

Announcements

- Mid-term exam: 02/01, Wed, in class
 - Chapters 7 and 8
 - Open book and open lecture notes but no personal notes
 - 5 questions
 - 2 questions from Chapter 8 conceptual questions 1-24 on p.338 -339.
 - More conceptual, simple calculations if any.
 - Review session, 30th, Monday room 356, 5:30-7 pm
- Homework Two No. 5
 - Orthogonal condition: $(p_x)^* p_y = 0$
- Homework Two No. 4

$$\Phi_{\pm 1} = \frac{1}{\sqrt{2\pi}} e^{\pm i\phi}$$
$$\Phi_{\pm 2} = \frac{1}{\sqrt{2\pi}} e^{\pm 2i\phi}$$

Lecture 8 Topics

- Wave function for a system of particles
 - Identical particles
 - Exclusion principle for fermions
- Multi-electron atoms
 - Energy levels by n
 - Energy levels by l at a given n
 - Energy levels by electron symmetric and antisymmetric configurations at a given l and n
- Periodic table
 - Valence electrons
 - Nuclear charge screening

Periodic Table

Group	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
Period 1	1																	2
1	H																	He
2	3	4											5	6	7	8	9	10
	Li	Be											B	C	N	O	F	Ne
3	11	12											13	14	15	16	17	18
	Na	Mg											Al	Si	P	S	Cl	Ar
4	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36
	K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
5	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54
	Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
6	55	56	57*	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86
	Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
7	87	88	89**	104	105	106	107	108	109	110	111	112	113	114	115	116	117	118
	Fr	Ra	Ac	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Uut	Uuq	Uup	Uuh	Uus	Uuo

○ Non Metals	● Noble Gases
● Alkali Metals	● Metalloids
● Alkaline Metals	● Halogens
● Transition Metals	● Other Metals
● Rare Earth Elements	

*Lanthanides

58	59	60	61	62	63	64	65	66	67	68	69	70	71
Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu

**Actinides

90	91	92	93	94	95	96	97	98	99	100	101	102	103
Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr

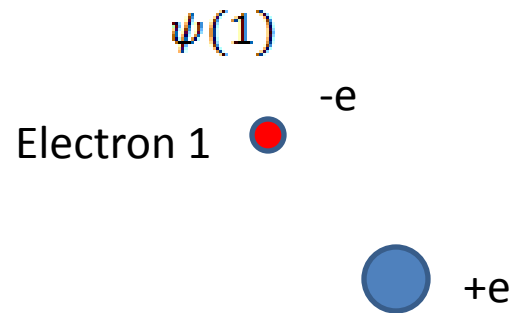
What we know so far:

- Number of electrons in each atom
- Electrons should be in one of the orbitals determined by n , l , and m_l
- n limits what types of l orbitals an electron can occupy.
- Each l orbital has $2l+1$ possible m_l states:
 - s orbital = 1
 - p orbital = $2 \times 1 + 1 = 3$
 - d orbital = $2 \times 2 + 1 = 5$
 - f orbital = $2 \times 3 + 1 = 7$
- Due to electron's spin where $\frac{1}{2}$ and $-\frac{1}{2}$ are possible, each m_l orbital can have two additional possible states.
- As a result, in each n , there are $2n^2$ possible states.

Questions

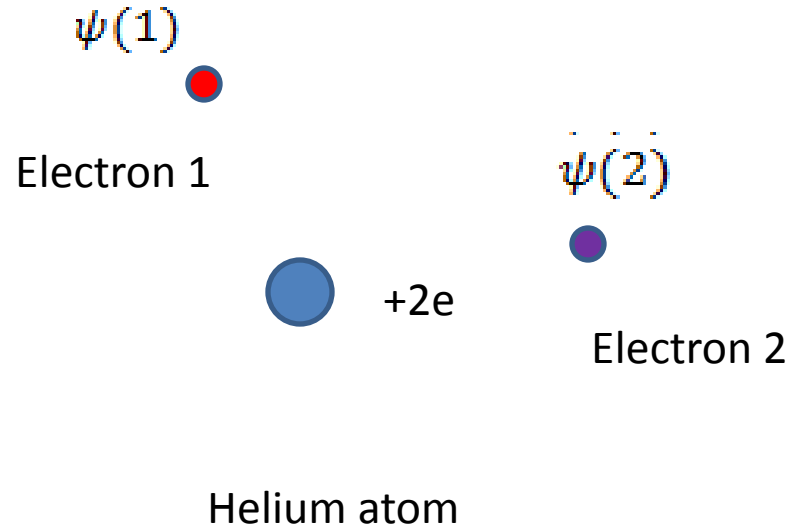
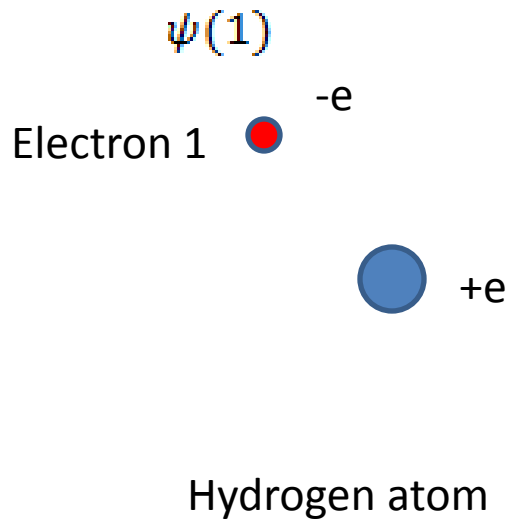
- How to construct a wave function with multi-electrons in an atom (wave function question)
- How to stack electrons across all possible orbitals? (energy question)
 - n
 - By l at a given n
 - By m_l at a given l and n

