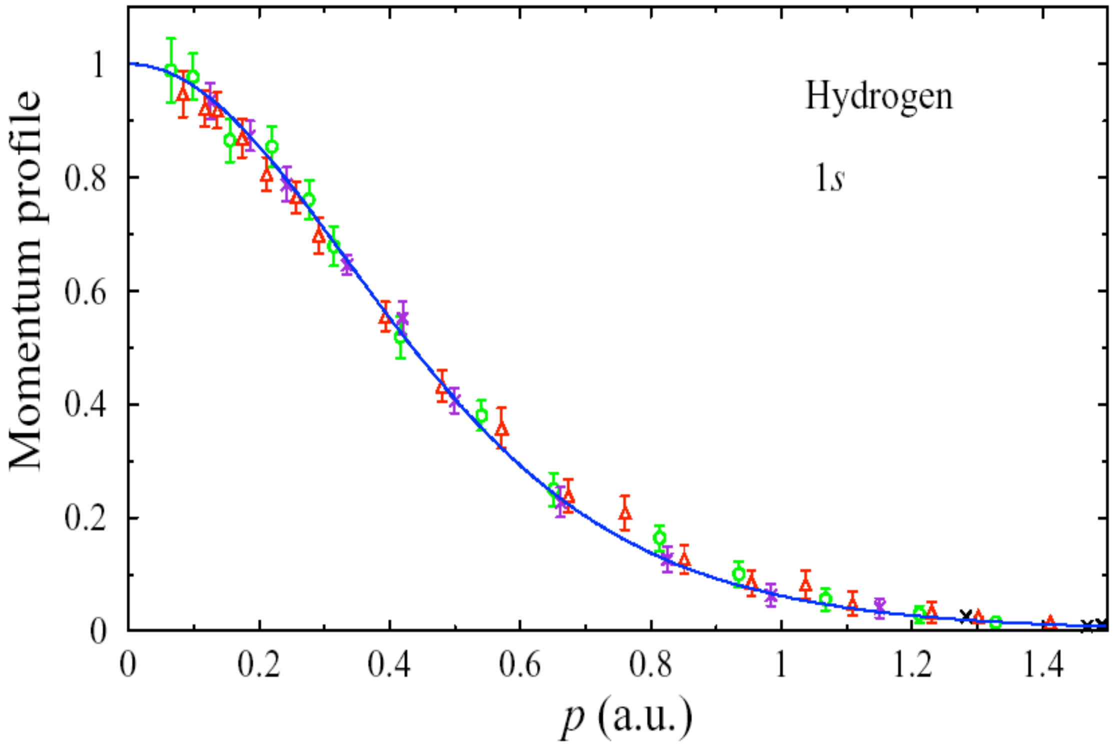
Direct knockout reactions

- 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)

Electrons in atoms

- Atomic units (a.u.) --> standard usage
  - electron mass m_e unit of mass
  - elementary charge e unit of charge
  - length and time such that numerical values of $\hbar$ and $4\pi\epsilon_0$ are unity
  - then atomic unit of length Bohr radius

$$\text{a.u. (length)} = a_0 = \frac{4\pi\epsilon_0\hbar^2}{e^2 m_e} \approx 5.29177 \times 10^{-11}\ \text{m}$$

  - and time $$\text{a.u. (time)} = \frac{a_0}{\alpha c} \approx 2.41888 \times 10^{-17}\ \text{s}$$
  - where $$\alpha = \frac{e^2}{4\pi\epsilon_0\hbar c} \approx \frac{1}{137.036}$$ is the fine structure constant
  - energy unit = Hartree $$E_H = \frac{\hbar^2}{m_e a_0^2} \approx 27.2114\ \text{eV}$$

Hamiltonian in a.u.

- Most of atomic physics can be understood on the basis of

$$H_N = \sum_{i=1}^{N} \frac{\boldsymbol{p}_i^2}{2} - \sum_{i=1}^{N} \frac{Z}{|\boldsymbol{r}_i|} + \frac{1}{2} \sum_{i \neq j}^{N} \frac{1}{|\boldsymbol{r}_i - \boldsymbol{r}_j|} + V_{mag}$$

- for most applications $V_{mag} \Rightarrow V_{so}^{eff} = \sum_i \zeta_i \, \boldsymbol{\ell}_i \cdot \boldsymbol{s}_i$

- Relativistic description required for heavier atoms
  - binding sizable fraction of electron rest mass
  - binding of lowest s state generates high-momentum components
- Sensible calculations up to Kr without V_{mag}
- Shell structure well established

