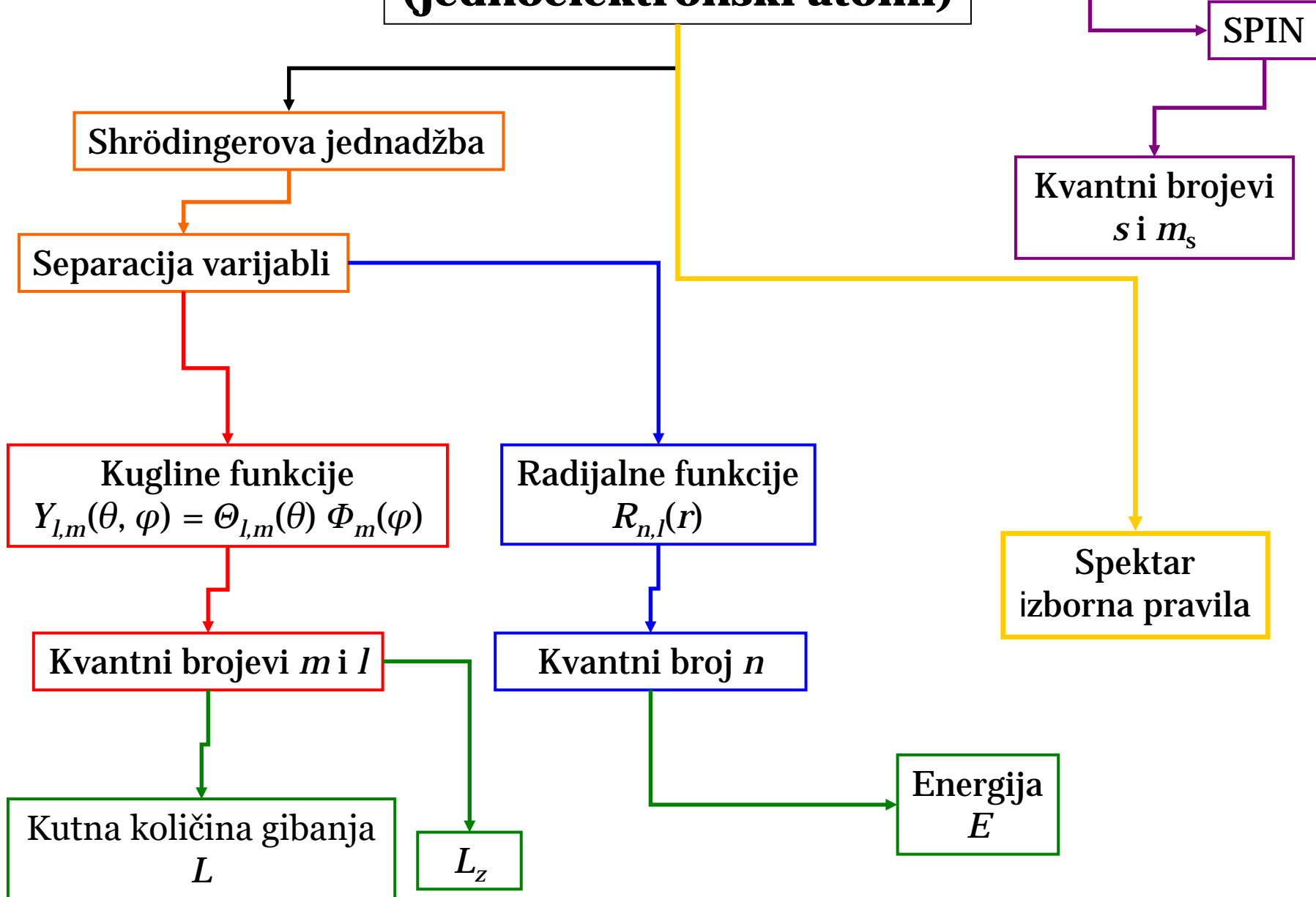


# VODIKOV ATOM H (jednoelektronski atomi)



Shrödingerova jednađba

Separacija varijabli

Kugline funkcije

$$Y_{l,m}(\theta, \varphi) = \Theta_{l,m}(\theta) \Phi_m(\varphi)$$

Kvantni brojevi  $m$  i  $l$

Kutna količina gibanja  
 $L$

$L_z$

Radijalne funkcije

$$R_{n,l}(r)$$

Kvantni broj  $n$

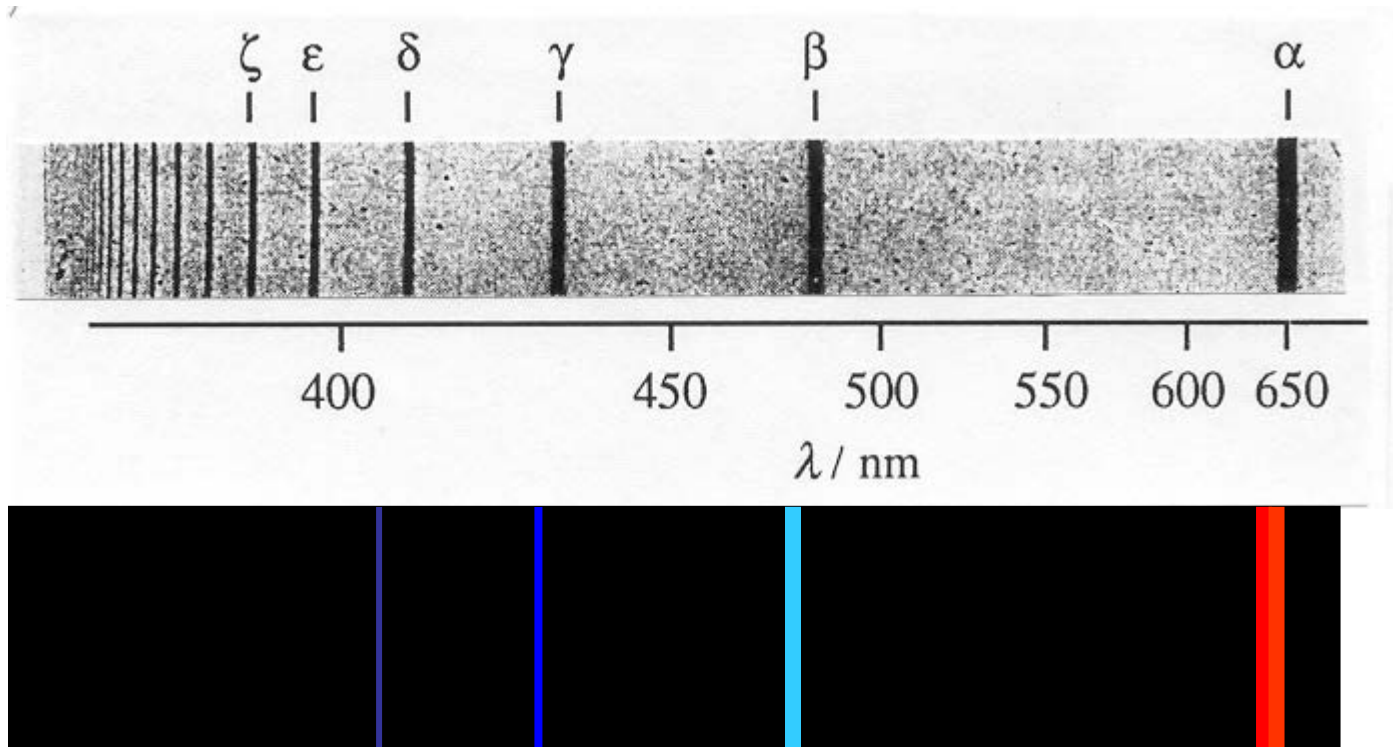
Energija  
 $E$

SPIN

Kvantni brojevi  
 $s$  i  $m_s$

Spektar  
izborna pravila

# Atomski spektri - Balmerova serija



$$E_e = -hcR_\infty \frac{\mu}{m_e} \cdot \frac{1}{n^2}$$

# Shrödingerova jednadžba za jednoelektronske atome

$$i) \quad H = \frac{p_e^2}{2m_e} + \frac{p_N^2}{2m_N} - \frac{1}{4\pi\epsilon_0} \frac{Ze^2}{r}$$


$$ii) \quad \hat{H} = -\frac{\hbar^2}{2m_e} \nabla_e^2 + -\frac{\hbar^2}{2m_N} \nabla_N^2 - \frac{1}{4\pi\epsilon_0} \frac{Ze^2}{r}$$

$$iii) \quad \hat{H} \Psi = -\frac{\hbar^2}{2m_e} \nabla_e^2 \Psi + -\frac{\hbar^2}{2m_N} \nabla_N^2 \Psi - \frac{1}{4\pi\epsilon_0} \frac{Ze^2}{r} \Psi = E\Psi$$

-odvajanje translacije od internog gibanja i uvođenje reducirane mase

$$iv) \quad X = \frac{m_e x_e + m_N x_N}{m_e + m_N}, \quad Y = \frac{m_e y_e + m_N y_N}{m_e + m_N}, \quad Z = \frac{m_e z_e + m_N z_N}{m_e + m_N}$$

$$x = x_e - x_N, \quad y = y_e - y_N, \quad z = z_e - z_N$$


$$\Psi(X, Y, Z, x, y, z) = \Psi(X)\Psi(Y)\Psi(Z)\psi(x, y, z)$$

Schrödingerova jednadžba za interno gibanje → separacija varijabli → polarne koordinate

$$v) \quad \hat{H} = -\frac{\hbar^2}{2\mu} \nabla^2 \psi - \frac{1}{4\pi\epsilon_0} \frac{Ze^2}{r} \psi = E_e \psi$$

# Polarne koordinate

$$r = \sqrt{x^2 + y^2 + z^2}$$

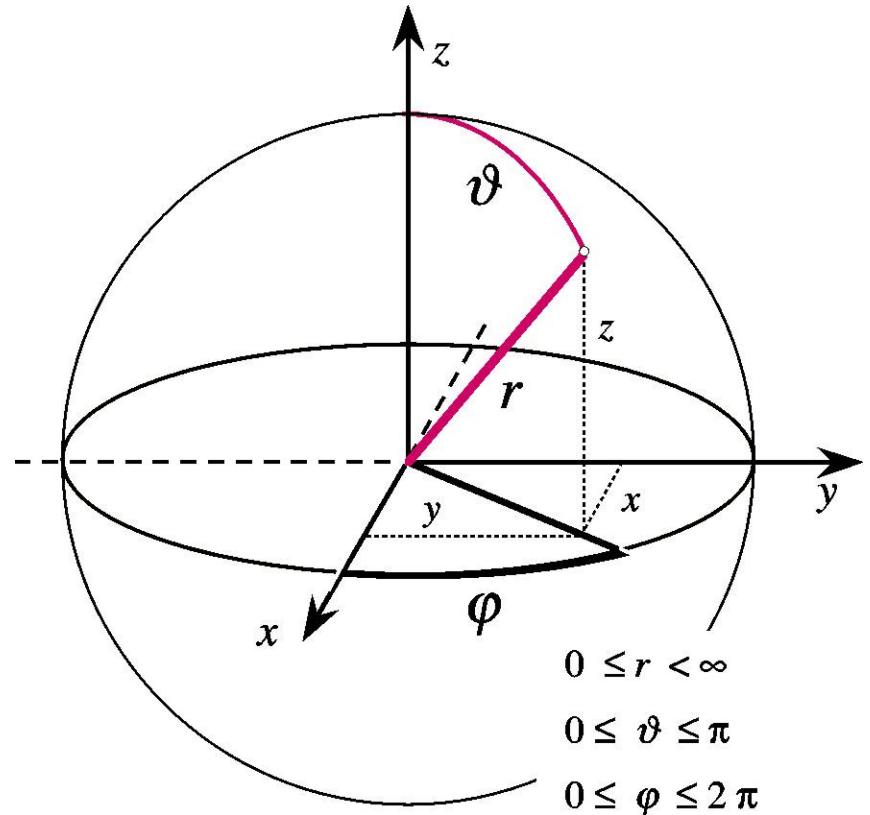
$$\vartheta = \arctan \left\{ \left( \frac{x^2 + y^2}{z^2} \right)^{1/2} \right\}$$

