

# Kvantová čísla

$$\frac{d^2\Phi}{d\varphi^2} + m^2\Phi = 0$$

$$\frac{1}{\sin\vartheta} \frac{d}{d\vartheta} \left( \sin\vartheta \frac{d\Theta}{d\vartheta} \right) + \left[ l(l+1) - \frac{m^2}{\sin^2\vartheta} \right] \Theta = 0$$

$$\frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{dR}{dr} \right) + \left[ \frac{2m_e}{\hbar^2} (E - U) - \frac{l(l+1)}{r^2} \right] R = 0$$

# Kvantová čísla

$$\Phi(\varphi) \quad \Phi(\varphi) = Ae^{im\varphi} \quad Ae^{im\varphi} = Ae^{im(\varphi+2\pi)}$$
$$m = 0, \pm 1, \pm 2, \pm 3, \dots$$

$$\Theta(\vartheta) \quad \text{Legendrovy polynomy} \quad l \geq |m|$$
$$m = 0, \pm 1, \pm 2, \dots, \pm l$$

$$R(r) \quad \text{Laguerovy polynomy} \quad n \geq l + 1$$
$$l = 0, 1, 2, \dots, (n - 1)$$

$$E_n = -\frac{me^4}{8\varepsilon_0^2 h^2} \frac{1}{n^2} \quad E > 0$$

# Kvantová čísla

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$$n = 1, 2, 3, \dots$$

Hlavní kvantové číslo

$$l = 0, 1, 2, \dots, (n - 1)$$

Orbitální kvantové číslo

$$m = 0, \pm 1, \pm 2, \dots, \pm l$$

Magnetické kvantové číslo

$$\psi = R_{n,l} \Theta_{l,m} \Phi_m$$

# Orbitální kvantové číslo

$$E = T_{rad} + T_{orb} + U$$

$$T_{orb} = \frac{\hbar^2 l(l+1)}{2m_e r^2} \quad T_{orb} = \frac{L^2}{2m_e r^2}$$

$$L = \sqrt{l(l+1)}\hbar$$

$l = 0 \ 1 \ 2 \ 3 \ 4 \ 5 \ 6 \ \dots$   
 $s \ p \ d \ f \ g \ h \ i \ \dots$

stavy momentu hybnosti

	s	p	d	f	g	h
	$l=0$	$l=1$	$l=2$	$l=3$	$l=4$	$l=5$
<b>n=1</b>	1s					
<b>n=2</b>	2s	2p				
<b>n=3</b>	3s	3p	3d			
<b>n=4</b>	4s	4p	4d	4f		
<b>n=5</b>	5s	5p	5d	5f	5g	
<b>n=6</b>	6s	6p	6d	6f	6g	6h

Symbolické značení stavů  
atomu vodíku

# Magnetické kvantové číslo

$$\mu = iA \quad \mu = -ef\pi r^2 \quad v = 2\pi fr$$

$$L = m_e v r = 2\pi m_e f r^2$$

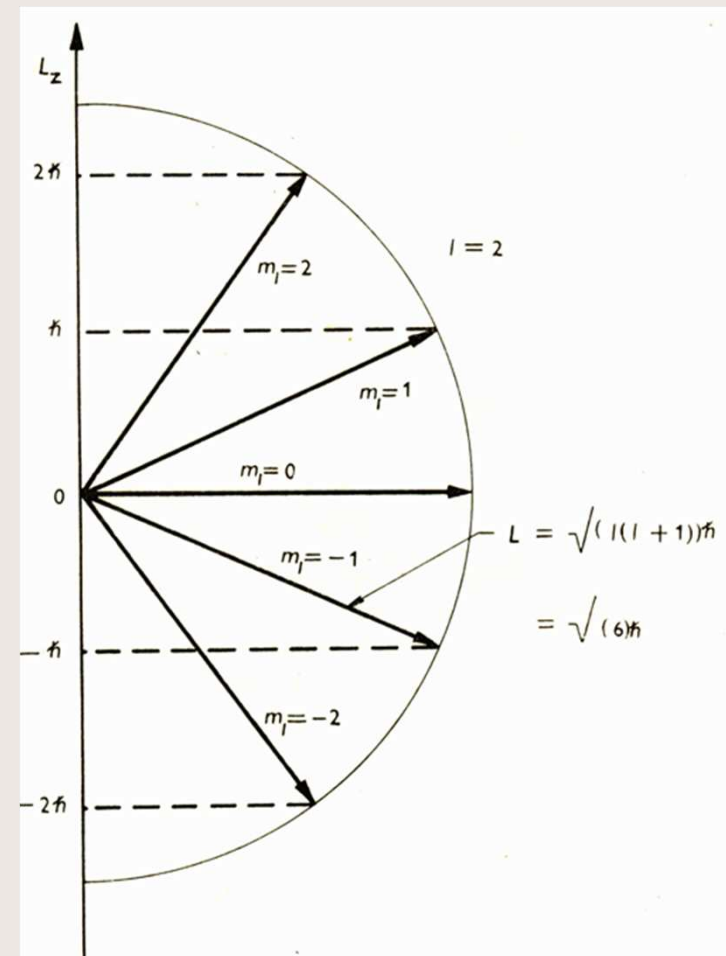
$$\vec{\mu} = -\left(\frac{e}{2m_e}\right)\vec{L}$$