Identical particles



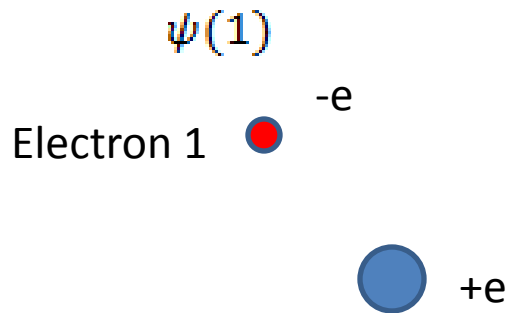
Hydrogen atom

Identical particles

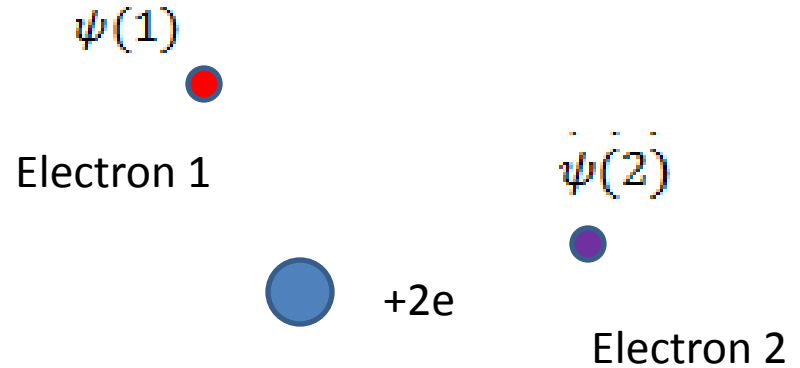


$$|\psi(1,2)\rangle = \psi(1)\psi(2)$$

Identical particles



Hydrogen atom

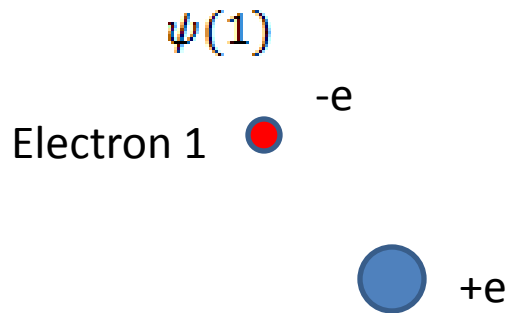


Helium atom

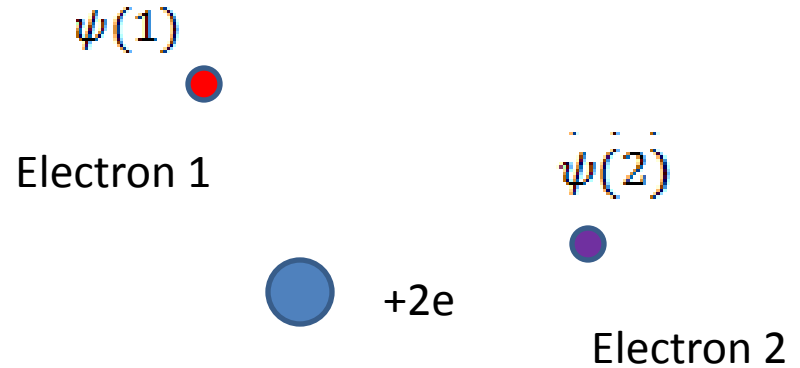
$$|\psi(1,2)\rangle = \psi(1)\psi(2)$$

After exchanging two particles

Identical particles



Hydrogen atom



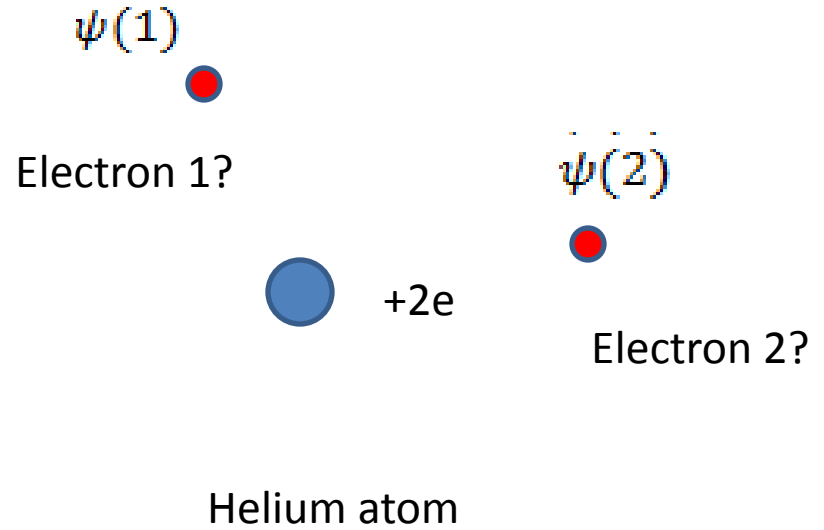
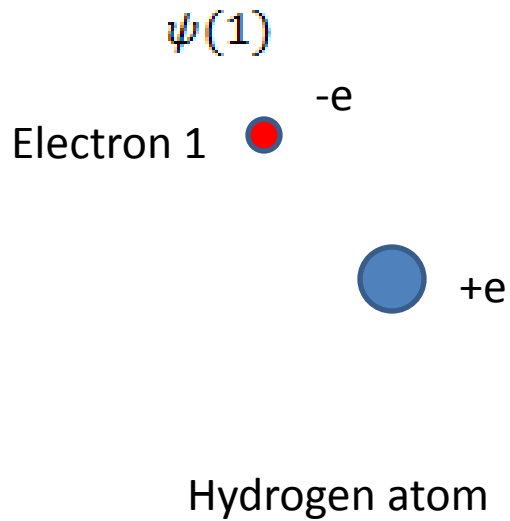
Helium atom