Shell structure

- Simulate with

$$H_0^N = \sum_{i=1}^{N} H_0(i)$$

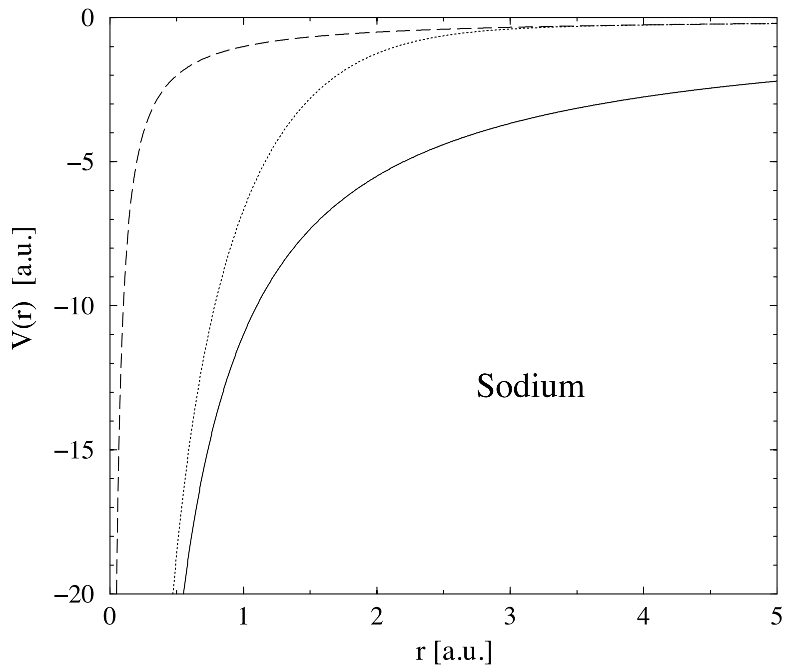
- with

$$H_0(i) = \frac{\boldsymbol{p}_i^2}{2} - \frac{Z}{r_i} + U(\boldsymbol{r}_i)$$

- even without auxiliary potential $\Rightarrow$ shells
  - hydrogen-like: $(2\ell + 1) * (2s + 1)$ degeneracy
  - but $\varepsilon_n = -\frac{Z^2}{2n^2}$ does not give correct shell structure (2,10,28...
  - degeneracy must be lifted
  - how?

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

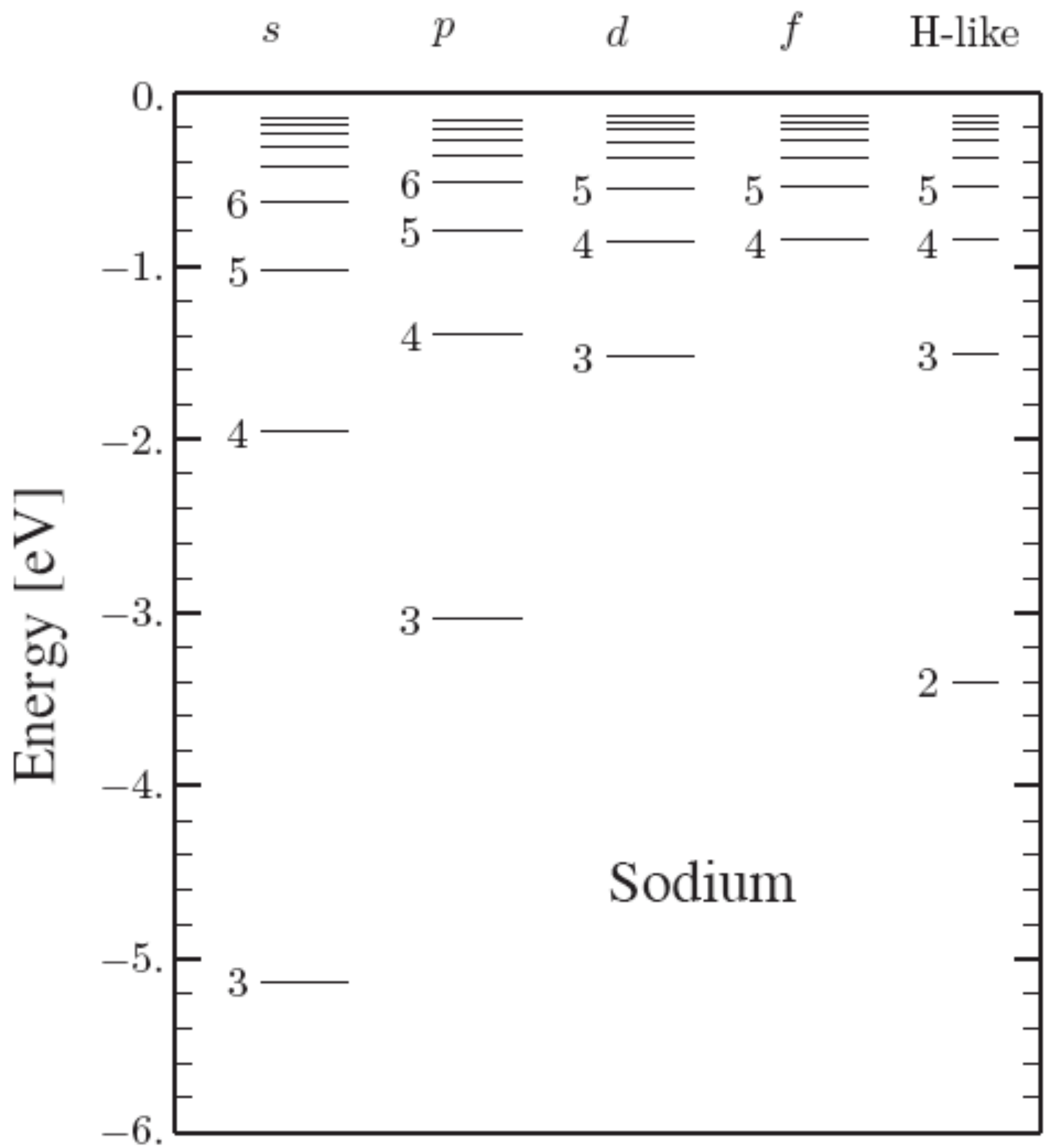
- Fill the lowest shells
- Use schematic potential

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

- Ground state: fill lowest orbits according to Pauli

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

- Excited states?