gyromagnetický poměr

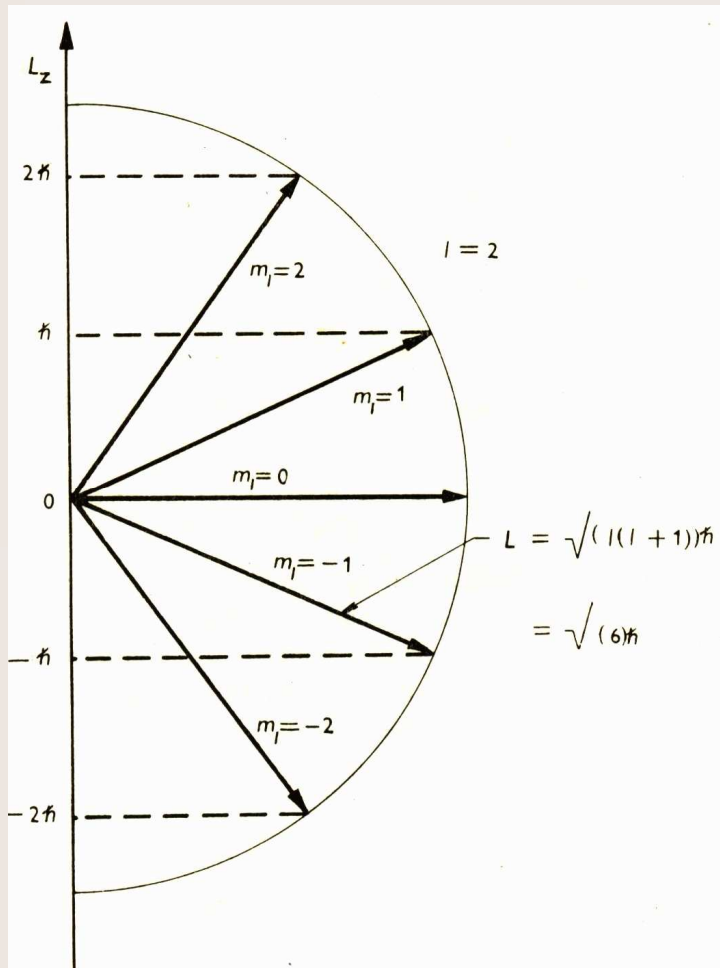
$$L = \sqrt{l(l+1)}\hbar$$

$$L_z = m\hbar$$

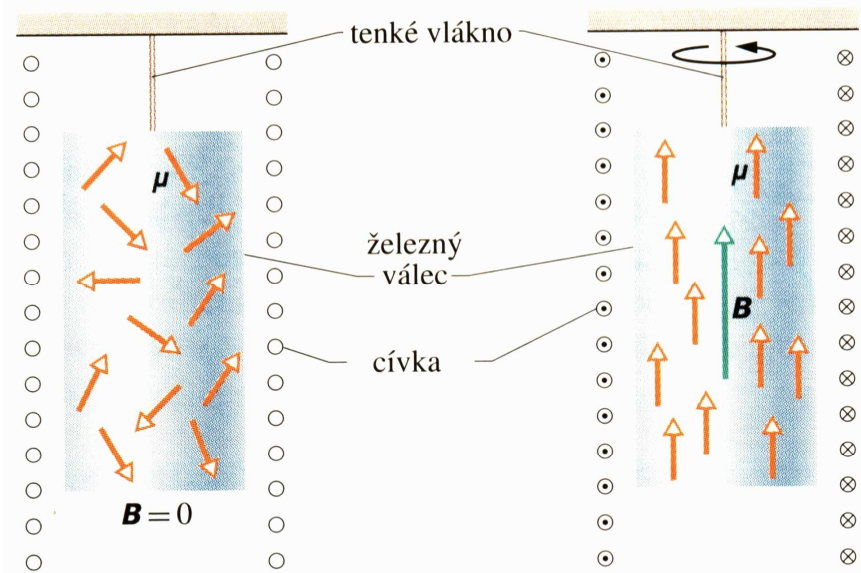
prostorové kvantování



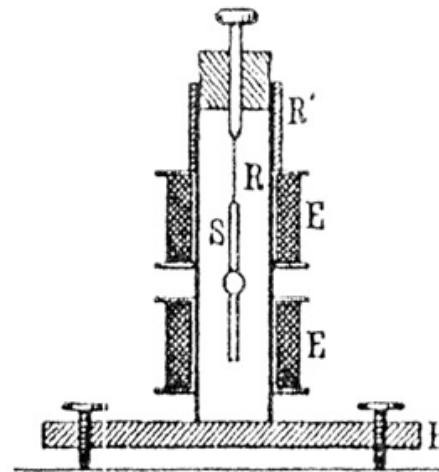
# Magnetické kvantové číslo



v obr. 41.4b).