$$|\psi(1,2)\rangle = \psi(1)\psi(2)$$

After exchanging two particles

$$|\psi(2,1)\rangle = \psi(2)\psi(1)$$

Identical particles

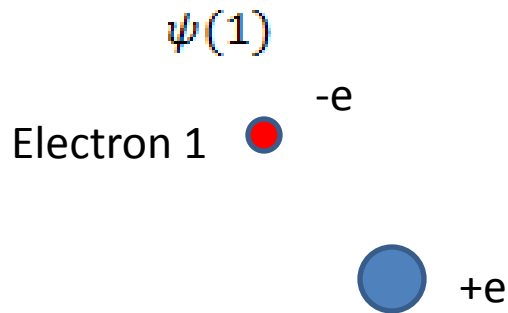


$$|\psi(1,2)\rangle = \psi(1)\psi(2)$$

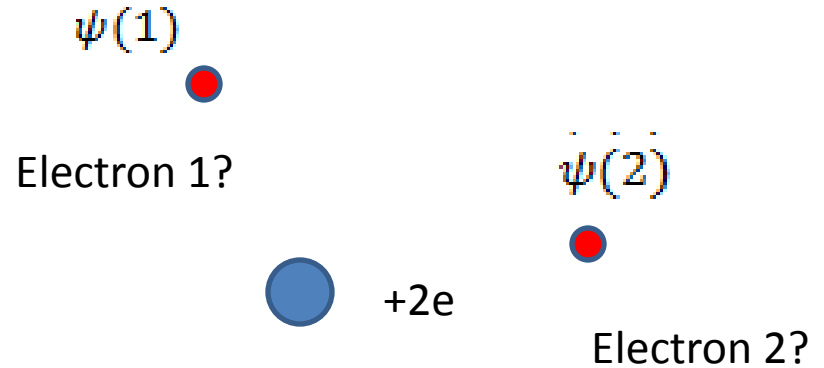
After exchanging two particles

$$|\psi(2,1)\rangle = \psi(2)\psi(1)$$

Identical particles



Hydrogen atom



Helium atom

$$|\psi(1,2)|^2 = |\psi(2,1)|^2$$

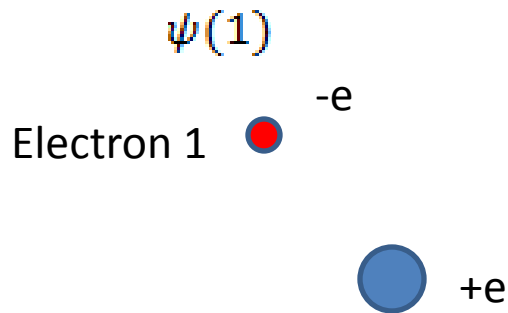
$$\begin{aligned} \psi(1,2) &= \psi(2,1) \\ \psi(1,2) &= -\psi(2,1) \end{aligned}$$