Closed-shell atoms

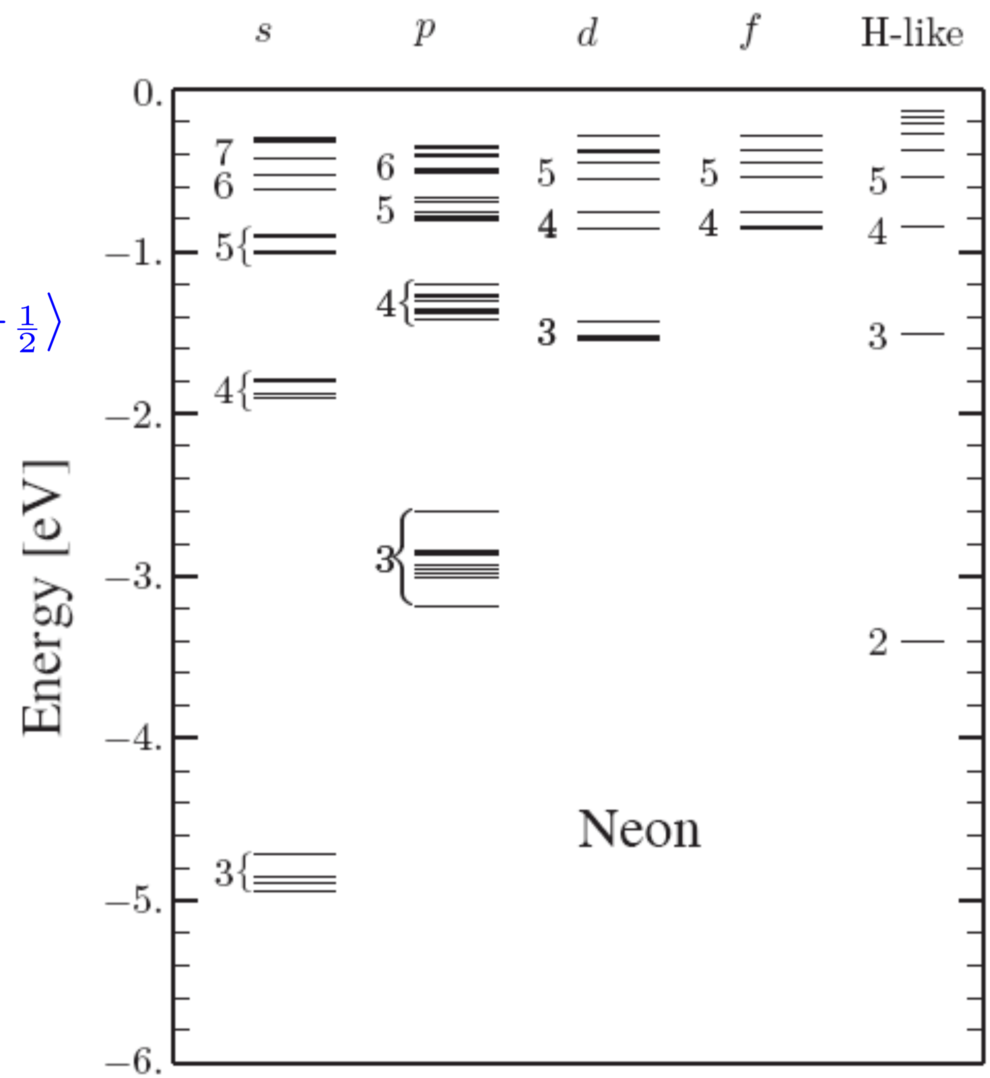
- Neon
- Ground state

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

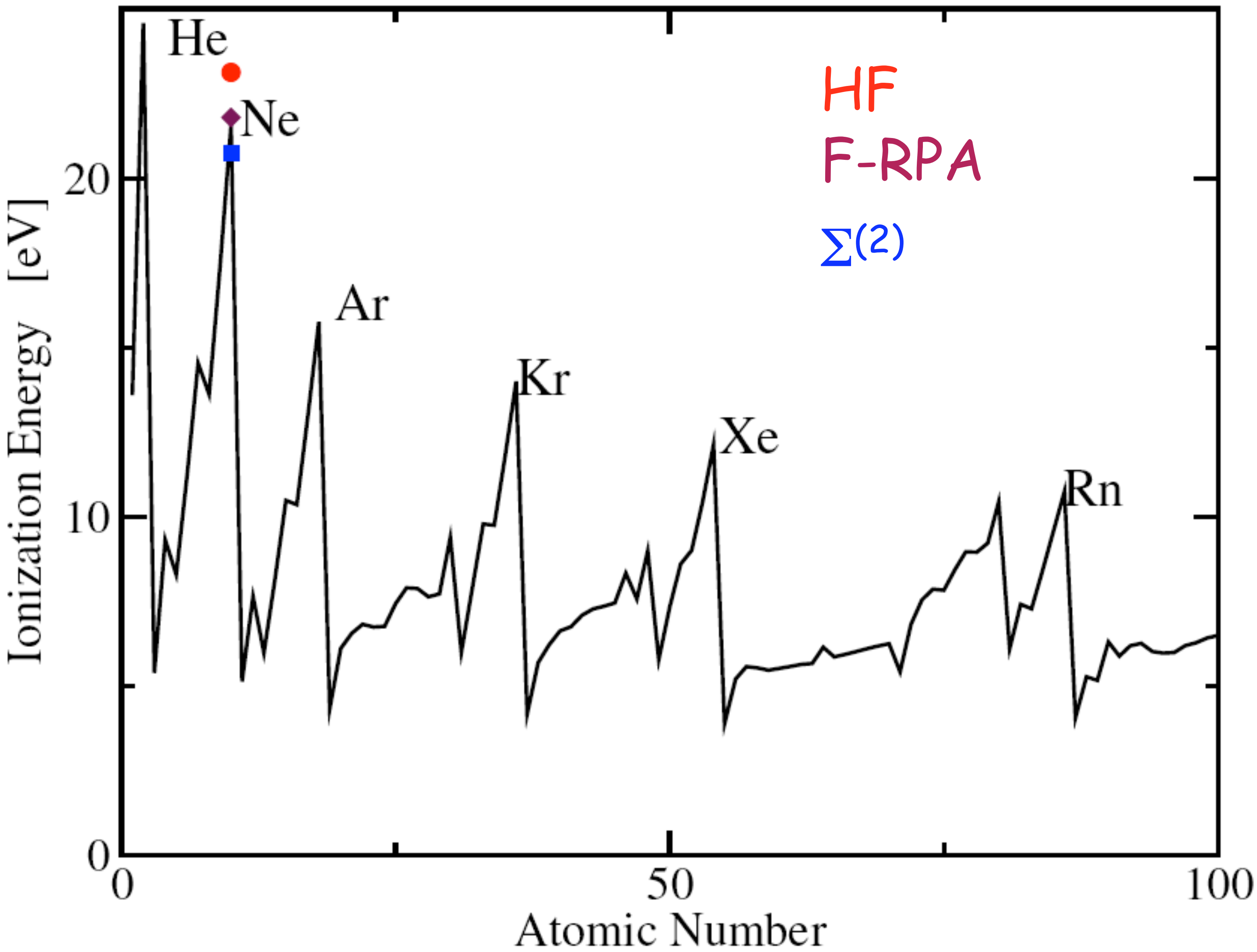
- Excited states

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