(a) Einstein de Haasův pokus (b)

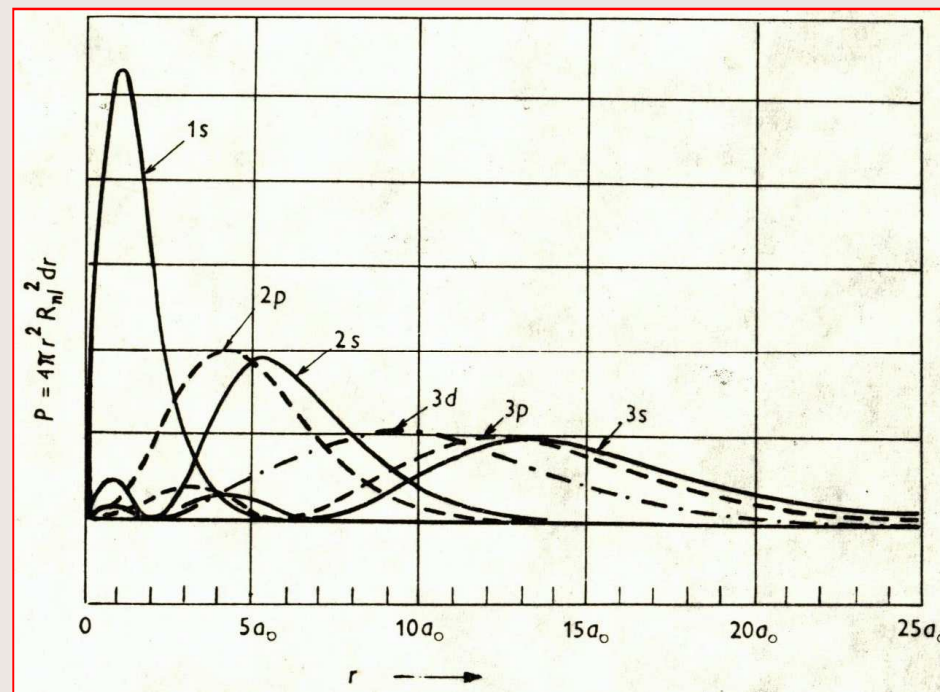
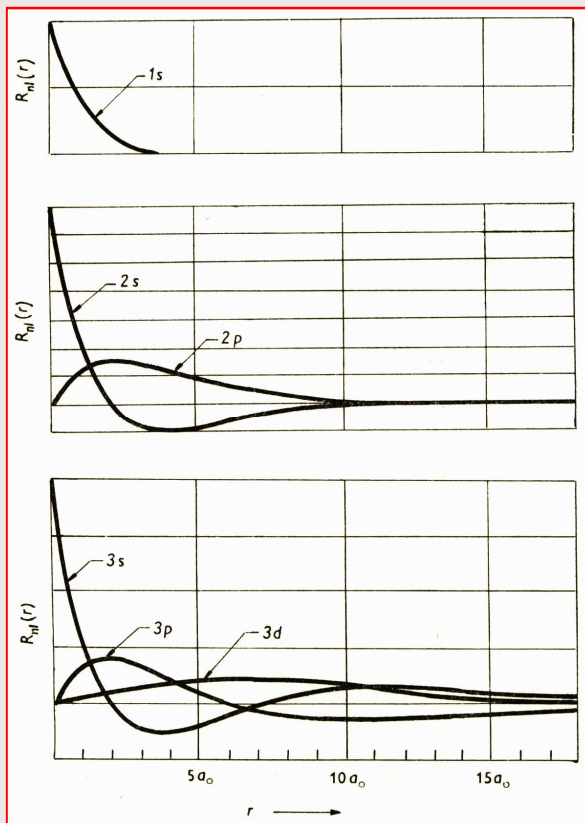