$$\psi(1,2) = \psi(1)\psi(2)$$

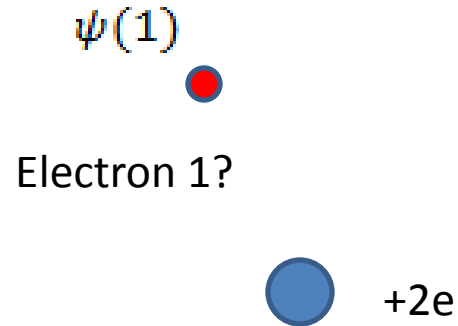
After exchanging two particles

$$\psi(2,1) = \psi(2)\psi(1)$$

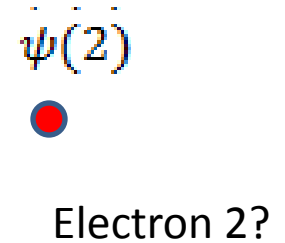
Identical particles



Hydrogen atom



Helium atom



$$|\psi(1,2)|^2 = |\psi(2,1)|^2$$

$$\psi(1,2) = \psi(2,1)$$
$$\psi(1,2) = -\psi(2,1)$$

Symmetric under exchange operation

Anti-symmetric

When Particle 1 is in n state and Particle 2 is in n' state

$$\psi_I = \psi_n(1)\psi_{n'}(2)$$

When Particle 2 is in n state and Particle 1 is in n' state

$$\psi_{II} = \psi_n(2)\psi_{n'}(1)$$

$$|\psi(1,2)|^2 = |\psi(2,1)|^2$$

$$\psi_{Symmetric} = \frac{1}{\sqrt{2}}[\psi_n(1)\psi_{n'}(2) + \psi_n(2)\psi_{n'}(1)]$$

$$\psi_{Anti-Symmetric} = \frac{1}{\sqrt{2}}[\psi_n(1)\psi_{n'}(2) - \psi_n(2)\psi_{n'}(1)]$$

Bosons

$\psi_{\text{Symmetric}}$ satisfies $\psi(1,2) = \psi(2,1)$

- Systems of bosons are described by wave functions that are symmetric upon the exchange of any pair of bosons.
- Bosons are integer spin particles such as
 - Photon ($s=1$) Deuteron ($s=1$)
 - Pion ($s=0$)
 - Helium nucleus (alpha particle; $s=0$)
- Bosons can occupy the same quantum state.

Fermions

$\psi_{\text{Anti-Symmetric}}$ satisfies $\psi(1,2) = -\psi(2,1)$

- Systems of fermions are described by wave functions that reverse sign upon the exchange of any pair of electrons.
- Fermions' spin numbers are half-integer:
 - Electron, proton, and neutron = $\frac{1}{2}$
- If $n = n'$, $\psi_{\text{Anti-Symmetric}} = ???$

$$\psi_{\text{Anti-Symmetric}} = \frac{1}{\sqrt{2}} [\psi_n(1)\psi_{n'}(2) - \psi_n(2)\psi_{n'}(1)]$$

Fermions

$\psi_{\text{Anti-Symmetric}}$ satisfies $\psi(1,2) = -\psi(2,1)$

- Systems of fermions are described by wave functions that reverse sign upon the exchange of any pair of electrons.
- Fermions' spin numbers are half-integer:
 - Electron, proton, and neutron = $\frac{1}{2}$
- If $n = n'$, $\psi_{\text{Anti-Symmetric}} = 0$.

$$\psi_{\text{Anti-Symmetric}} = \frac{1}{\sqrt{2}} [\psi_n(1)\psi_{n'}(2) - \psi_n(2)\psi_{n'}(1)]$$

Two fermions of the same type cannot occupy the same quantum state in an isolated system.

→ Exclusion Principle

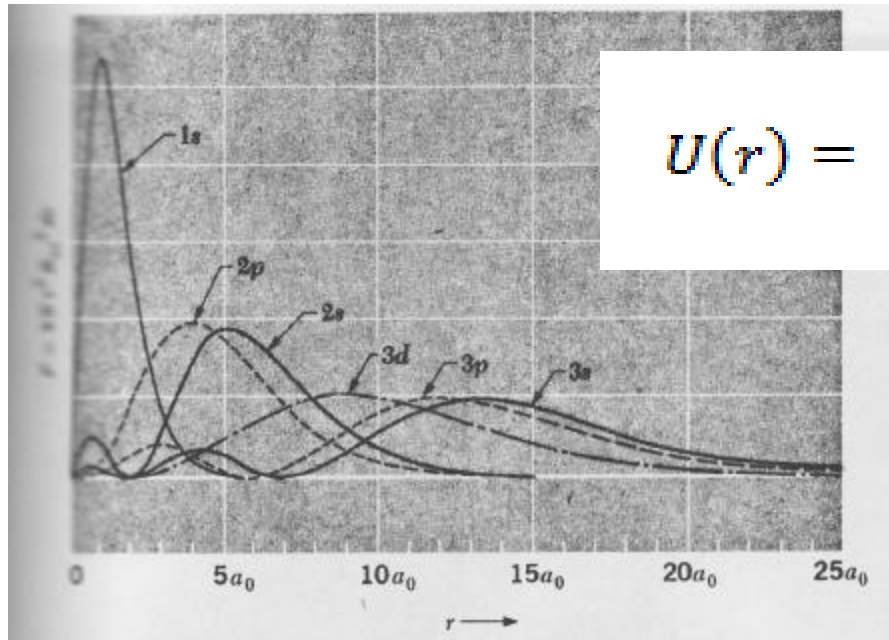
Periodic Table: Two basic rules

- A system of particles is stable when its total energy is a minimum
- Only one electron can exist in any particular quantum state in an atom (exclusion principle).