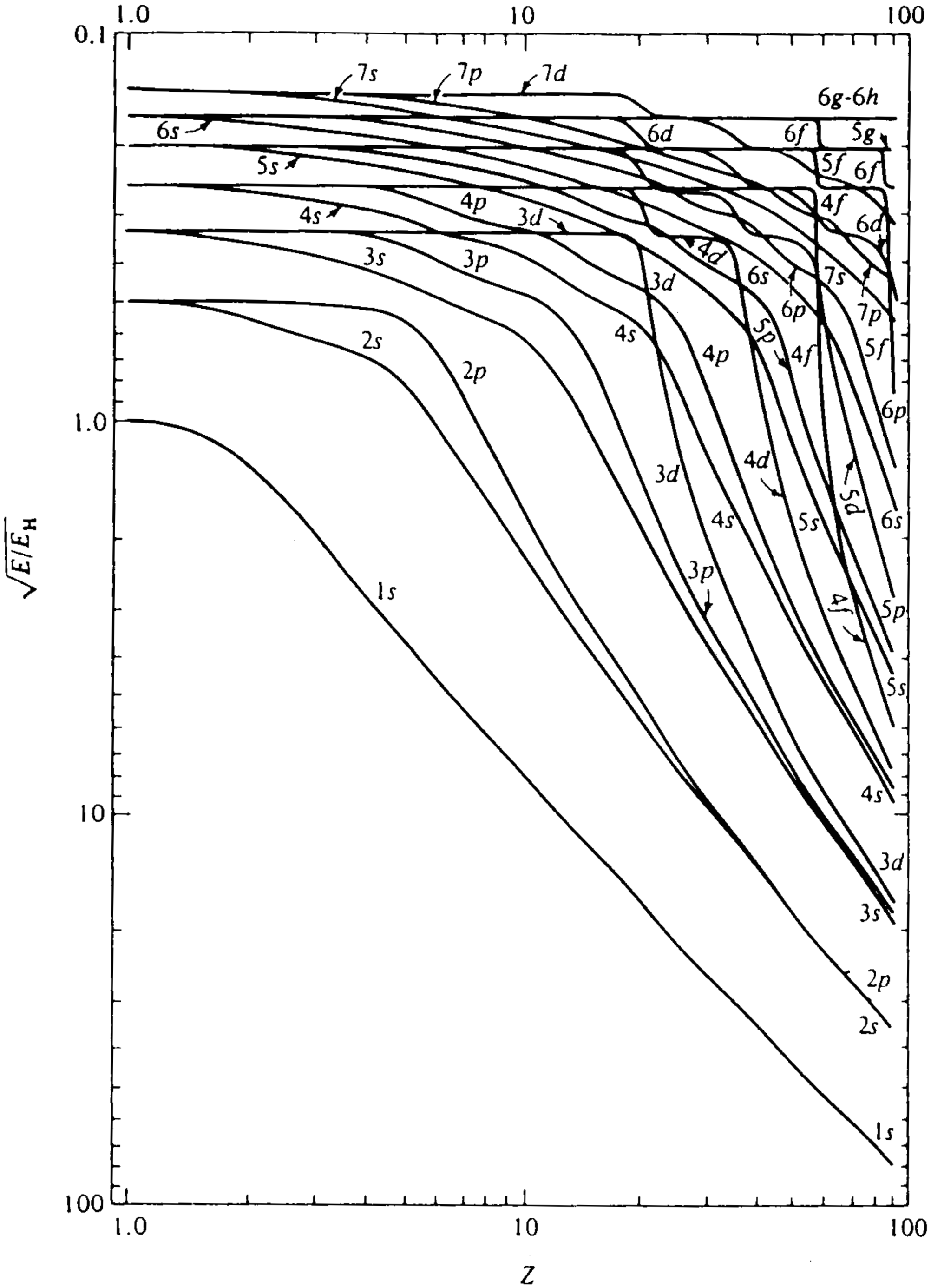
- operators: see later
- Note the H-like states
- Splitting?
- Basic shell structure of atoms understood $\Rightarrow$ IPM



Periodic table



Level sequence (approximately)