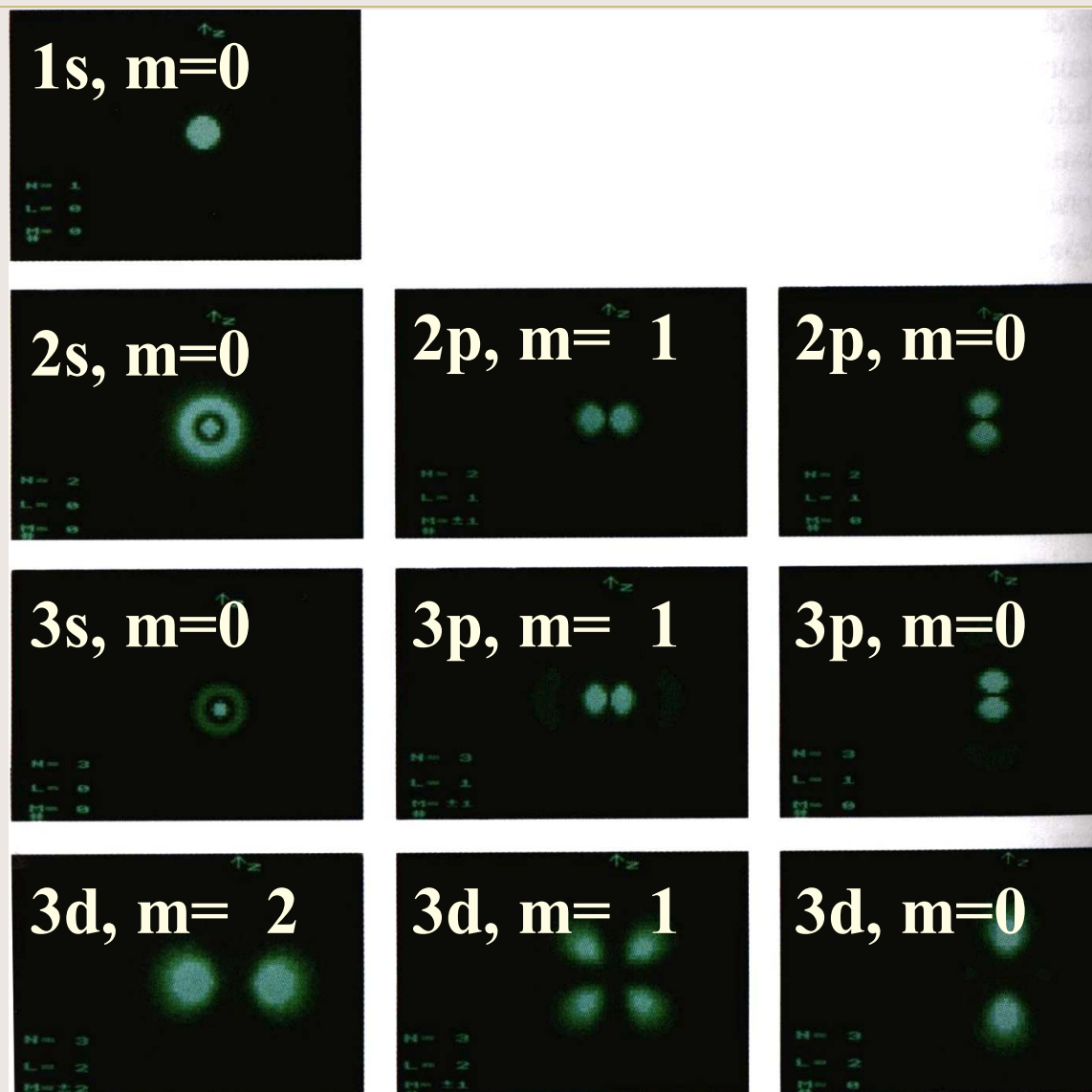
# Hustota pravděpodobnosti výskytu elektronu

$$\psi = R\Theta\Phi$$

$$|\psi|^2 = |R|^2 |\Theta|^2 |\Phi|^2$$



# Hustota pravděpodobnosti výskytu elektronu





# Mnohaelektronové atomy

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**Nesoulad předcházející kvantově mechanické teorie se dvěma experimentálními fakty.**

**1. Jemná struktura spektrálních čar. První čára Balmerovy série (přechod mezi hladinami  $n = 3$  a  $n = 2$ ) s  $\lambda = 6563 \text{ \AA}$  je ve skutečnosti tvořena dvěma čarami vzdálenými od sebe  $1,4 \text{ \AA}$ .**