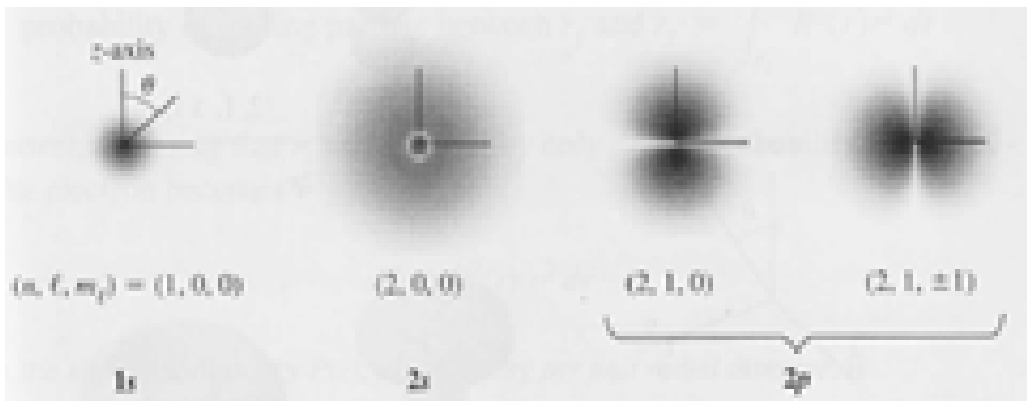
Which quantum state has a lower energy?

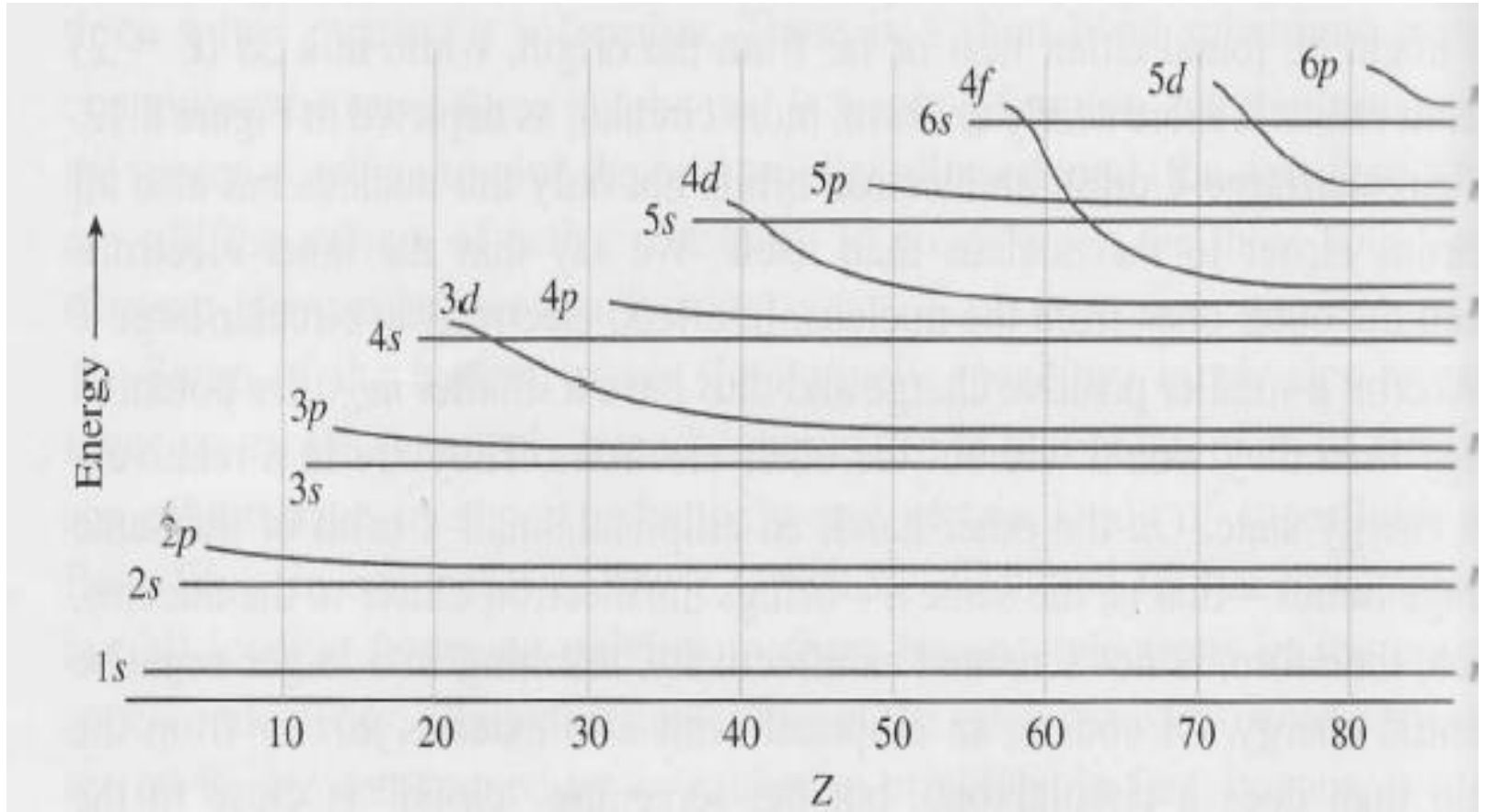
- When n is lower.
- With a given n , when l is lower.
- With a given l , parallel spin arrangements lower energy.