(e,2e) data for atoms

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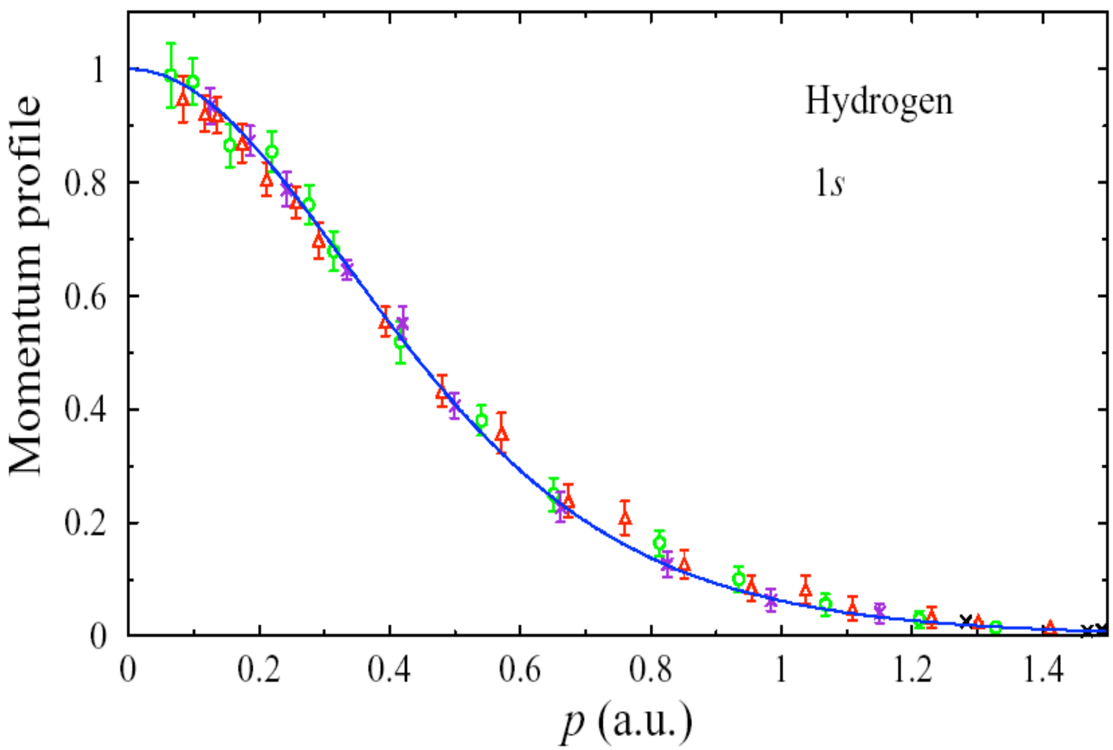
- (e,2e) removal amplitude

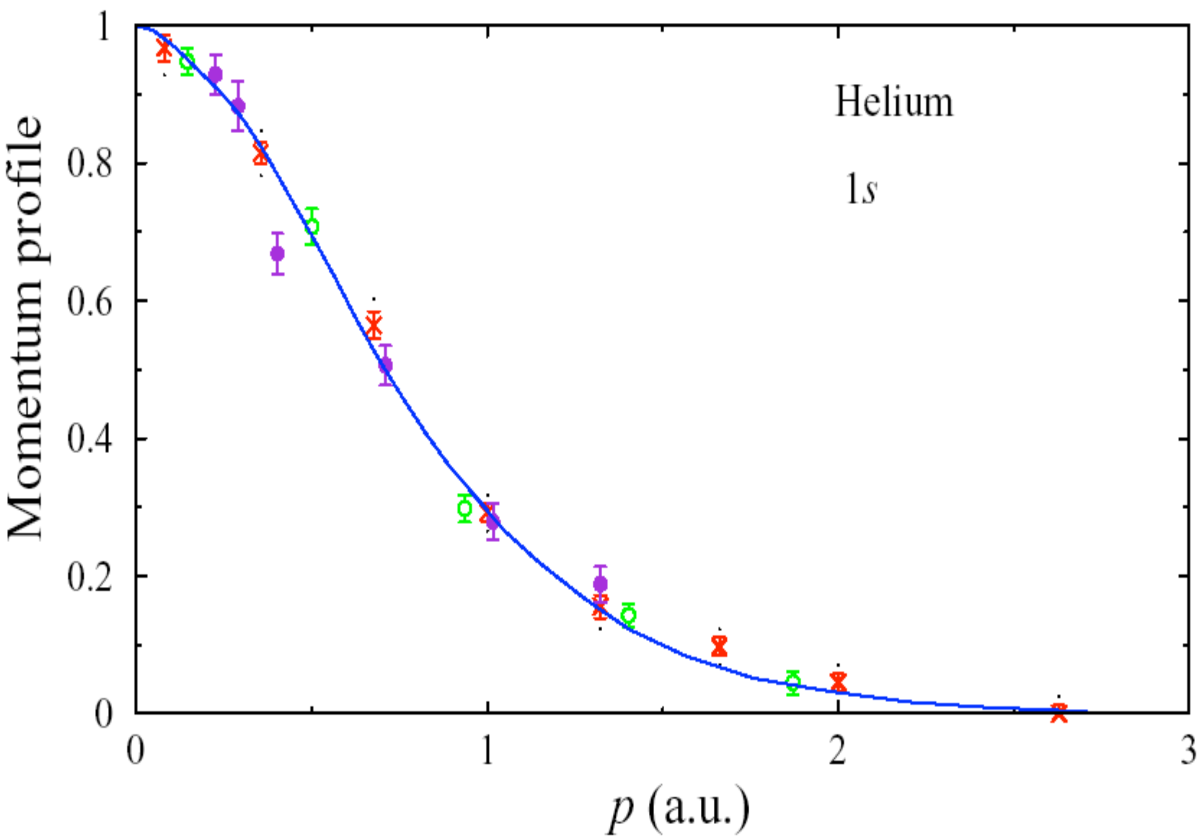
$$\langle 0 | \, a_{\boldsymbol{p}} \, | n=1, \ell=0 \rangle = \langle \boldsymbol{p} \, | n=1, \ell=0 \rangle = \phi_{1s}(\boldsymbol{p})$$