$$\varphi = \arctan \left( \frac{y}{x} \right)$$

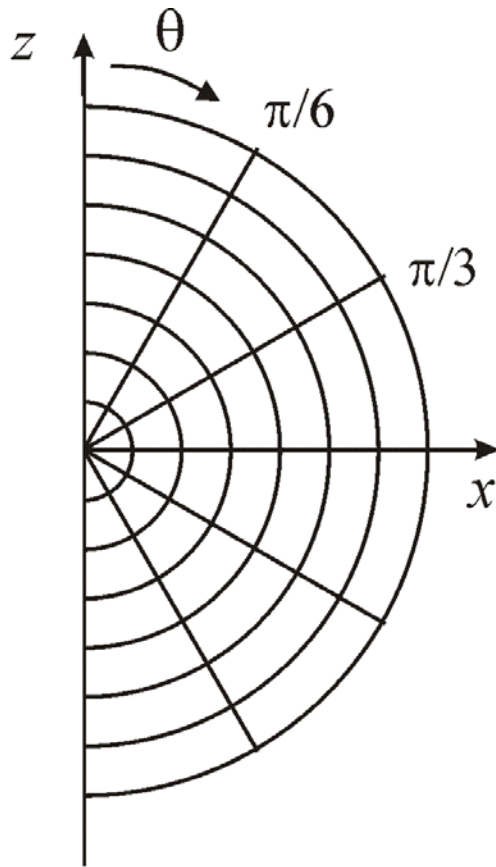
$$x = r \sin \vartheta \cos \varphi$$

$$y = r \sin \vartheta \sin \varphi$$

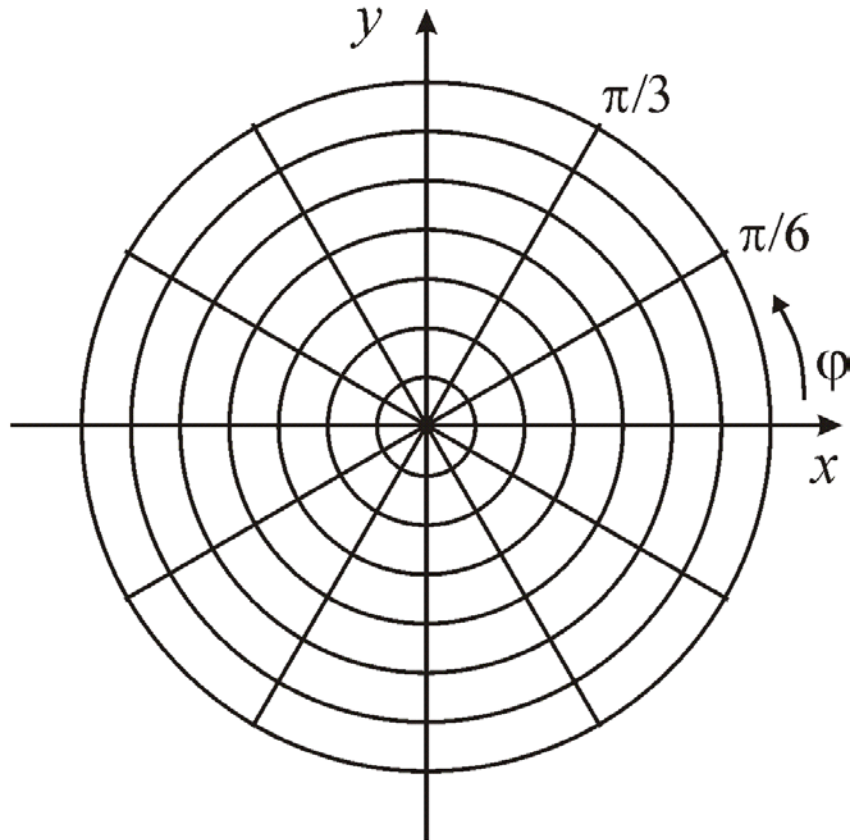
$$z = r \cos \vartheta$$



# Polare koordinate



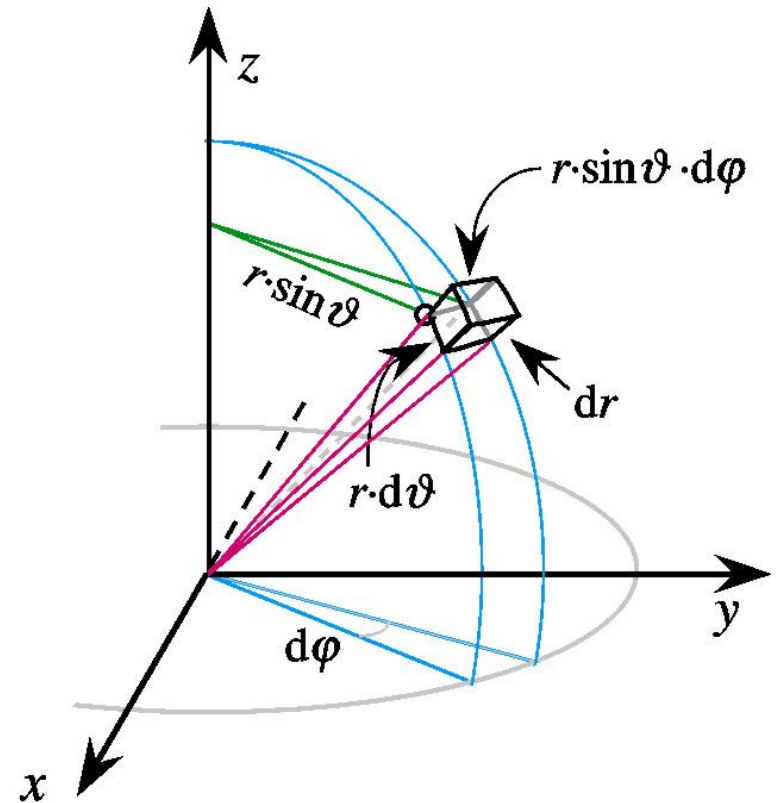
$\theta$

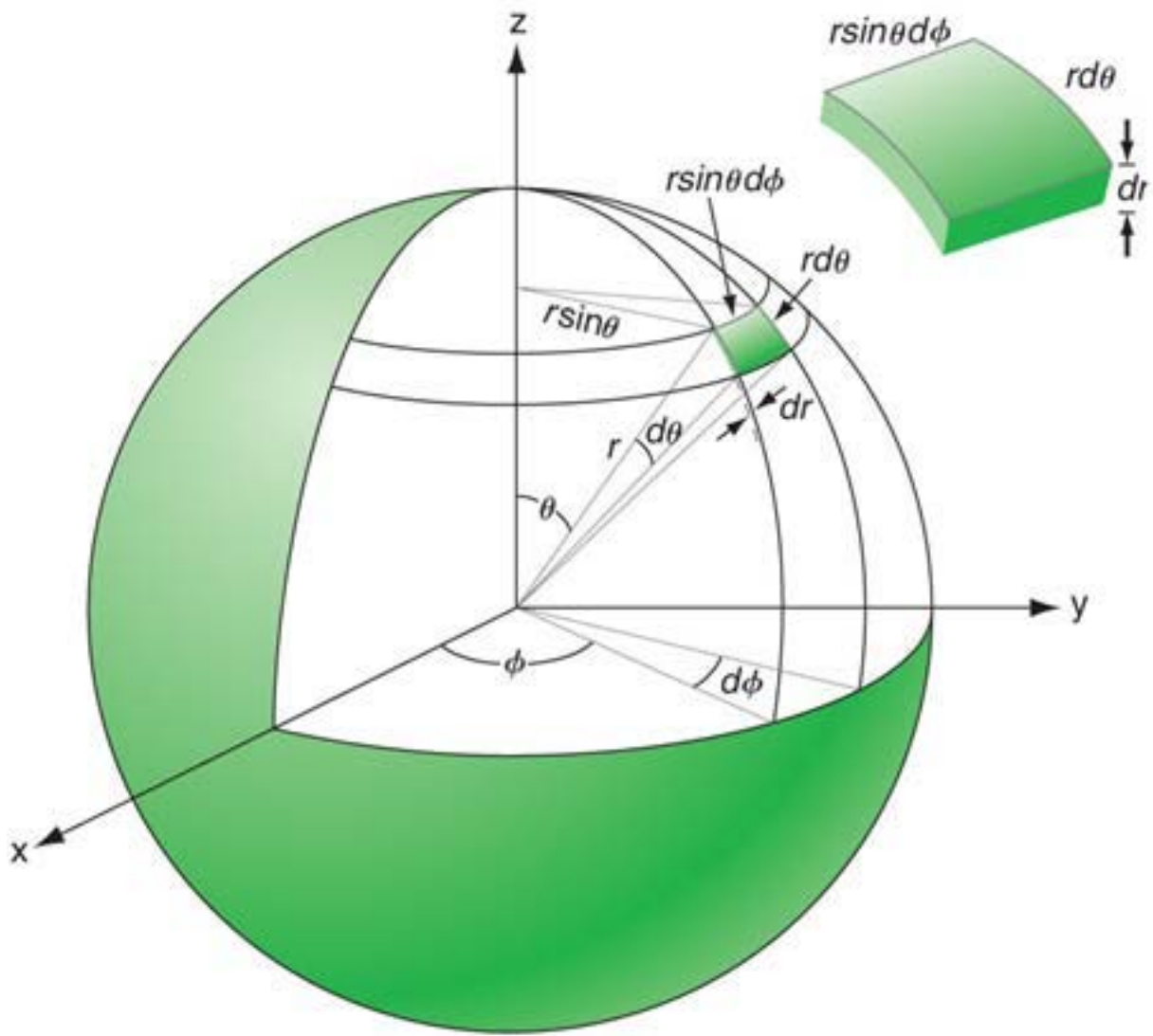


$\varphi$

# Element prostora

$$\begin{aligned}d\tau &= dr \cdot r d\vartheta \cdot r \sin \vartheta d\varphi \\ &= r^2 \sin \vartheta d\varphi d\vartheta dr\end{aligned}$$





$$\nabla^2 = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) - \frac{1}{r^2} \frac{\hat{L}^2}{\hbar^2}$$

$$\hat{L}^2 = -\hbar^2 \left\{ \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \varphi^2} \right\}$$

$$\Psi(r, \vartheta, \varphi) = R(r) \cdot \Phi(\varphi) \cdot \Theta(\vartheta)$$

$$\frac{-\hbar^2}{2\mu r^2} \left\{ \frac{\partial}{\partial r} \left( r^2 \frac{\partial \psi}{\partial r} \right) - \frac{\hat{L}^2 \psi}{\hbar^2} \right\} - \frac{1}{4\pi\epsilon_0} \frac{Ze^2 \psi}{r} = E_e \psi$$

$$-\hbar^2 \left\{ \frac{\partial}{\partial r} \left( r^2 \frac{\partial R(r)}{\partial r} \right) \right\} \cdot \Phi(\varphi) \cdot \Theta(\vartheta) - \frac{1}{4\pi\epsilon_0} \frac{Ze^2 R(r) \cdot \Phi(\varphi) \cdot \Theta(\vartheta)}{r} - 2\mu r^2 E_e R(r) \cdot \Phi(\varphi) \cdot \Theta(\vartheta) = \hat{L}^2 R(r) \cdot \Phi(\varphi) \cdot \Theta(\vartheta)$$

$$\frac{-\hbar^2}{R(r)} \left\{ \frac{\partial}{\partial r} \left( r^2 \frac{\partial R(r)}{\partial r} \right) \right\} - \frac{1}{4\pi\epsilon_0} \frac{Ze^2}{r} - 2\mu r^2 E_e = \frac{\hat{L}^2 \Phi(\varphi) \cdot \Theta(\vartheta)}{\Phi(\varphi) \cdot \Theta(\vartheta)}$$

$$\frac{-\hbar^2}{2\mu r^2} \left\{ \frac{d^2 R(r)}{dr^2} + \frac{2}{r} \frac{dR(r)}{dr} + \frac{\beta}{r^2} R(r) \right\} - \frac{1}{4\pi\epsilon_0} \frac{Ze^2 R(r)}{r} = E_e R(r)$$

$$\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial Y}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2 Y}{\partial \varphi^2} = -\beta Y; \quad Y = \Phi(\varphi) \cdot \Theta(\vartheta)$$



$$Y(\theta, \varphi) = \Phi(\varphi) \cdot \Theta(\mathcal{G})$$

$$\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial Y}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2 Y}{\partial \varphi^2} = -\beta Y$$

$$\frac{\sin \theta}{\Theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial \Theta}{\partial \theta} \right) + \beta \sin^2 \theta = -\frac{1}{\Phi} \frac{\partial^2 \Phi}{\partial \varphi^2} = \alpha$$

$$\frac{d^2 \Phi(\varphi)}{d\varphi^2} = -\alpha \Phi(\varphi)$$

$$\frac{\sin \theta}{\Theta(\mathcal{G})} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial \Theta(\mathcal{G})}{\partial \theta} \right) + \beta \sin^2 \theta = -\frac{1}{\Phi} \frac{\partial^2 \Phi(\varphi)}{\partial \varphi^2} = \alpha$$

$$\frac{d^2 \Theta(\mathcal{G})}{d\theta^2} + \frac{\cos \theta}{\sin \theta} \frac{d\Theta(\mathcal{G})}{d\theta} - \frac{\alpha}{\sin^2 \theta} \Theta(\mathcal{G}) + \beta \Theta(\mathcal{G}) = 0$$