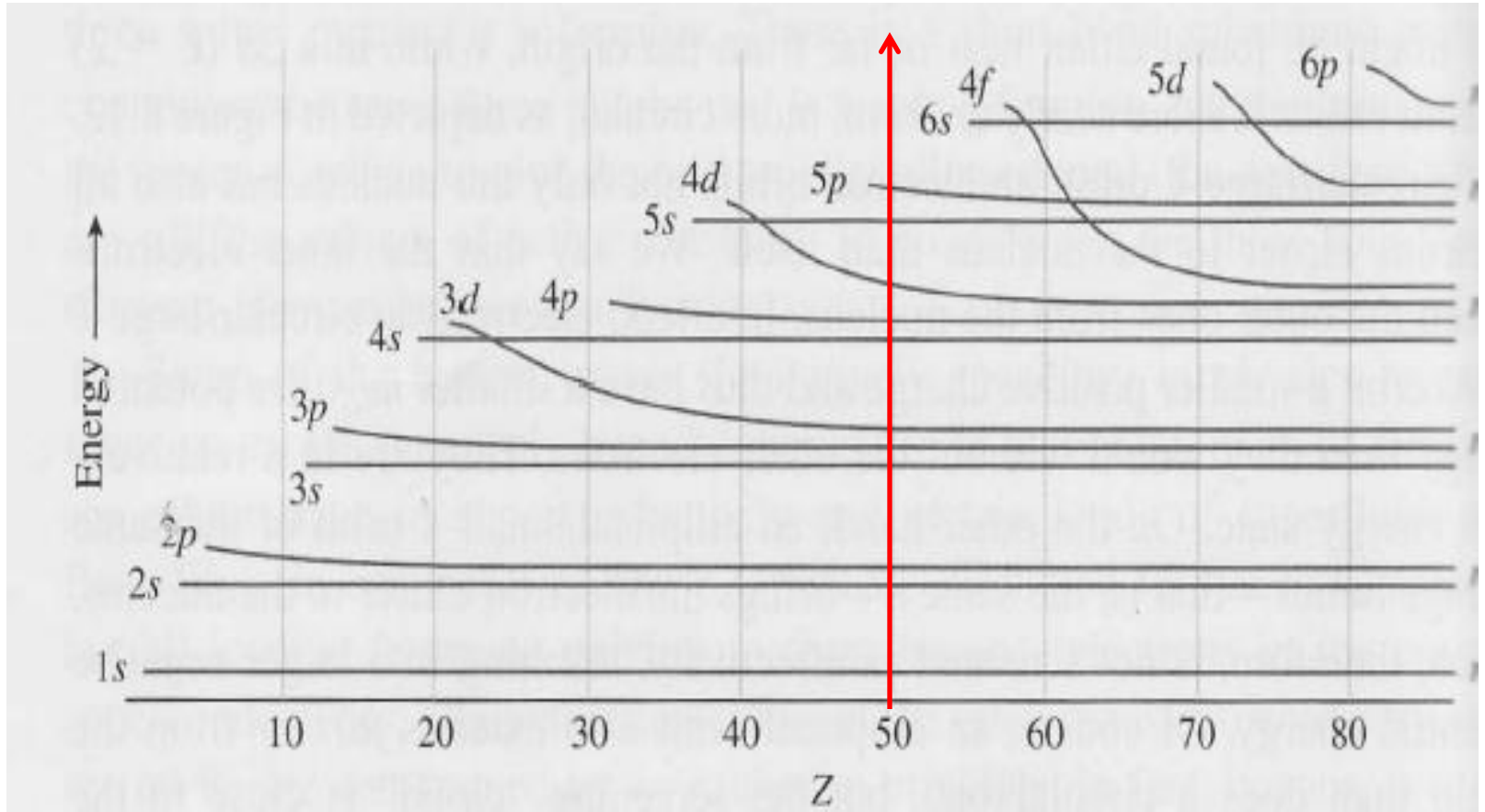
With a given n , when l is lower



$$U(r) = \frac{1}{4\pi\epsilon_0} \frac{(\text{electron charge})(\text{nucleus charge})}{r}$$







With a given l , parallel spin arrangements lower energy.

wave function where electron 1 occupies n state and electron occupies n' state:

$$\psi(1,2) = \psi_{n n'}(1,2) \uparrow\uparrow$$

If we exchange electron 1 and electron 2, a wave function becomes

$$\psi(2,1) = \psi_{n n'}(2,1) \uparrow\uparrow$$

According to the exclusion principle,

$$\psi(1,2) = -\psi(2,1)$$

$$\psi_{n n'}(1,2) \uparrow\uparrow = -\psi_{n n'}(2,1) \uparrow\uparrow$$

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If $n = n'$?

$$\psi_{n n}(1,2) = -\psi_{n n}(2,1) = 0$$

$$\psi_{n n'}(1,2) \uparrow\uparrow = -\psi_{n n'}(2,1) \uparrow\uparrow$$

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→ Lower Coulomb Interaction (by decreasing repulsive interaction between two electrons)