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)



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

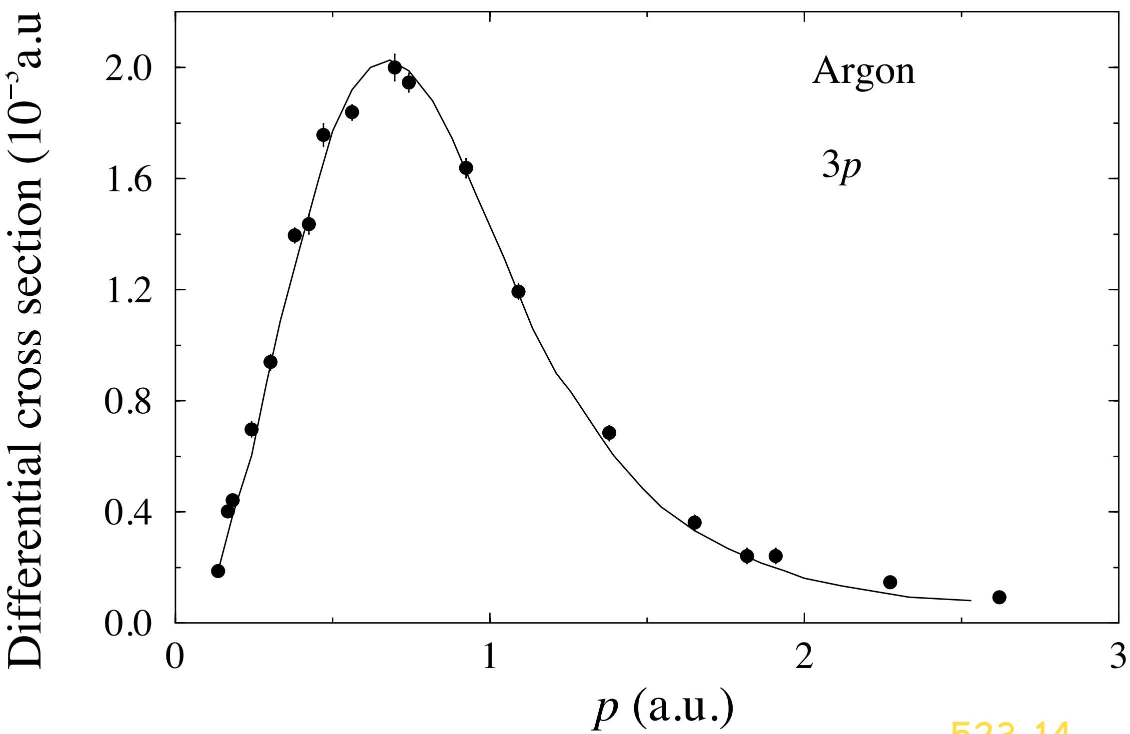
agreement with IPM!

$\rightarrow 1$

Phys. Rev. A8, 2494 (1973)