$$\frac{d^2\Phi(\varphi)}{d\varphi^2} = -\alpha\Phi(\varphi)$$

$\Phi(\varphi)$  periodička za  $\alpha = m^2; m = 0, \pm 1, \pm 2, \dots$

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

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

$$l \geq |m|$$



$$l = 0, 1, \dots, n-1$$

$n$  iznosi minimalno  $l+1$

$$m_l = -l, -l+1, \dots, +l$$

$$\Psi_{n,l,m}(r, \vartheta, \varphi) = \Phi_m(\varphi) \cdot \Theta_{l,m}(\vartheta) \cdot R_{n,l}(r)$$

$$E_e = -hcZ^2 R_\infty \frac{\mu}{m_e} \cdot \frac{1}{n^2}$$

# Rješenja $\Phi$

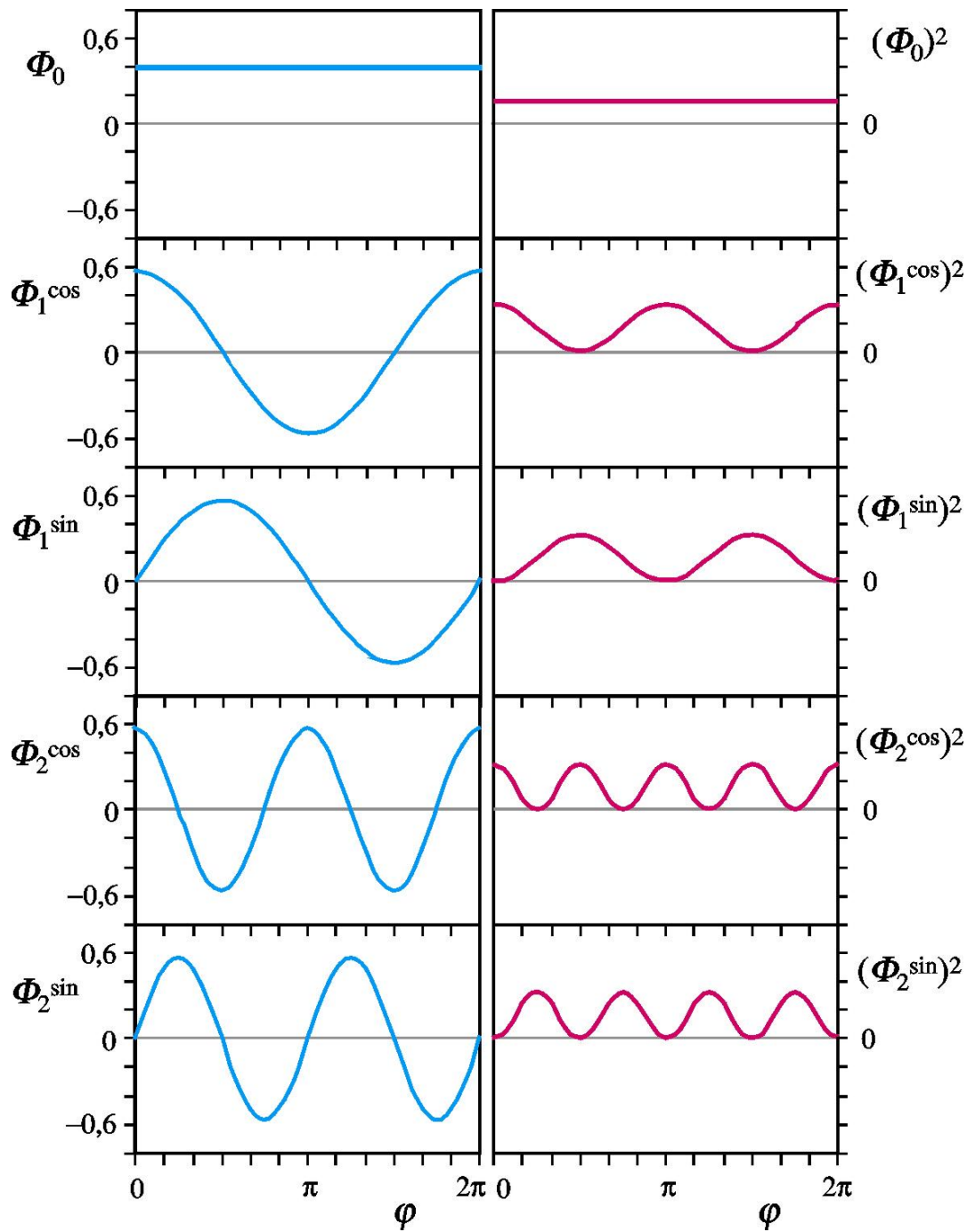
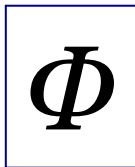
$$\Phi_m(\varphi) = \frac{1}{\sqrt{2\pi}} e^{im\varphi}$$

$$\Phi_m(\varphi) = \frac{1}{\sqrt{2\pi}} (\cos m\varphi + i \sin m\varphi)$$

$$\Phi_{|m|}^{\cos} = \frac{1}{\sqrt{2\pi}} \left\{ \Phi_{|m|} + \Phi_{-|m|} \right\} = \frac{1}{\sqrt{\pi}} \cos(|m|\varphi)$$

$$\Phi_{|m|}^{\sin} = \frac{-i}{\sqrt{2}} \left\{ \Phi_{|m|} - \Phi_{-|m|} \right\} = \frac{1}{\sqrt{\pi}} \sin(|m|\varphi)$$

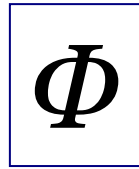
$$m = 0, \pm 1, \pm 2, \pm 3, \dots \pm l$$



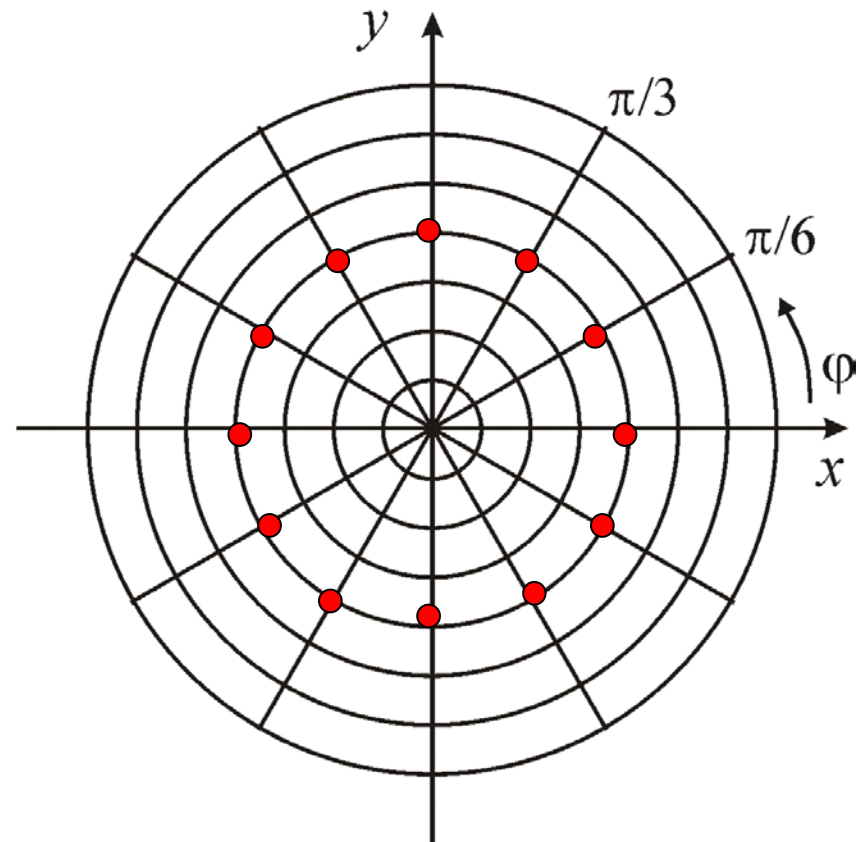
$$\Phi_m(\varphi) = \frac{1}{\sqrt{2\pi}} e^{im\varphi}$$

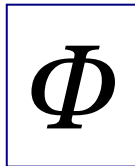
$$m = 0$$

$$\Phi_m(\varphi) = \frac{1}{\sqrt{2\pi}}$$

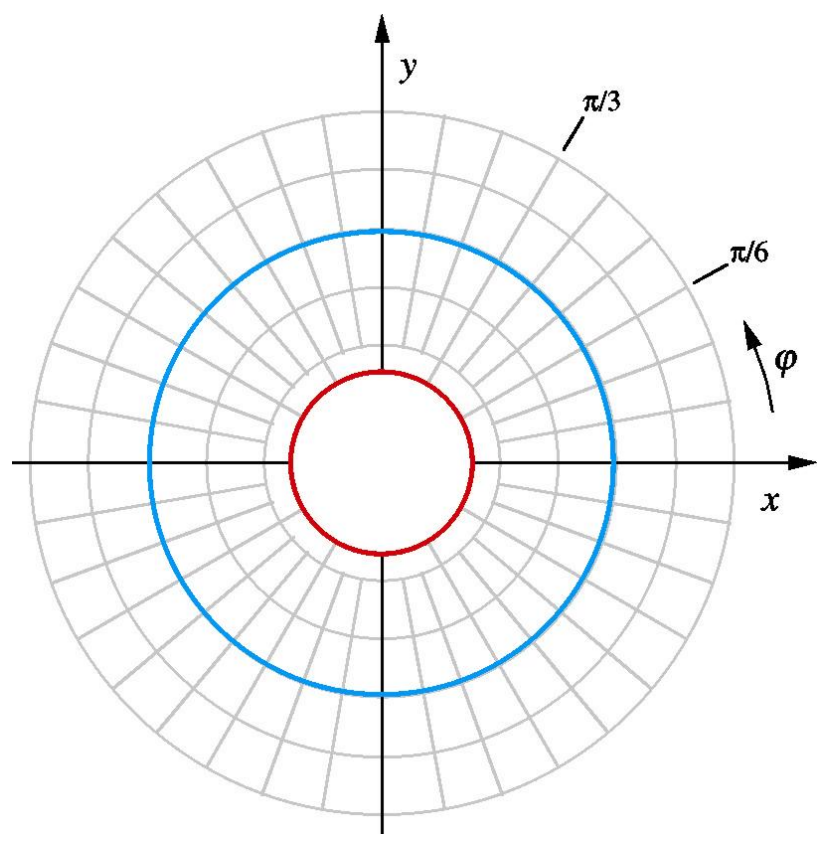
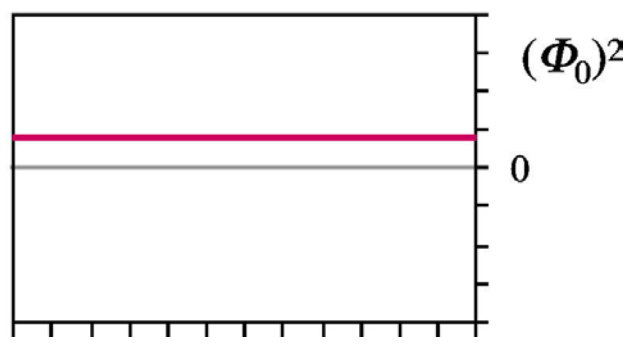
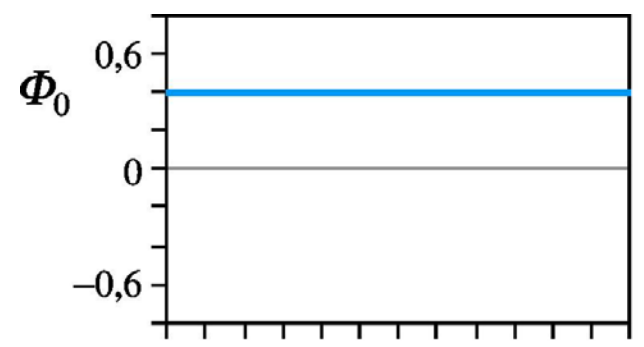


$\varphi$	$\varphi$	$\Phi$
0	0	0,399
$\pi/6$	30°	0,399
$\pi/3$	60°	0,399
$\pi/2$	90°	0,399
$4\pi/6$	120°	0,399
$5\pi/6$	150°	0,399
$\pi$	180°	0,399
$7\pi/6$	210°	0,399
$8\pi/6$	240°	0,399
$3\pi/2$	270°	0,399
$10\pi/6$	300°	0,399
$11\pi/6$	330°	0,399