**2. Anomální Zeemanův jev.**

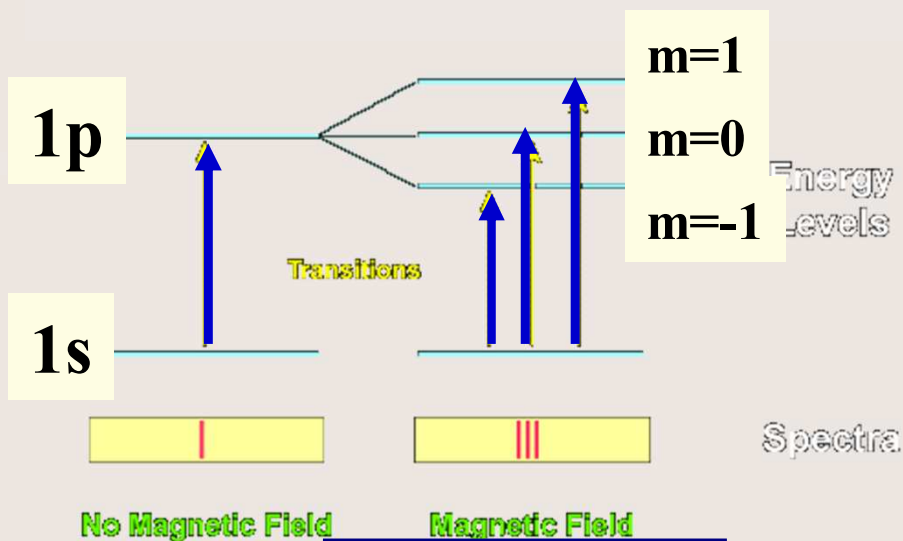
# Normální Zeemanův jev

$$\vec{\mu} = -\left(\frac{e}{2m_e}\right)\vec{L}$$

$$U = -\vec{\mu}\vec{B} = \mu B \cos \vartheta$$

$$\cos \vartheta = \frac{m}{\sqrt{l(l+1)}}$$

$$L = \sqrt{l(l+1)}\hbar$$



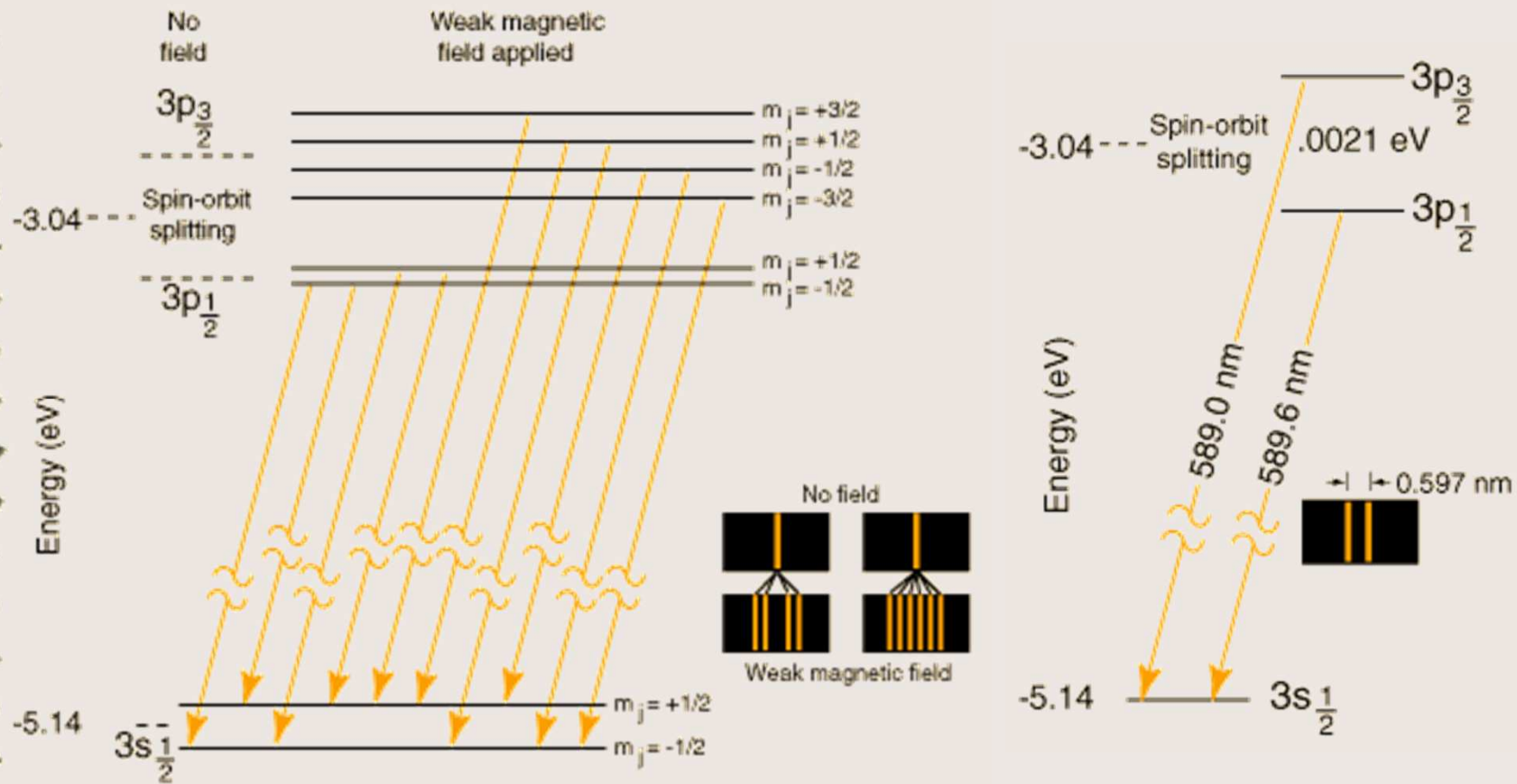
$$U = m \frac{e\hbar}{2m_e} B$$

$$f_1 = f_0 - \frac{e}{4\pi m_e} B$$

$$f_2 = f_0$$

$$f_3 = f_0 + \frac{e}{4\pi m_e} B$$

# Anomální Zeemanův jev



# Spin elektronu

**S.A. Goudsmit a G.E. Uhlenbeck:**  
elektron má vlastní, vnitřní moment hybnosti