P orbital spin arrangements

	p_x	p_y	p_z
Lower E	↑		
Higher E			

P orbital spin arrangements

	p_x	p_y	p_z
Lower E	↑		
	↑	↑	
	↑	↑	↑
	↑↓	↑	↑
Higher E	↑↓	↑↓	↑
	↑↓	↑↓	↑↓

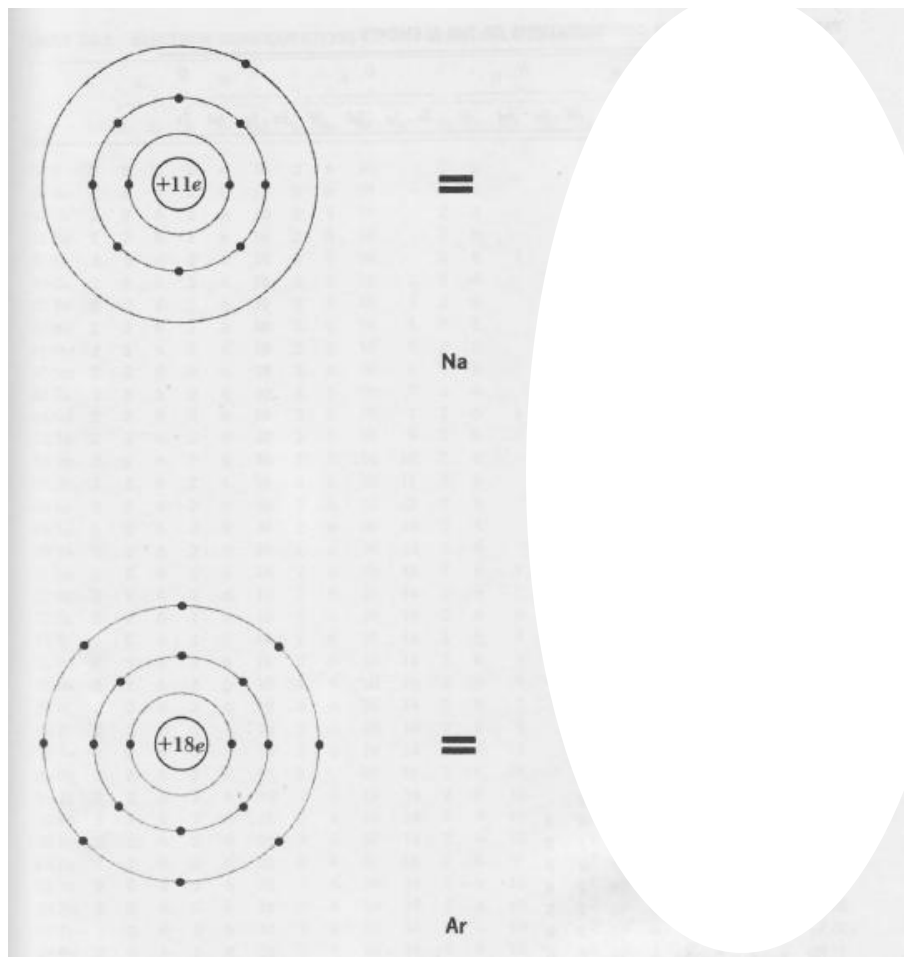
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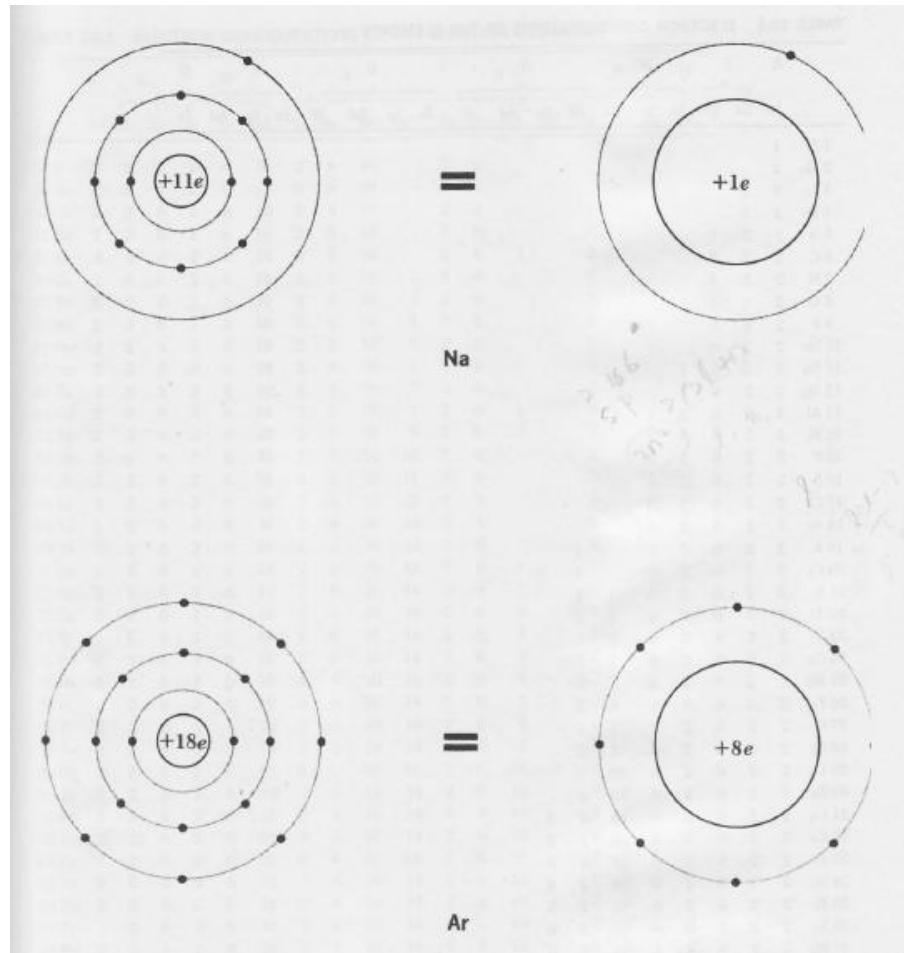