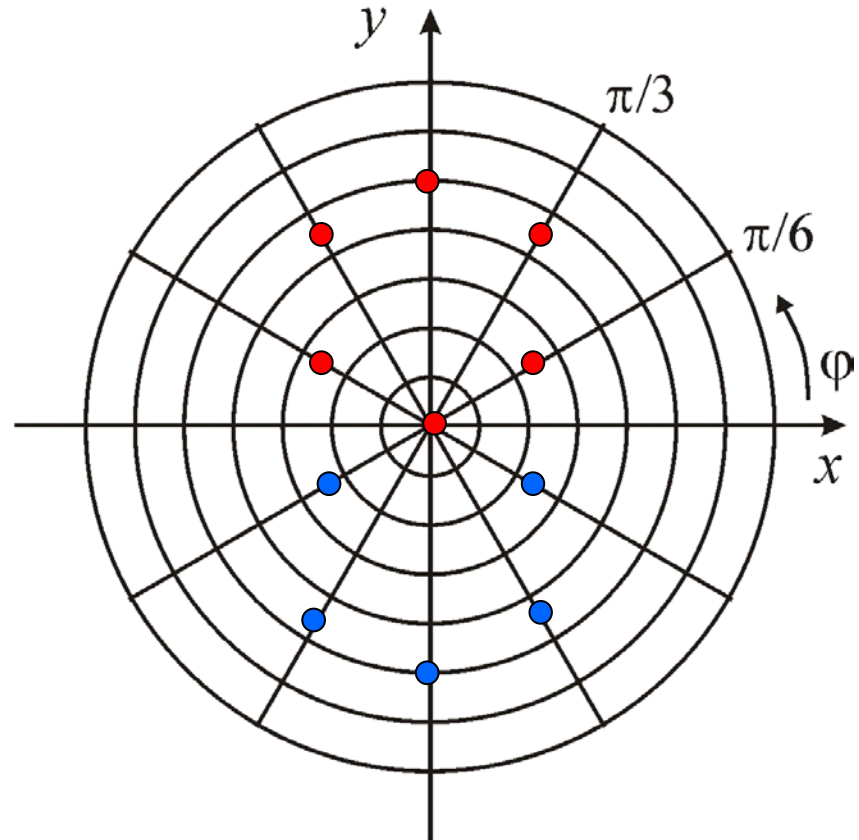
$$m = 0 \quad \Phi_0(\varphi) = \frac{1}{\sqrt{2\pi}}$$



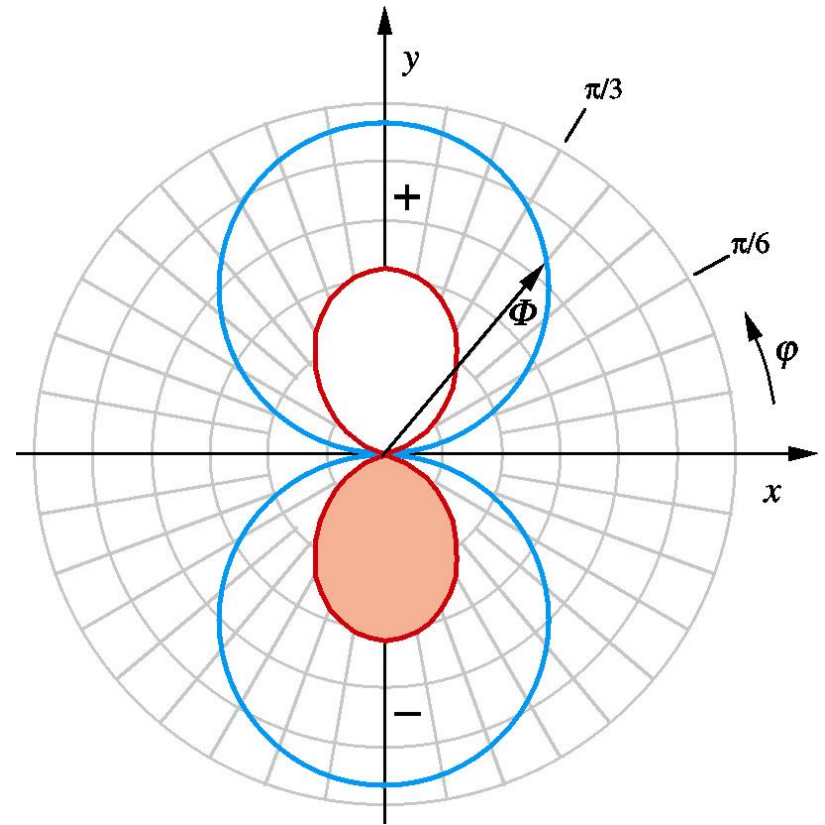
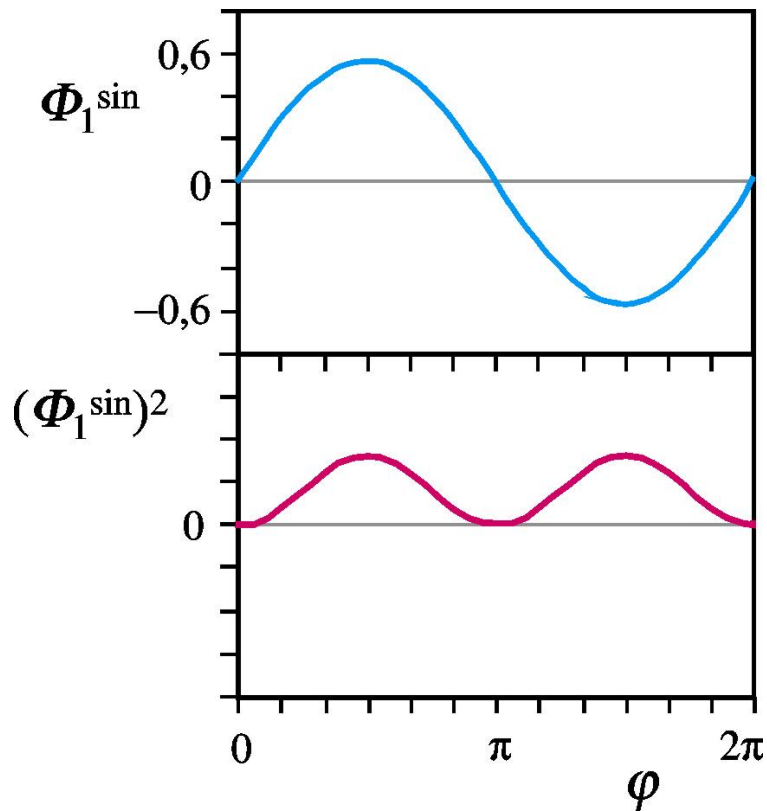
$$m = -1$$

$$\Phi_1^{\sin} = \frac{1}{\sqrt{\pi}} \sin(\varphi)$$

$\varphi$	$\varphi$	$\Phi$
0	0	0
$\pi/6$	30°	0.28
$\pi/3$	60°	0.49
$\pi/2$	90°	0.56
$\pi/6$	120°	0.49
$5\pi/6$	150°	0.28
$\pi$	180°	0
$7\pi/6$	210°	-0.28
$8\pi/6$	240°	-0.49
$3\pi/2$	270°	-0.56
$10\pi/6$	300°	-0.49
$11\pi/6$	330°	-0.28

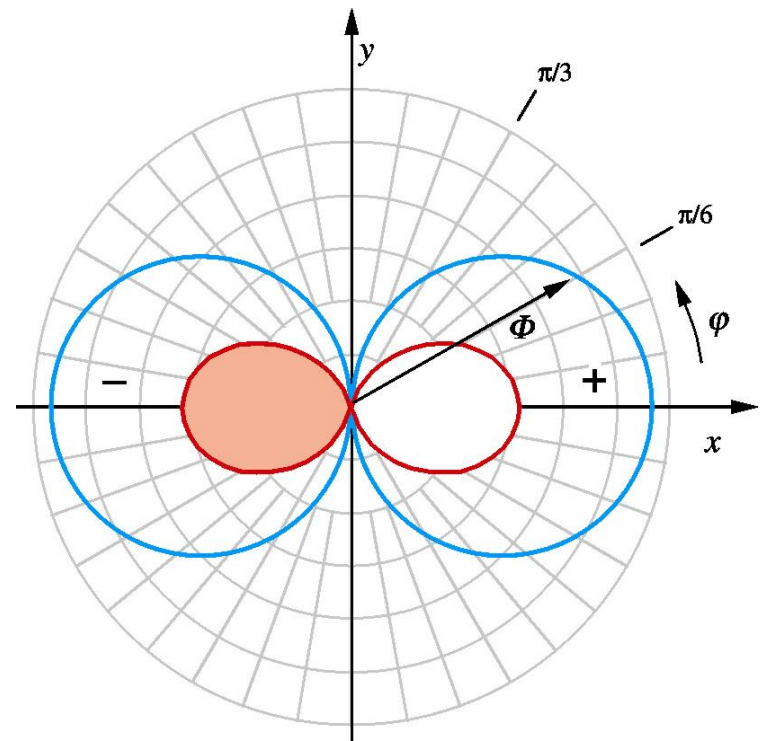
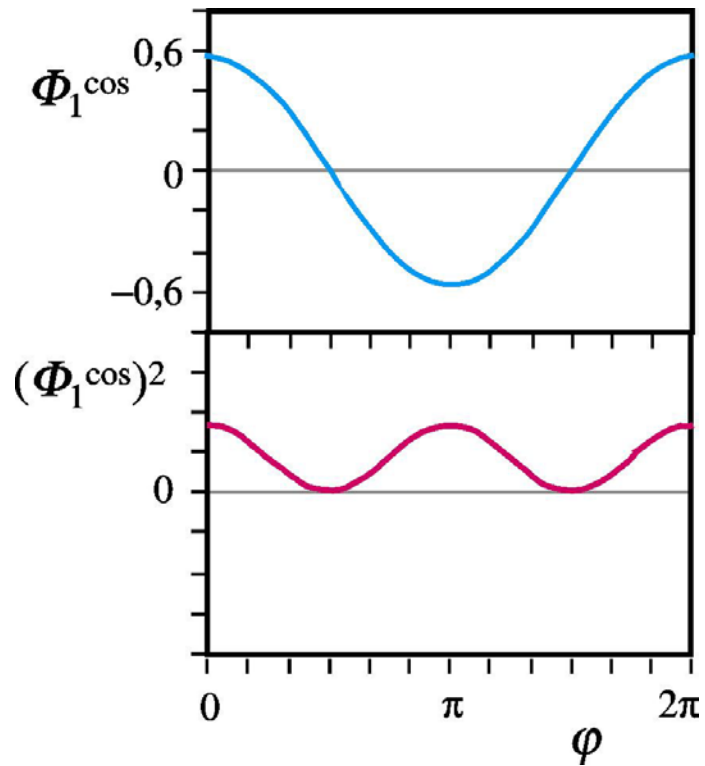


$$m = -1 \quad \Phi_1^{\sin} = \frac{1}{\sqrt{\pi}} \sin(\varphi)$$





$$m = +1 \quad \Phi_1^{\cos} = \frac{1}{\sqrt{\pi}} \cos(\varphi)$$



# Rješenja $\Theta$

$$l = 0; \quad m = 0; \quad \Theta_{0,0} = \frac{1}{\sqrt{2}}$$

$$l = 1; \quad m = 0; \quad \Theta_{1,0} = \frac{\sqrt{6}}{2} \cos \vartheta$$

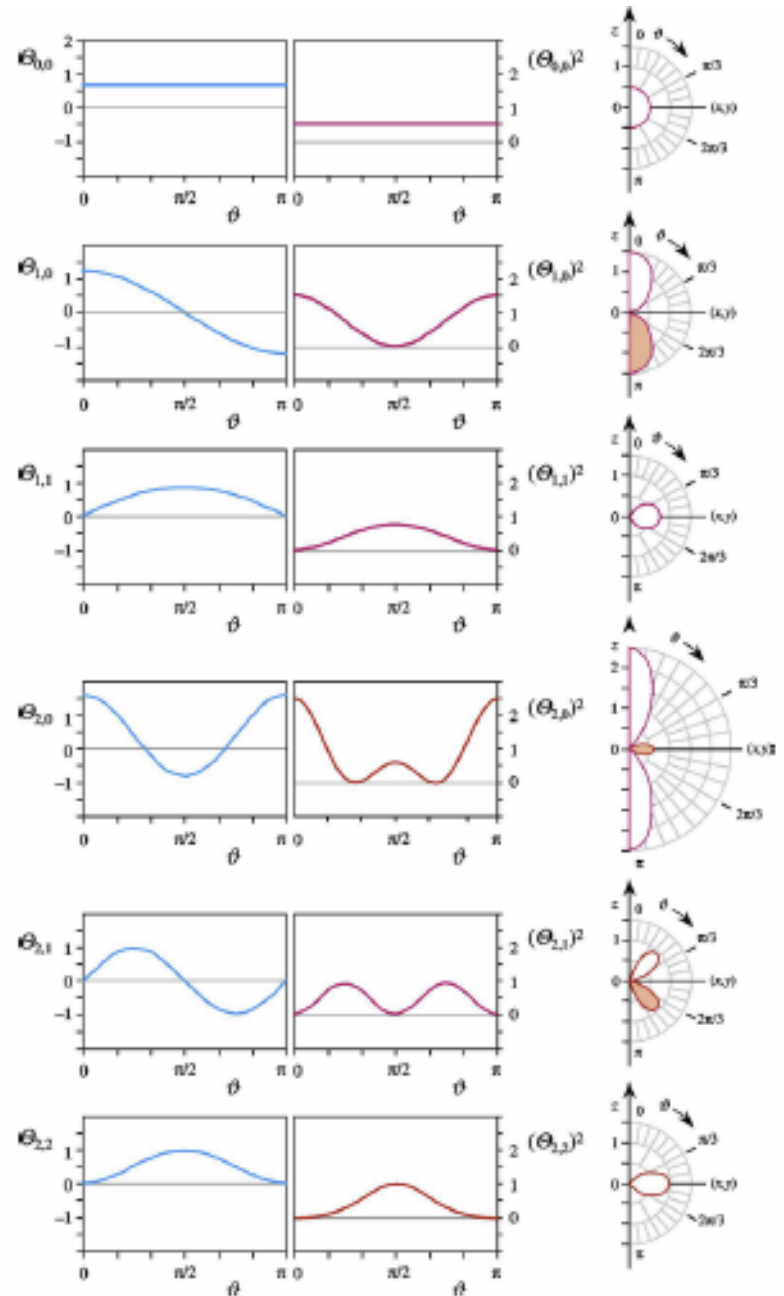
$$m = 1; \quad \Theta_{1,1} = \frac{\sqrt{3}}{2} \sin \vartheta$$

$$l = 2; \quad m = 0; \quad \Theta_{2,0} = \frac{\sqrt{10}}{4} (3 \cos^2 \vartheta - 1)$$

$$m = 1; \quad \Theta_{2,1} = \frac{\sqrt{15}}{2} \sin \vartheta \cos \vartheta$$