$$S = \sqrt{s(s+1)}\hbar = \frac{\sqrt{3}}{2}\hbar$$

$$s = \frac{1}{2}$$

$$S_z = m_s\hbar = \pm\frac{1}{2}\hbar$$

$$\vec{\mu}_s = \frac{e}{m}\vec{S}$$

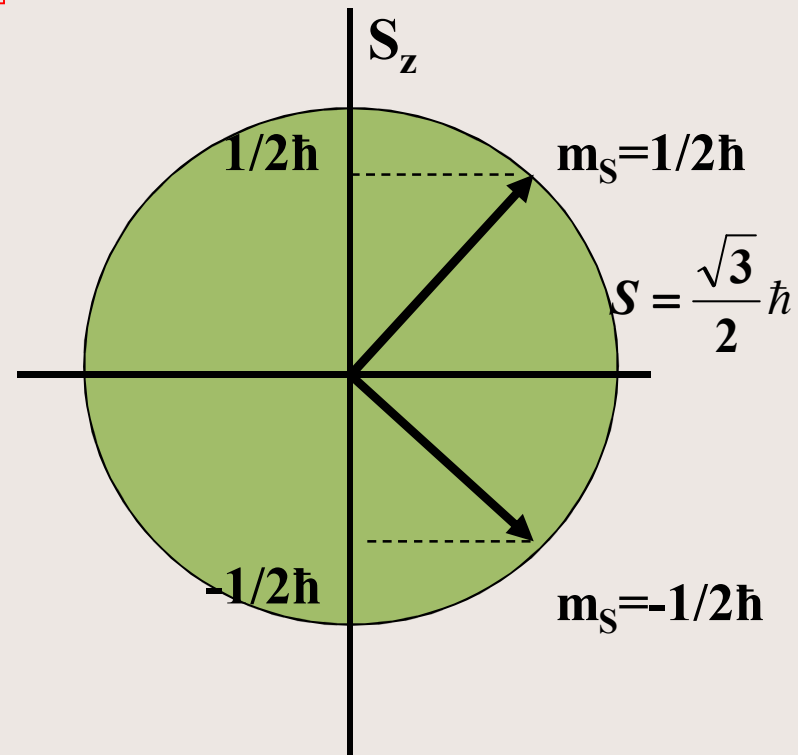
$$\mu_{S_z} = \pm\frac{e\hbar}{2m_e}$$

**Kvantová čísla**

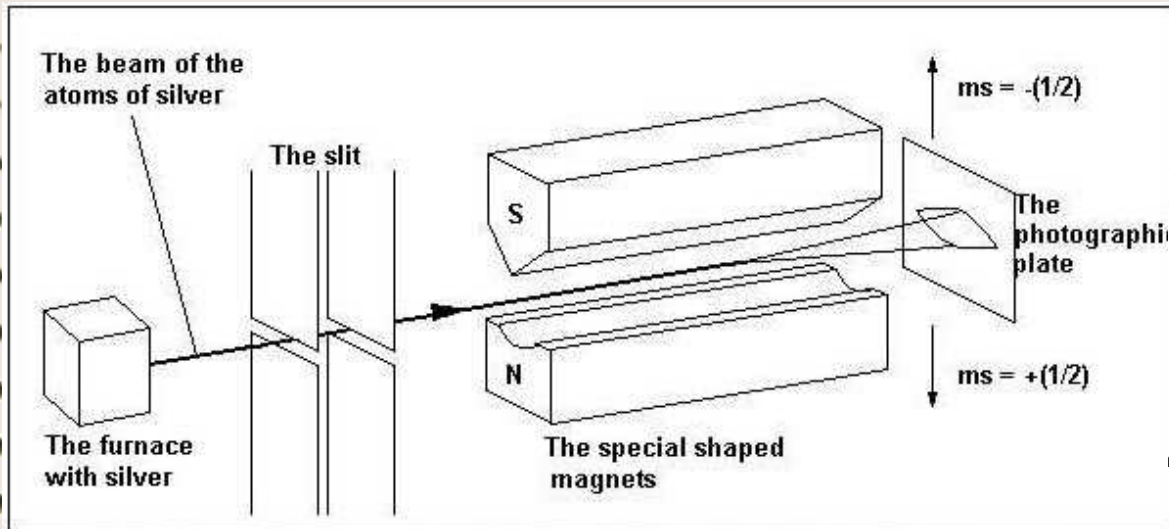
**n**

**l, m<sub>L</sub>**

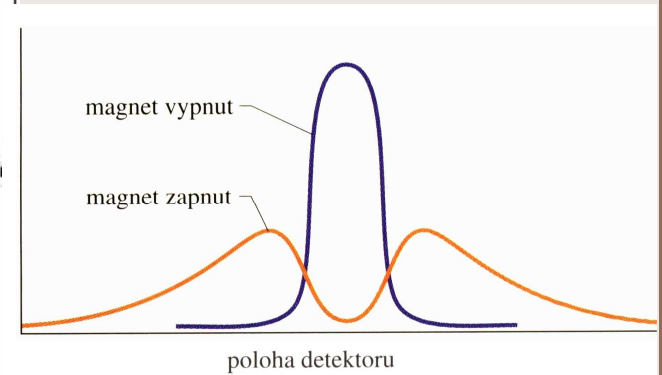
**s, m<sub>S</sub>**



# Stern-Gerlachův pokus

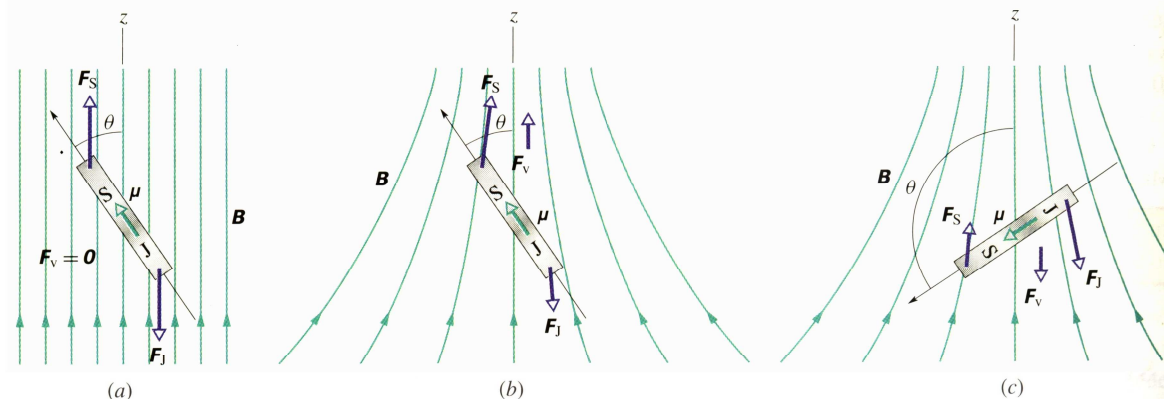


The Stern-Gerlach experiment. On the photographic plate are two clear tracks.