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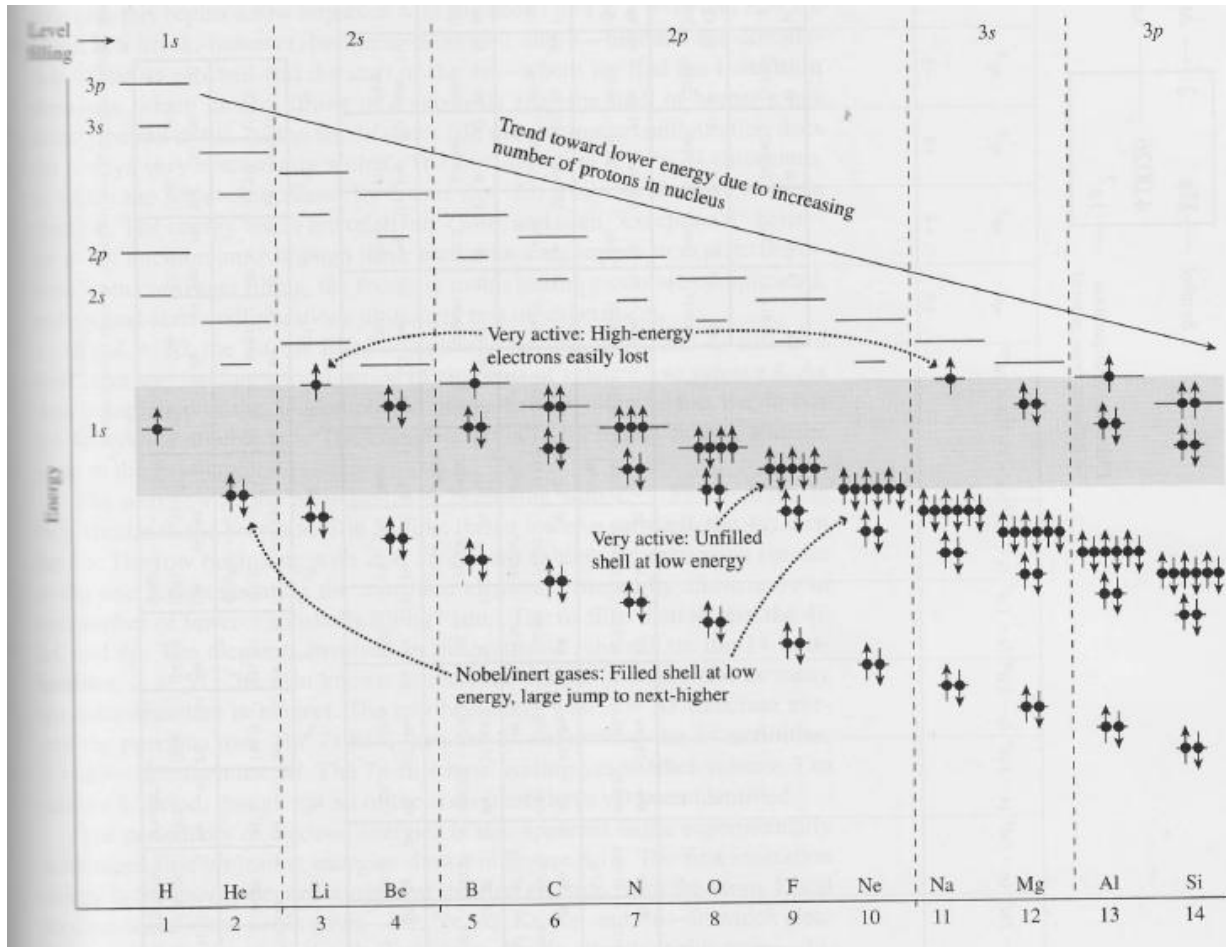
Effective charge of the nucleus



Effective charge of the nucleus



Orbital Energy levels



Ionization Energy

Figure 8.16 First ionization energies of the elements.