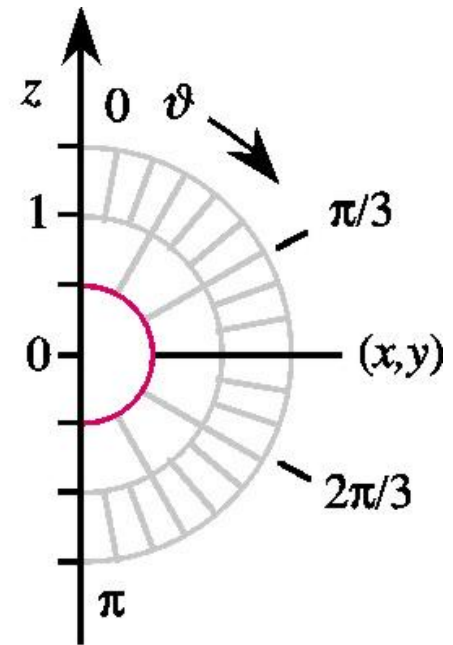
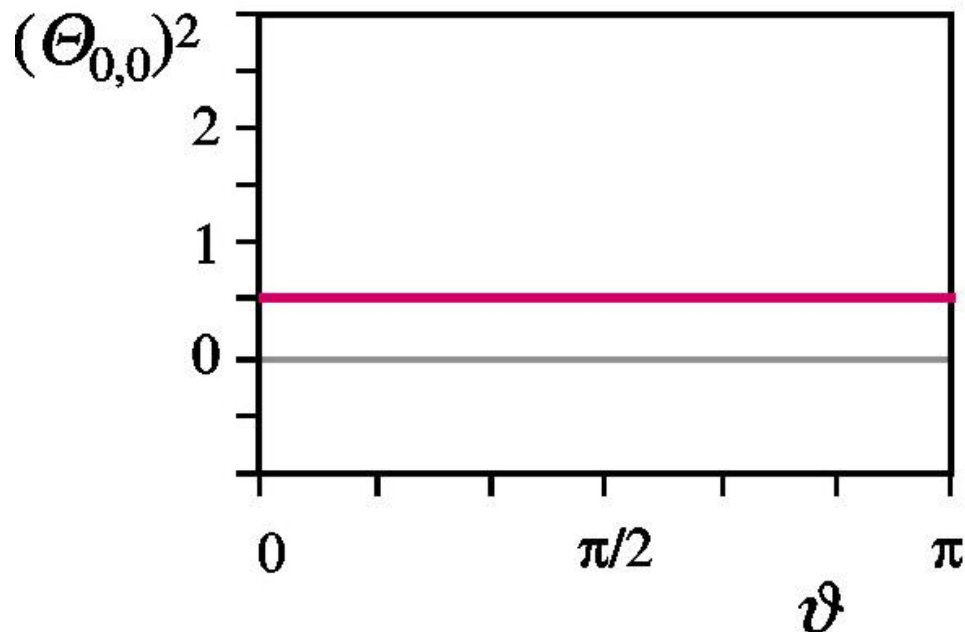
$$m = 2; \quad \Theta_{2,2} = \frac{\sqrt{15}}{4} \sin^2 \vartheta$$

$$l = 0, 1, 2, 3, \dots, n-1$$





$$l = 0, m = 0 \quad \Theta_{0,0} = \frac{1}{\sqrt{2}}$$

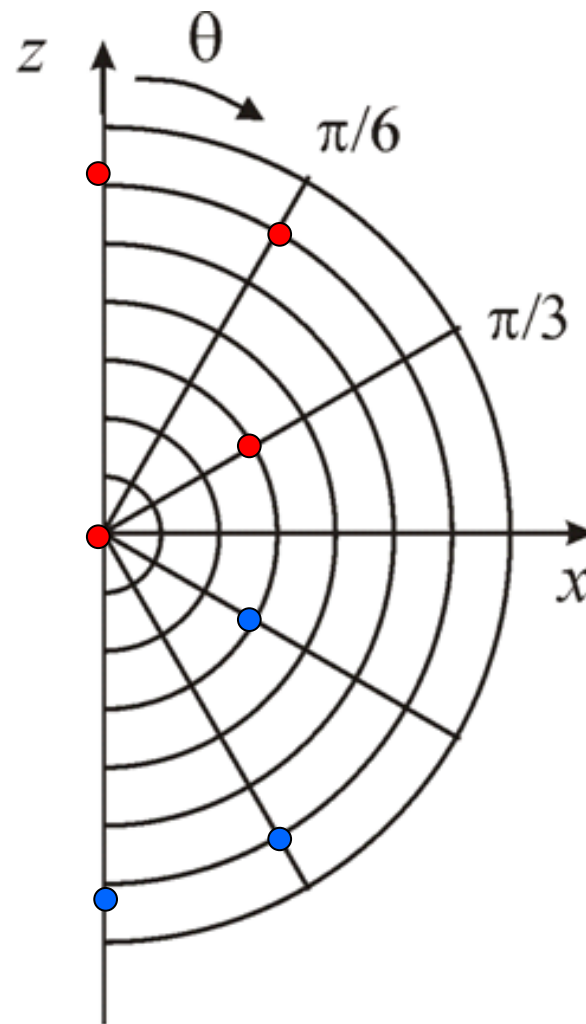


$$l = 1, m = 0$$

$$\Theta_{1,0} = \frac{\sqrt{6}}{2} \cos \vartheta$$



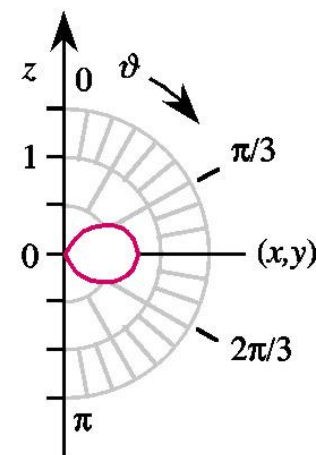
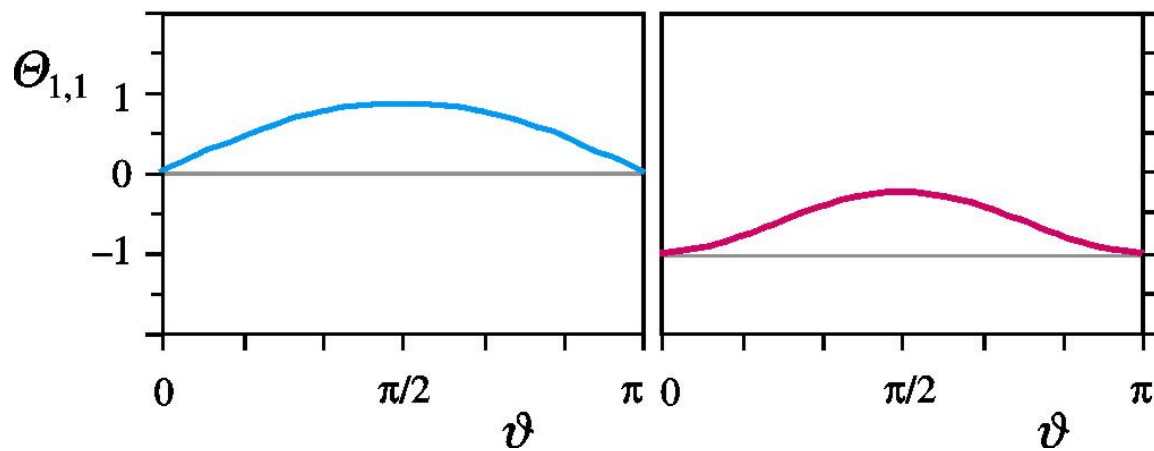
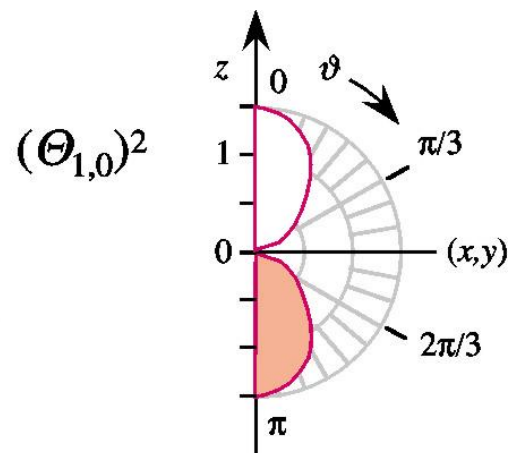
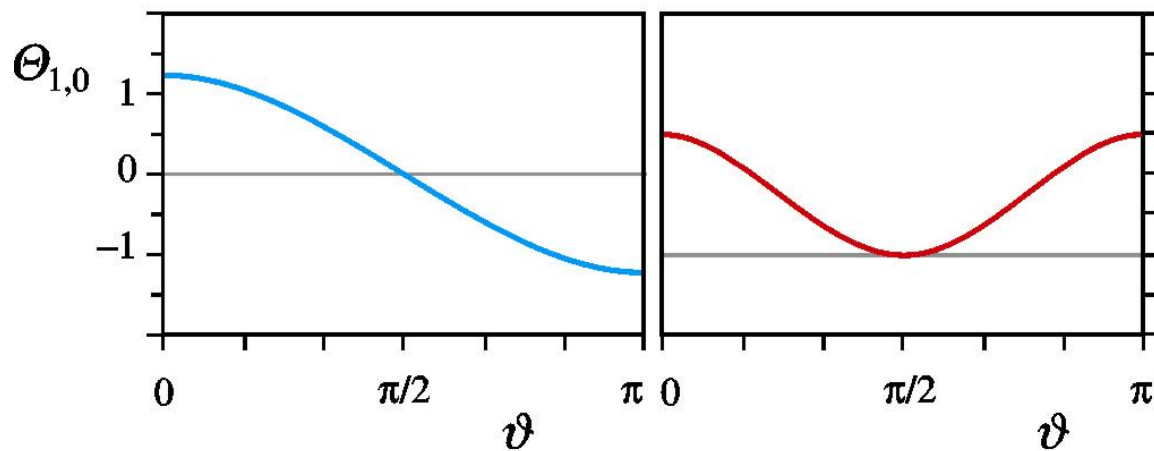
$\vartheta$	$\vartheta$	$\theta$
0	0	1.2
$\pi/6$	30°	1.1
$\pi/3$	60°	0.6
$\pi/2$	90°	0
$4\pi/6$	120°	-0.6
$5\pi/6$	150°	-1.1
$\pi$	180°	-1.2