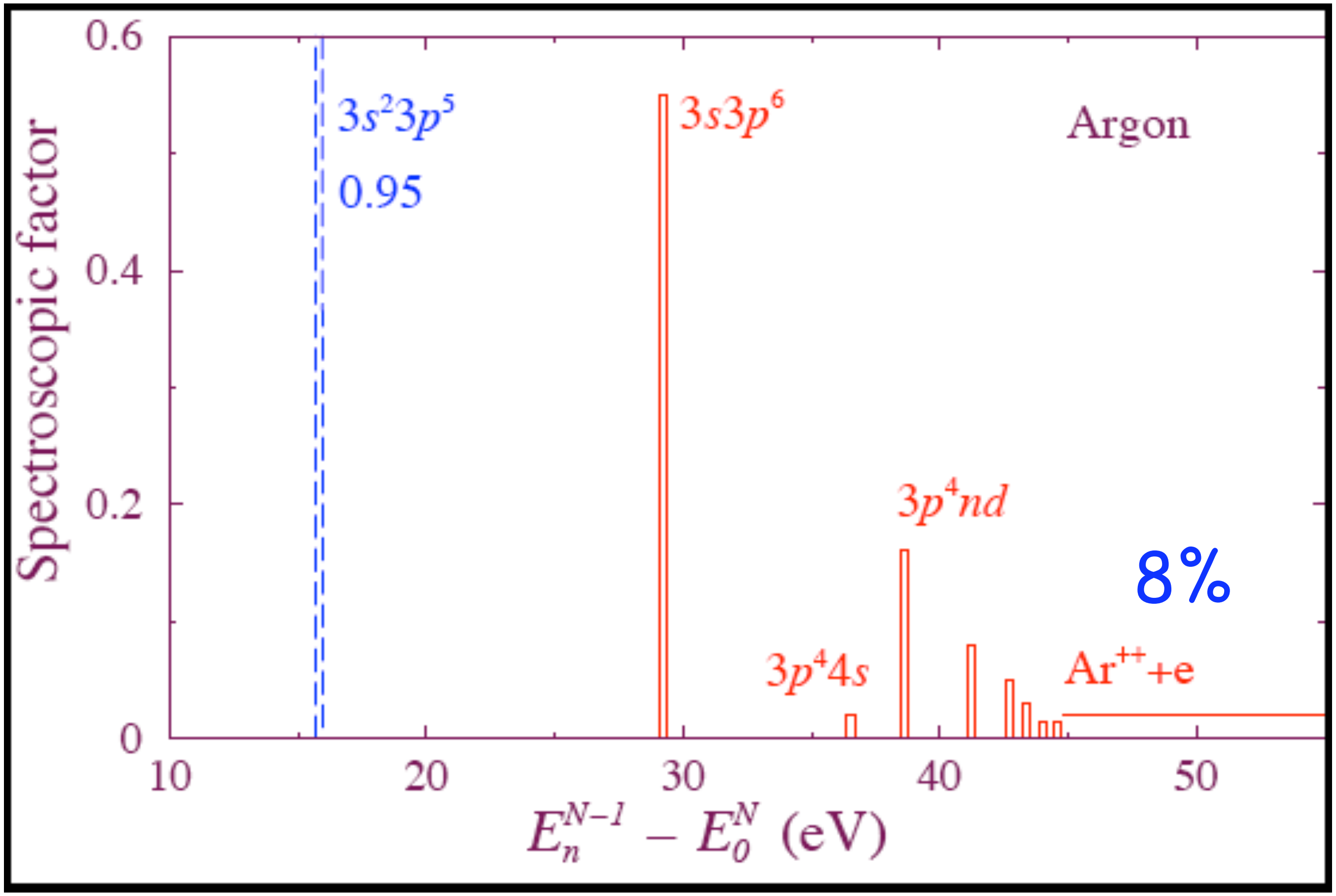
Other closed-shell atoms

- 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



Argon spectroscopic factors

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



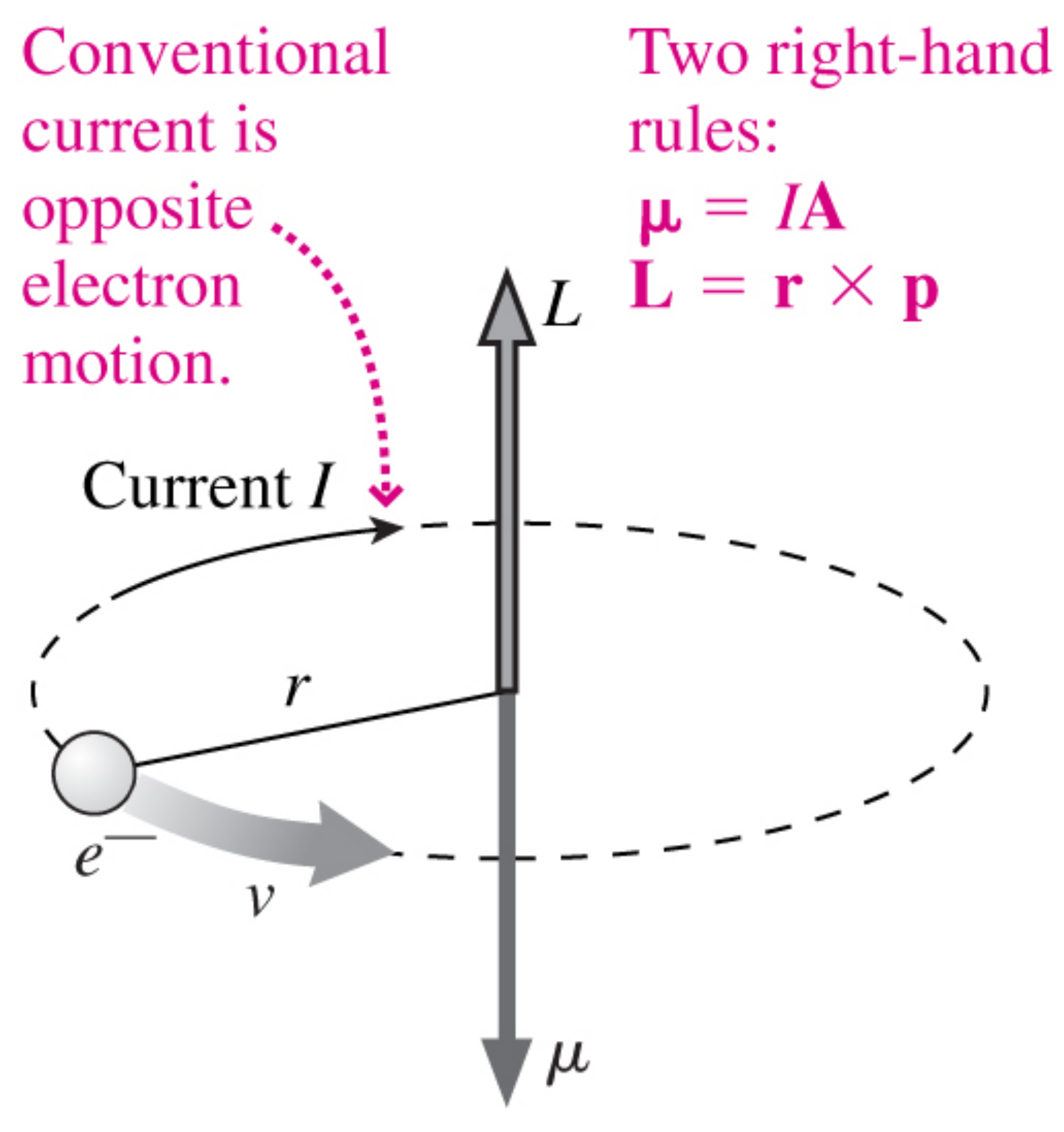
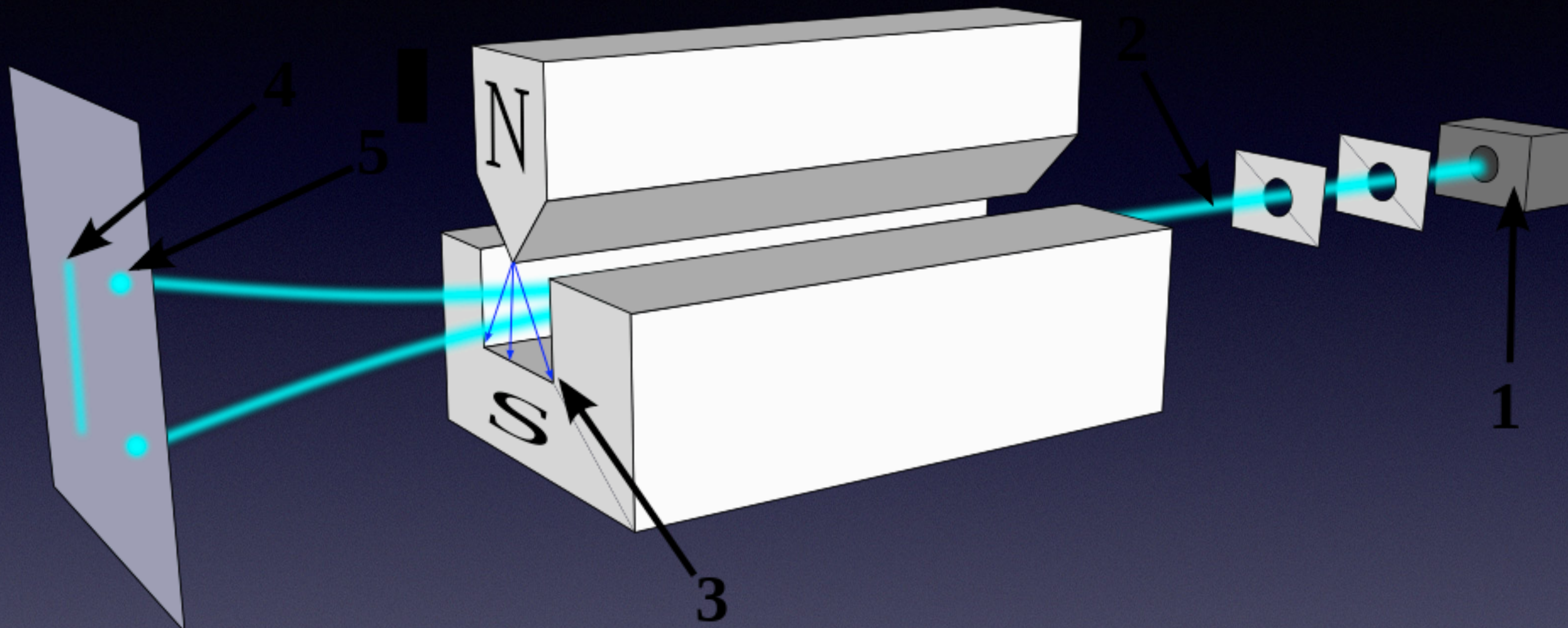