Obr. 41.10 Výsledky moderního opakování Sternova-Gerlachova pokusu.

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Obr. 41.9 Magnetický dipól, znázorněný jako tyčový magnet se dvěma póly (a) v homogenním magnetickém poli a (b, c) v

# Pauliho vylučovací princip

Žádné dva elektrony v atomu nemohou existovat ve stejném kvantovém stavu.

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

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

Symetrická vlnové funkce: bosony

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

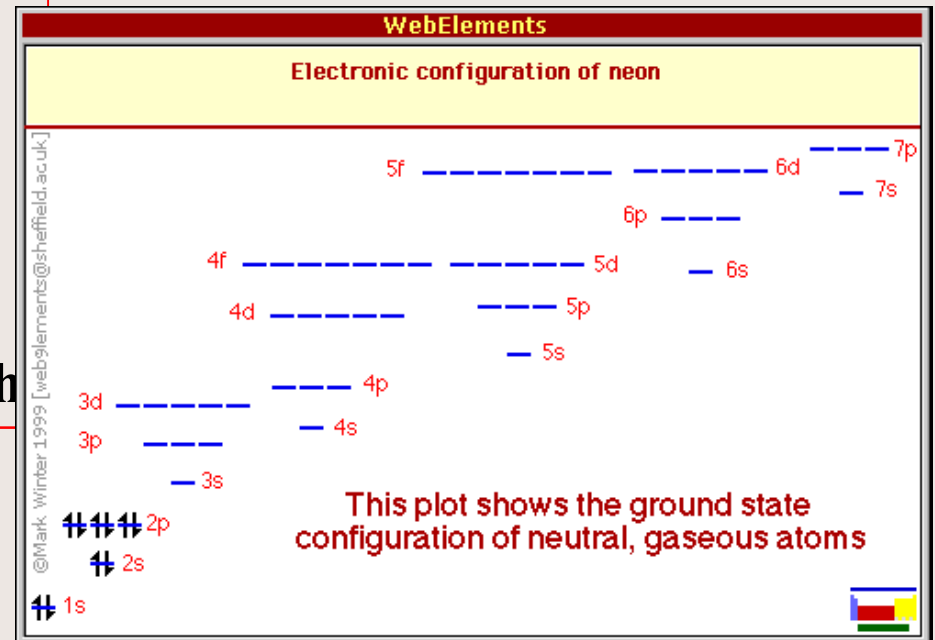
Asymetrická vlnové funkce: fermiony



# Elektronové konfigurace

1. Systém částic je stabilní, je-li jeho celková energie minimální.
2. V každém jednotlivém kvantovém stavu může existovat jen jeden elektron.

	s	p	d	f	g	h
	$l=0$	$l=1$	$l=2$	$l=3$	$l=4$	$l=5$
n=1	1s					
n=2	2s	2p				
n=3	3s	3p	3d			
n=4	4s	4p	4d	4f		
n=5	5s	5p	5d	5f	5g	
n=6	6s	6p	6d	6f	6g	6h



# Periodická soustava prvků

TABELLE II

REIHEN	GRUPPE I. — R <sup>2</sup> O	GRUPPE II. — RO	GRUPPE III. — R <sup>2</sup> O <sup>3</sup>	GRUPPE IV. RH <sup>4</sup> RO <sup>2</sup>	GRUPPE V. RH <sup>3</sup> R <sup>2</sup> O <sup>5</sup>	GRUPPE VI. RH <sup>2</sup> RO <sup>3</sup>	GRUPPE VII. RH R <sup>2</sup> O <sup>7</sup>	GRUPPE VIII. — RO <sup>4</sup>
1	H=1							
2	Li=7	Be=9,4	B=11	C=12	N=14	O=16	F=19	
3	Na=23	Mg=24	Al=27,3	Si=28	P=31	S=32	Cl=35,5	
4	K=39	Cd=40	—=44	Ti=48	V=51	Cr=52	Mn=55	Fe=56, Co=59, Ni=59, Cu=63.
5	(Cu=63)	Zn=65	—=68	—=72	As=75	Se=76	Br=80	
6	Rb=85	Sr=87	?Yt=88	Zr=90	Nb=94	Mo=96	—=100	Ru=104, Rh=104, Pd=106, Ag=108.
7	(Ag=108)	Cd=112	In=113	Sn=118	Sb=122	Te=125	J=127	
8	Cs=133	Ba=137	?Di=138	?Ce=140	—	—	—	— — — —
9	(—)	—	—	—	—	—	—	
10	—	—	?Er=178	?La=180	Ta=182	W=184	—	Os=195, Ir=197, Pt=198, Au=199.
11	(Au=199)	Hg=200	Tl=204	Pb=207	Bi=208	—	—	
12	—	—	—	Th=231	—	U=240	—	— — — —

**Figure 2.5** Dmitri Mendeleev's 1872 periodic table. The spaces marked with blank lines represent elements that Mendeleev deduced existed but were unknown at the time, so he left places for them in the table. The symbols at the top of the columns (e.g., R<sup>2</sup>O and RH<sup>4</sup>) are molecular formulas written in the style of the 19th century.