$$l = 1, m = 1$$

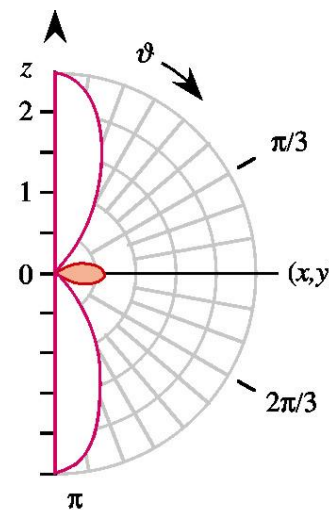
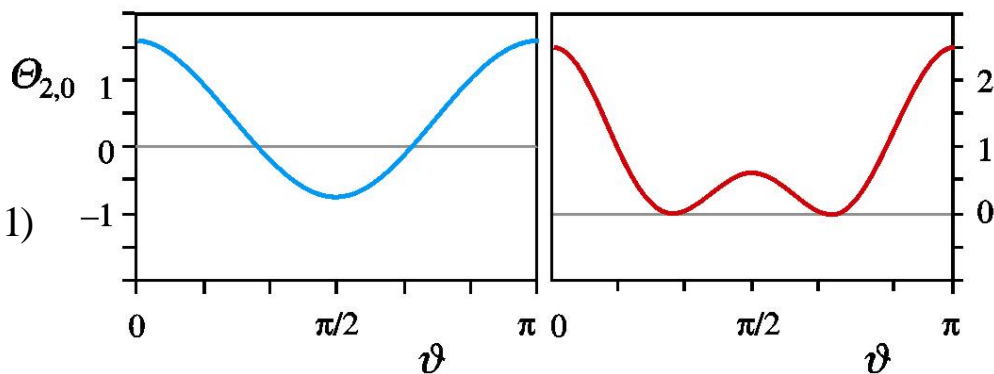
$$\Theta_{1,0} = \frac{\sqrt{6}}{2} \cos \vartheta$$

$$\Theta_{1,1} = \frac{\sqrt{3}}{2} \sin \vartheta$$

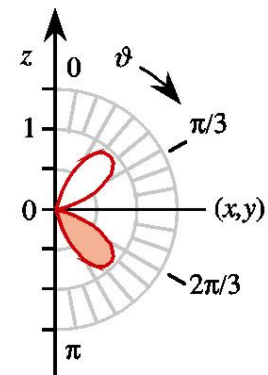
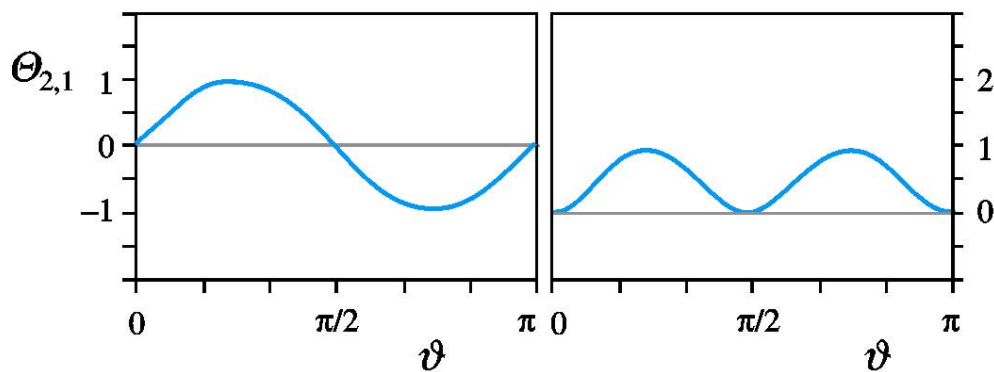


# $l = 2$

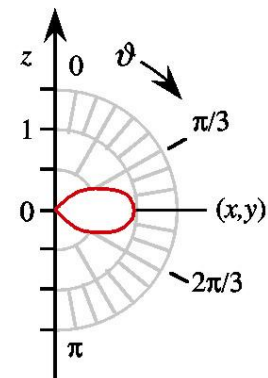
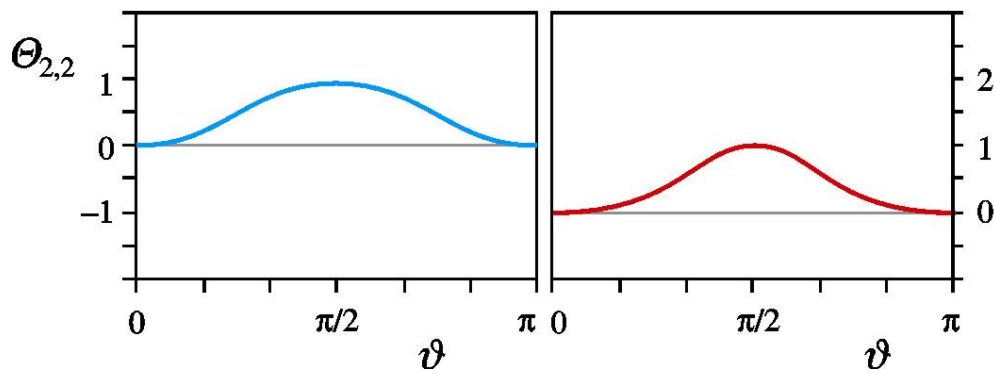
$$\Theta_{2,0} = \frac{\sqrt{10}}{4} (3\cos^2 \vartheta - 1)$$



$$\Theta_{2,1} = \frac{\sqrt{15}}{2} \sin \vartheta \cos \vartheta$$



$$\Theta_{2,2} = \frac{\sqrt{15}}{4} \sin^2 \vartheta$$

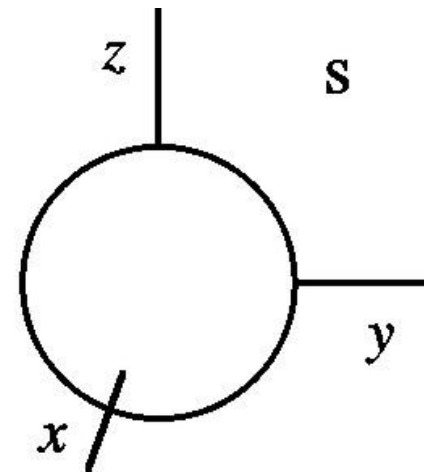


# Kugline funkcije

$$Y_{0,0} = \frac{1}{2\sqrt{\pi}}$$

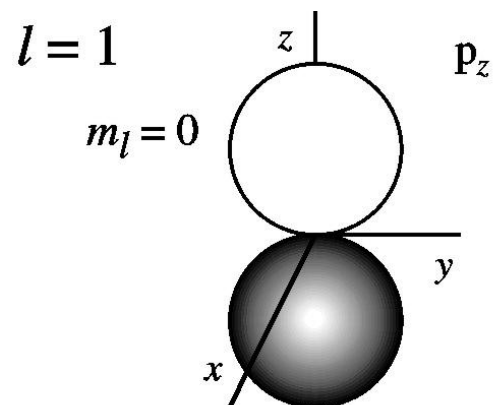
$$l = 0$$

$$m_l = 0$$

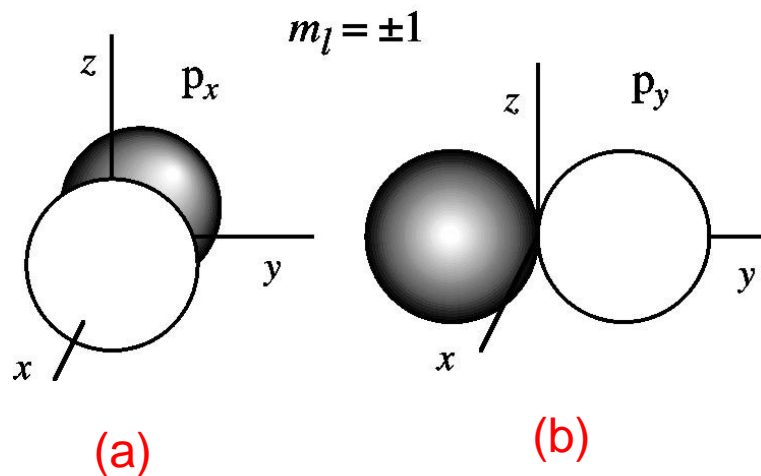


# Kugline funkcije

$$Y_{1,0} = \frac{1}{2} \sqrt{\frac{3}{\pi}} \cos \vartheta$$



(a)  $Y_{1,1}^{\cos} = \frac{1}{2} \sqrt{\frac{3}{\pi}} \sin \vartheta \cos \varphi$



(b)  $Y_{1,1}^{\sin} = \frac{1}{2} \sqrt{\frac{3}{\pi}} \sin \vartheta \sin \varphi$



# Kugline funkcije

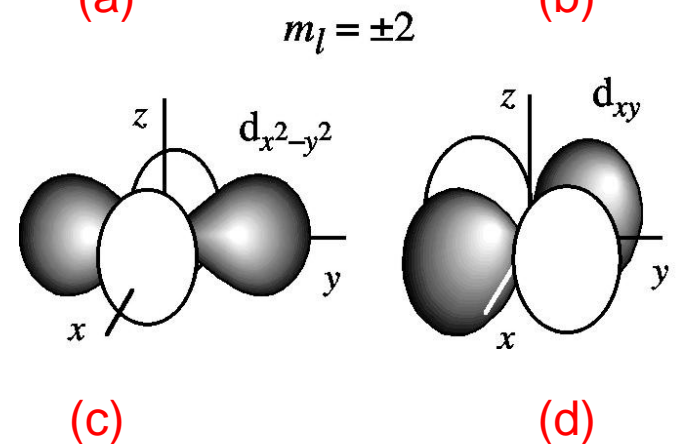
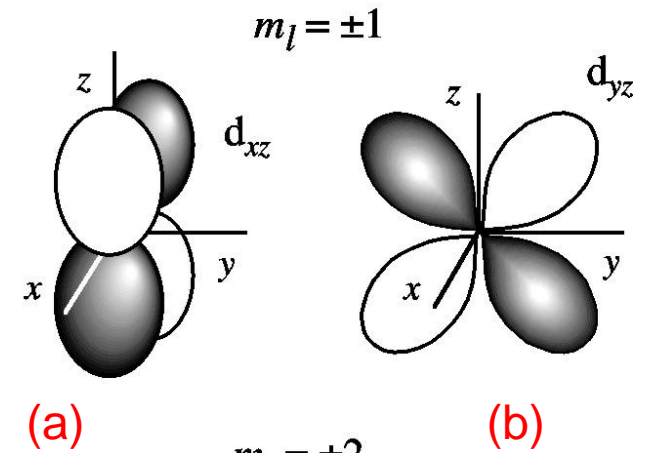
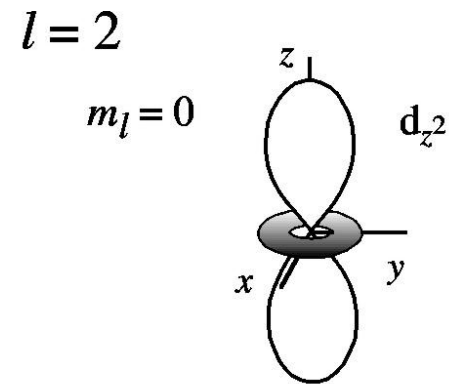
$$Y_{2,0} = \frac{1}{4} \sqrt{\frac{5}{\pi}} (3 \cos^2 \vartheta - 1)$$

(a)  $Y_{2,1}^{\cos} = \frac{1}{2} \sqrt{\frac{15}{\pi}} \sin \vartheta \cos \vartheta \cos \varphi$

(b)  $Y_{2,1}^{\sin} = \frac{1}{2} \sqrt{\frac{15}{\pi}} \sin \vartheta \cos \vartheta \sin \varphi$

(c)  $Y_{2,2}^{\cos} = \frac{1}{4} \sqrt{\frac{15}{\pi}} \sin^2 \vartheta \cos 2\varphi$

(d)  $Y_{2,2}^{\sin} = \frac{1}{4} \sqrt{\frac{15}{\pi}} \sin^2 \vartheta \sin 2\varphi$