Conventional current is opposite electron motion.
Two right-hand rules:
μ = IA
L = r × p
L
Current I
r
e⁻
v
μ

TABLE 8.2 Subshell ordering and capacity

Subshell $n\ell$	1*s*	2*s*	2*p*	3*s*	3*p*	4*s*	3*d*	4*p*	5*s*	4*d*	5*p*	6*s*	4*f*	5*d*	6*p*	7*s*	5*f*	6*d*
$n + \ell$	1	2	3	3	4	4	5	5	5	6	6	6	7	7	7	7	8	8
Number of electrons $2(2\ell + 1)$	2	2	6	2	6	2	10	6	2	10	6	2	14	10	6	2	14	10


N
S
1
2
3
4
5

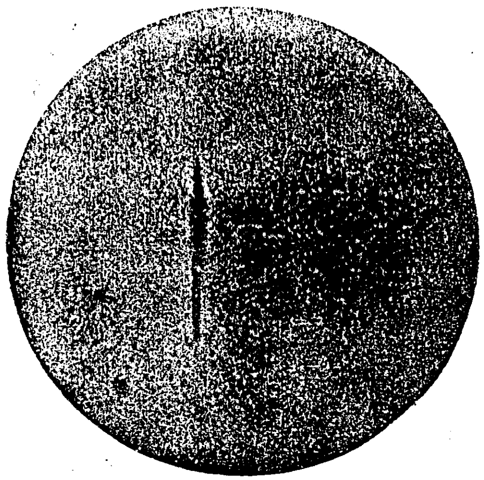


Fig. 2.

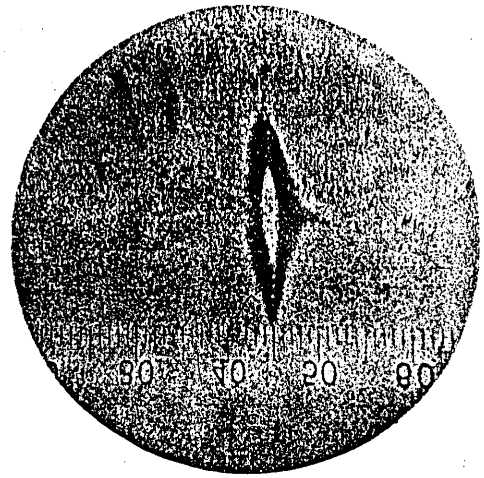


Fig. 3.