# Periodická soustava prvků

## Periodic Table of the Elements

1	New												18																																																										
1A	Original												VIIA																																																										
1 H Hydrogen (1.008)	2 He Helium (4.0026)											3 B Boron (10.81)	4 C Carbon (12.011)	5 N Nitrogen (14.007)	6 O Oxygen (15.999)	7 F Fluorine (18.998)	8 Ne Neon (20.180)	9 Li Lithium (6.941)	10 Be Beryllium (9.0122)	11 Na Sodium (22.990)	12 Mg Magnesium (24.305)	13 Al Aluminum (26.982)	14 Si Silicon (28.086)	15 P Phosphorus (30.974)	16 S Sulfur (32.06)	17 Cl Chlorine (35.453)	18 Ar Argon (39.948)																																												
19 K Potassium (39.098)	20 Ca Calcium (40.078)	21 Sc Scandium (44.956)	22 Ti Titanium (47.88)	23 V Vanadium (50.942)	24 Cr Chromium (52.00)	25 Mn Manganese (54.938)	26 Fe Iron (55.845)	27 Co Cobalt (58.933)	28 Ni Nickel (58.69)	29 Cu Copper (63.546)	30 Zn Zinc (65.38)	31 Ga Gallium (69.723)	32 Ge Germanium (72.63)	33 As Arsenic (74.922)	34 Se Selenium (78.96)	35 Br Bromine (79.904)	36 Kr Krypton (83.798)	37 Rb Rubidium (85.468)	38 Sr Strontium (87.62)	39 Y Yttrium (88.906)	40 Zr Zirconium (91.224)	41 Nb Niobium (92.906)	42 Mo Molybdenum (95.94)	43 Tc Technetium (98)	44 Ru Ruthenium (101.07)	45 Rh Rhodium (102.91)	46 Pd Palladium (106.42)	47 Ag Silver (107.87)	48 Cd Cadmium (112.41)	49 In Indium (114.82)	50 Sn Tin (118.71)	51 Sb Antimony (121.76)	52 Te Tellurium (127.6)	53 I Iodine (126.91)	54 Xe Xenon (131.29)	55 Cs Cesium (132.91)	56 Ba Barium (137.33)	57-71 Lanthanide series	72 Hf Hafnium (178.49)	73 Ta Tantalum (180.95)	74 W Tungsten (183.84)	75 Re Rhenium (186.21)	76 Os Osmium (190.23)	77 Ir Iridium (192.22)	78 Pt Platinum (195.08)	79 Au Gold (196.967)	80 Hg Mercury (200.59)	81 Tl Thallium (204.38)	82 Pb Lead (207.2)	83 Bi Bismuth (208.98)	84 Po Polonium (209)	85 At Astatine (210)	86 Rn Radon (222)	87 Fr Francium (223)	88 Ra Radium (226)	89-103 Actinide series	104 Rf Rutherfordium (261)	105 Db Dubnium (262)	106 Sg Seaborgium (263)	107 Bh Bohrium (264)	108 Hs Hassium (265)	109 Mt Meitnerium (266)	110 Ds Darmstadtium (271)	111 Rg Roentgenium (272)	112 Uub Ununbium (285)	113 Uut Ununtrium (288)	114 Uuq Ununquadium (289)	115 Uup Ununpentium (288)	116 Uuh Ununhexium (289)	117 Uue Ununseptium (289)	118 Uuo Ununoctium (289)

Atomic masses in parentheses are those of the most stable or common isotope.

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Note: This table is based on IUPAC's 2002 periodic table. The names of elements 112-118 are the IUPAC's temporary names.

57 La Lanthanum (138.905)	58 Ce Cerium (140.12)	59 Pr Praseodymium (140.908)	60 Nd Neodymium (144.24)	61 Pm Promethium (145)	62 Sm Samarium (150.36)	63 Eu Europium (151.964)	64 Gd Gadolinium (157.25)	65 Tb Terbium (158.925)	66 Dy Dysprosium (162.50)	67 Ho Holmium (164.930)	68 Er Erbium (167.259)	69 Tm Thulium (168.934)	70 Yb Ytterbium (173.054)	71 Lu Lutetium (174.967)
89 Ac Actinium (227)	90 Th Thorium (232.038)	91 Pa Protactinium (231.036)	92 U Uranium (238.029)	93 Np Neptunium (237)	94 Pu Plutonium (244)	95 Am Americium (243)	96 Cm Curium (247)	97 Bk Berkelium (247)	98 Cf Californium (251)	99 Es Einsteinium (252)	100 Fm Fermium (257)	101 Md Mendelevium (258)	102 No Nobelium (259)	103 Lr Lawrencium (260)

# Periodická soustava prvků

## Chrom