# Radijalne funkcije

Orbitala	$n$	$l$	Radijalna funkcija*, $R_{n,l}$	
1s	1	0	$2\left(\frac{Z}{a_0}\right)^{3/2} e^{-\rho}$	$\sim \rho^0 \exp(-\rho)$
2s	2	0	$\frac{1}{2\sqrt{2}} \left(\frac{Z}{a_0}\right)^{3/2} (2-\rho) e^{-\rho/2}$	$\sim \rho^1 \exp(-\rho)$
2p	2	1	$\frac{1}{2\sqrt{6}} \left(\frac{Z}{a_0}\right)^{3/2} \rho e^{-\rho/2}$	
3s	3	0	$\frac{2}{81\sqrt{3}} \left(\frac{Z}{a_0}\right)^{3/2} (27-18\rho+2\rho^2) e^{-\rho/3}$	$\sim \rho^2 \exp(-\rho)$
3p	3	1	$\frac{4}{81\sqrt{6}} \left(\frac{Z}{a_0}\right)^{3/2} (6\rho-\rho^2) e^{-\rho/3}$	
3d	3	2	$\frac{4}{81\sqrt{30}} \left(\frac{Z}{a_0}\right)^{3/2} \rho^2 e^{-\rho/3}$	

$$\rho = \frac{Zr}{a_0}$$

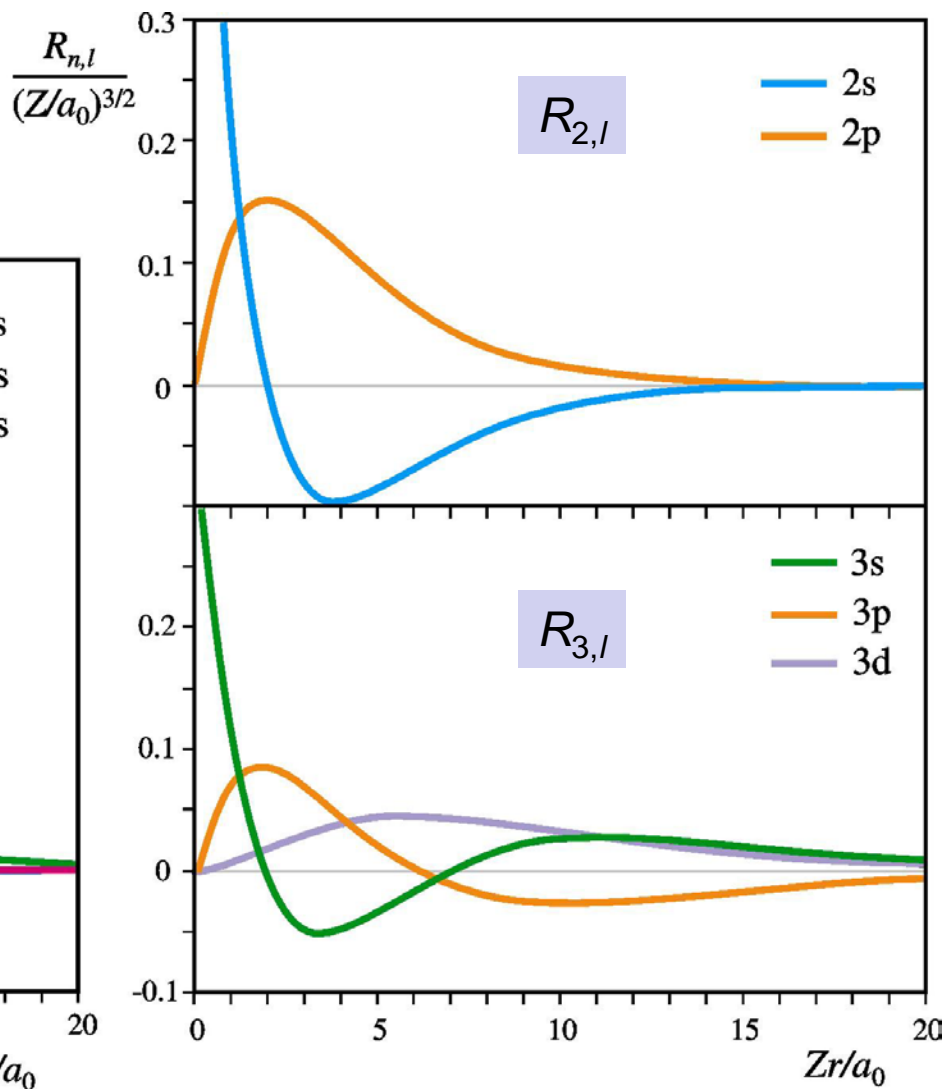
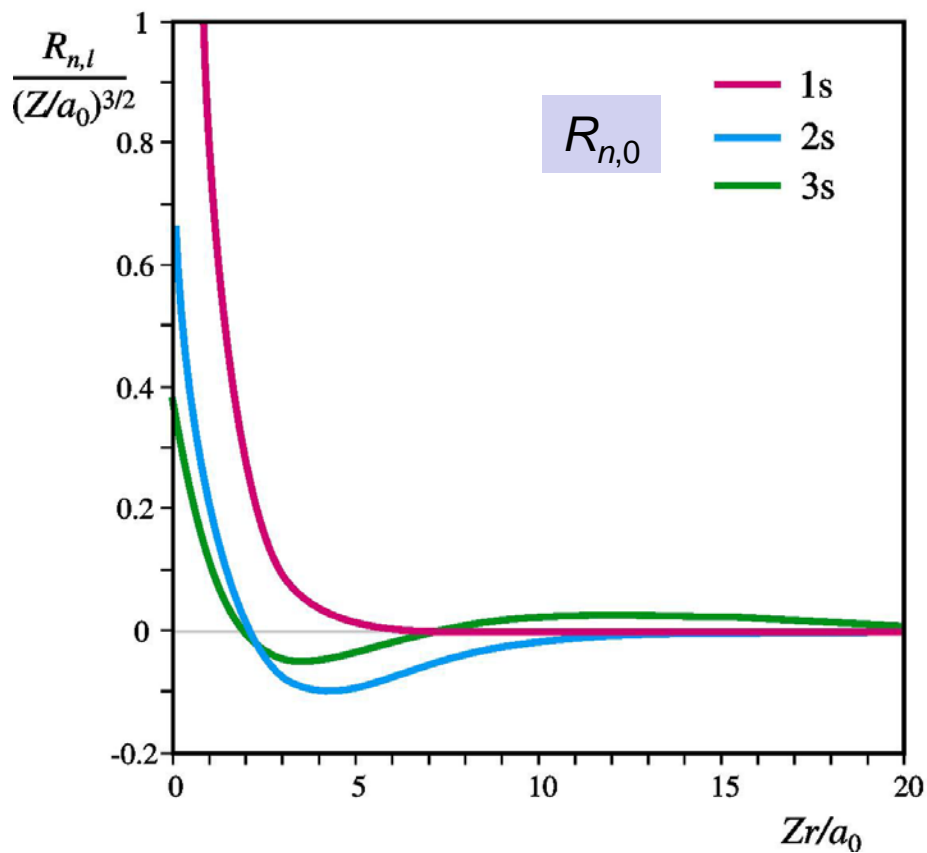
# Radijalne funkcije

$$R_{1,0} = 2 \left( \frac{Z}{a_0} \right)^{3/2} e^{-\rho}$$

$$R_{2,0} = \frac{1}{2\sqrt{2}} \left( \frac{Z}{a_0} \right)^{3/2} (2 - \rho) e^{-\rho/2}$$

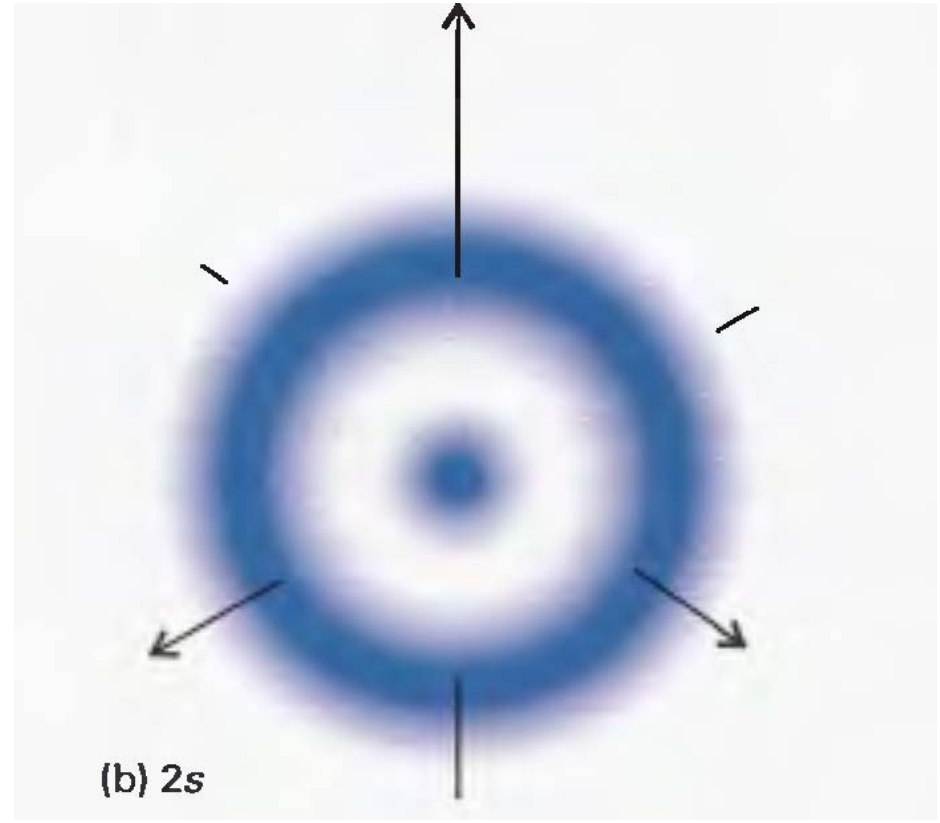
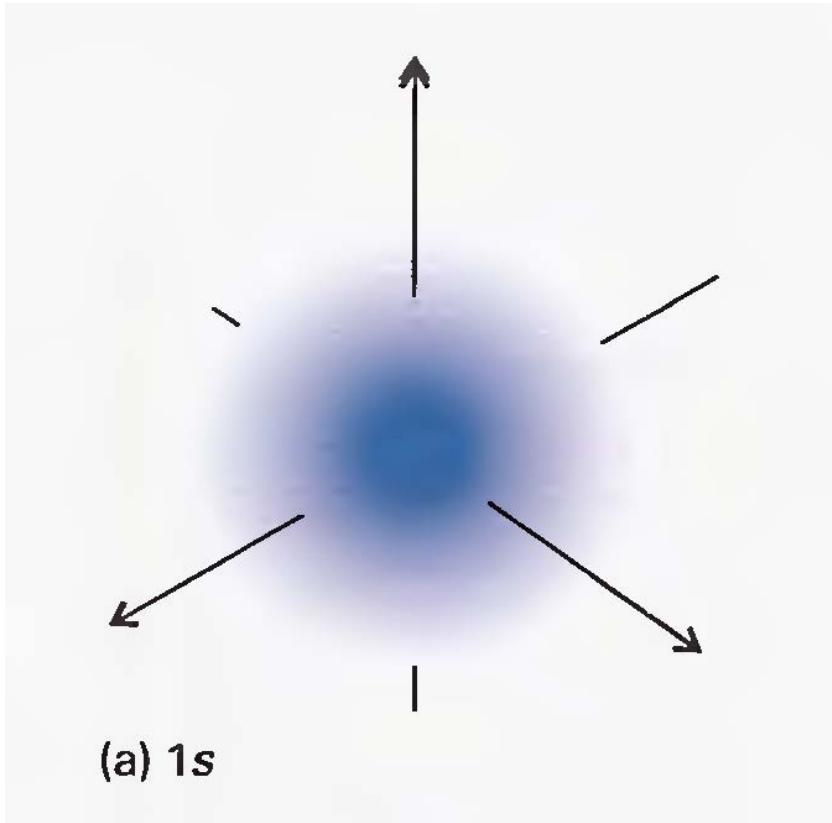
$$R_{2,1} = \frac{1}{2\sqrt{6}} \left( \frac{Z}{a_0} \right)^{3/2} \rho e^{-\rho/2}$$

# Radijalne funkcije



## Radijalne funkcije

- samo **s** orbitale ( $l = 0$ ) imaju značajniju vrijednost u blizini jezgre
- radijalne funkcije proporcionalne s  $r^l$  – elektroni s većim vrijednostima  $l$  sve se manje zadržavaju u blizini jezgre
- valna funkcija sve je položenija što su kvantni brojevi veći (položenija valna funkcija – manja kinetička energija)
- na jezgru djeluju **s**-elektroni i jezgra djeluje najviše na **s**-elektrone
- energija raste s brojem čvornih točaka (čvornih ploha) – za neki  $l$  broj čvornih ploha raste s glavnim kvantnim brojem  $n$ .



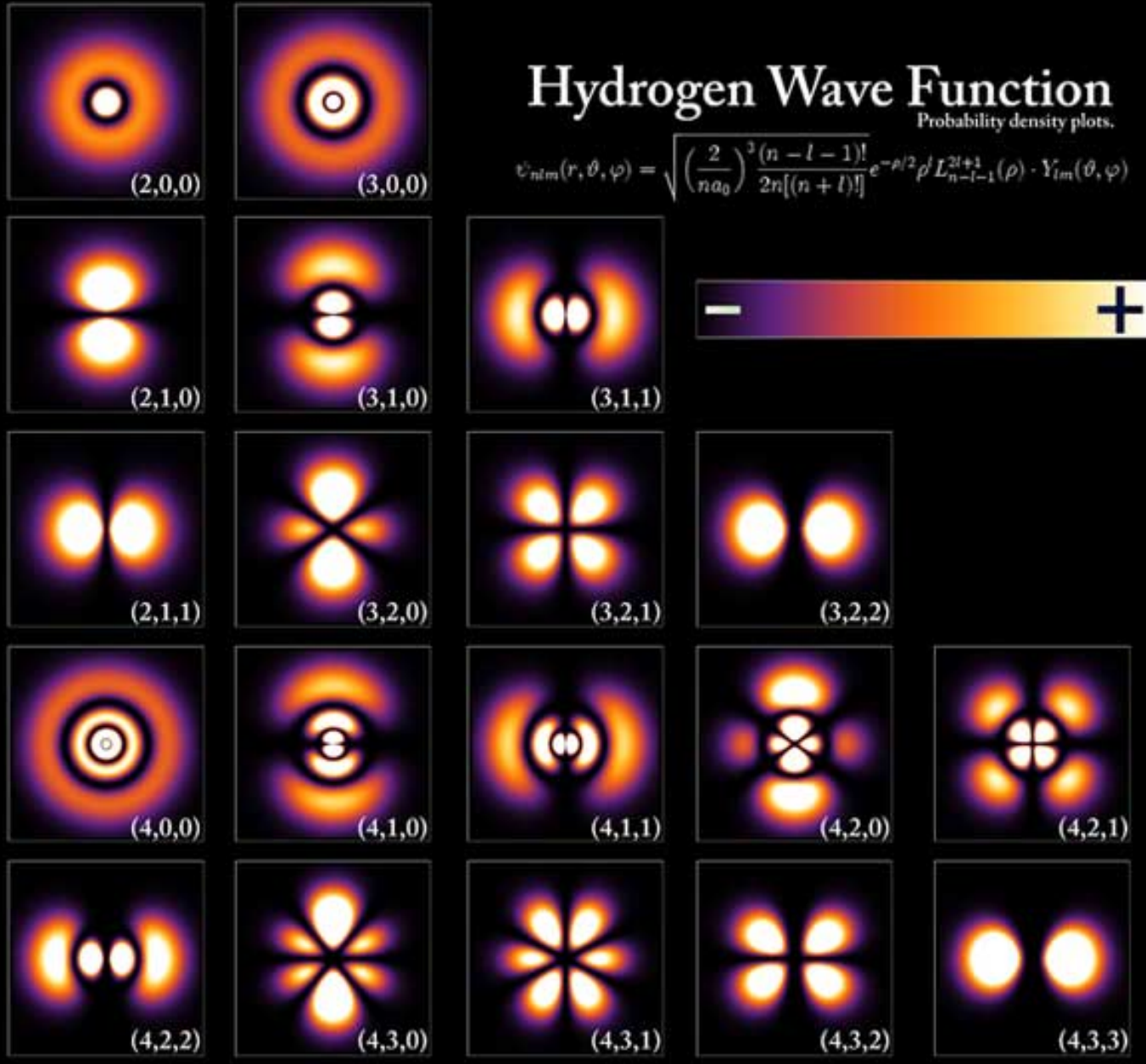
$$\Psi_{1s} = \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0}$$

$$\Psi_{2s} = \frac{1}{4\sqrt{2\pi a_0^3}} (2 - r/a_0) e^{-r/2a_0}$$

# Hydrogen Wave Function

Probability density plots.

$$\psi_{nlm}(r, \theta, \varphi) = \sqrt{\left(\frac{2}{na_0}\right)^3 \frac{(n-l-1)!}{2n[(n+l)!]}} e^{-\rho/2} \rho^l L_{n-l-1}^{2l+1}(\rho) \cdot Y_{lm}(\theta, \varphi)$$



## Radijalna funkcija

### Kvadrat radijalne funkcije (elektronska gustoća)

- vjerojatnost nalaženja elektrona u elementu prostora  $d\tau$  oko točke u prostoru s koordinatama  $r$ ,  $\vartheta$  i  $\varphi$ .

### Radijalna gustoća vjerojatnosti

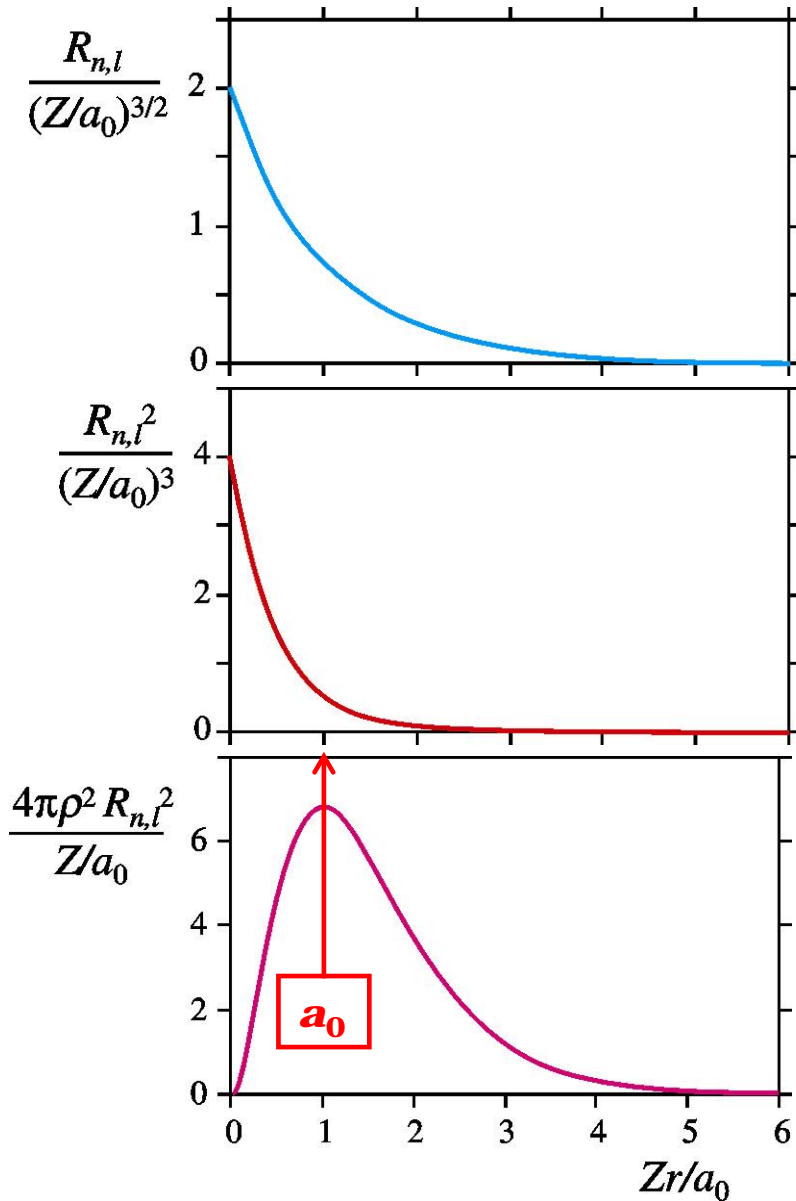
- na kojoj udaljenosti od jezgre  $r$  je najveća vjerojatnost nalaženja elektrona?  
- integracija preko svih  $\vartheta$  i  $\varphi$   
- volumen sloja kugle polumjera  $r$  i debljine  $dr$

$\psi^2 d\tau$  = vjerojatnost nalaženja elektrona u elementu prostora  $d\tau$

$$d\tau = dr \cdot r d\vartheta \cdot r \sin \vartheta d\varphi$$
$$= r^2 \sin \vartheta d\varphi d\vartheta dr$$

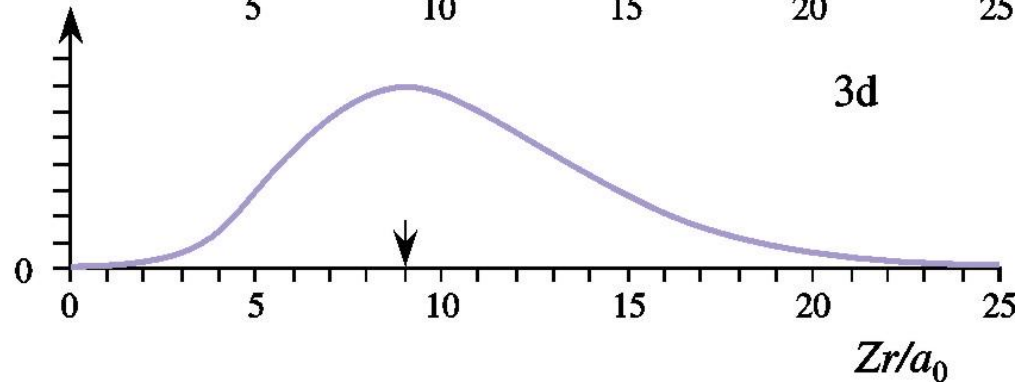
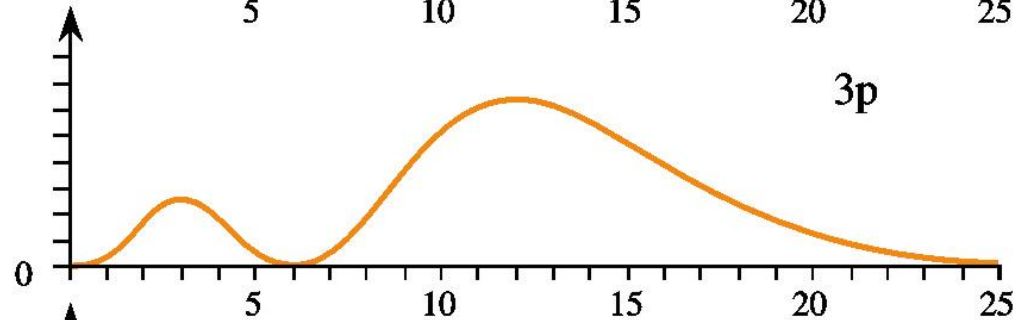
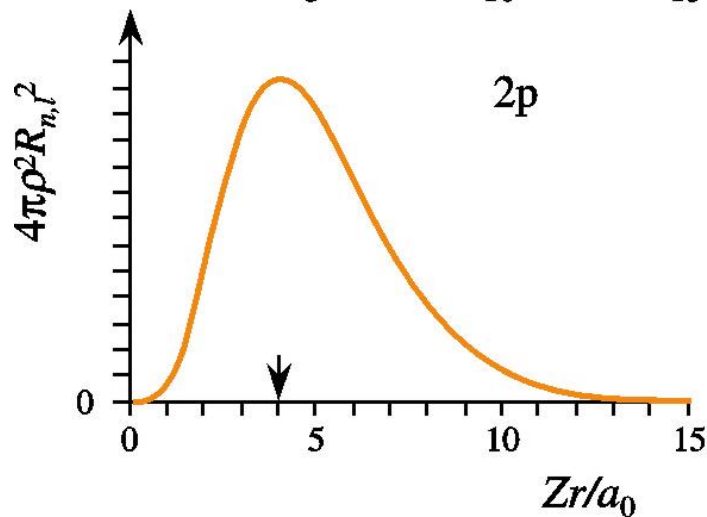
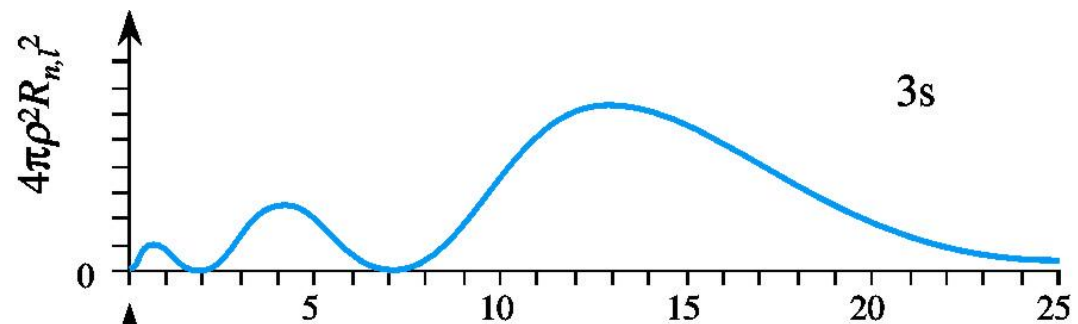
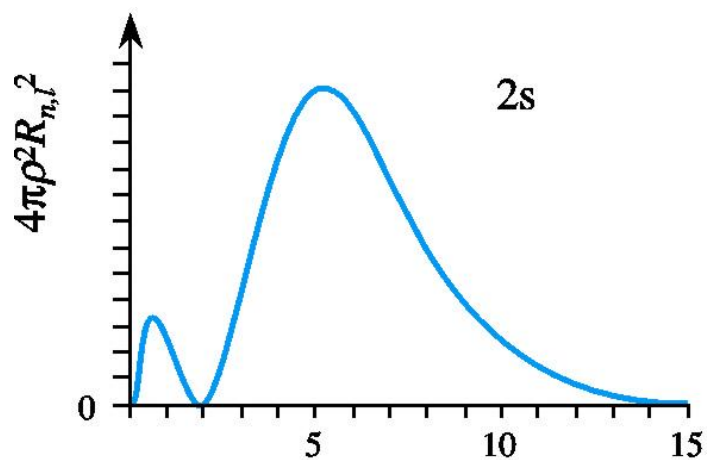
$$= r^2 dr \int_0^\pi \sin \vartheta d\vartheta \int_0^{2\pi} d\varphi$$

$$= 4\pi r^2 dr$$



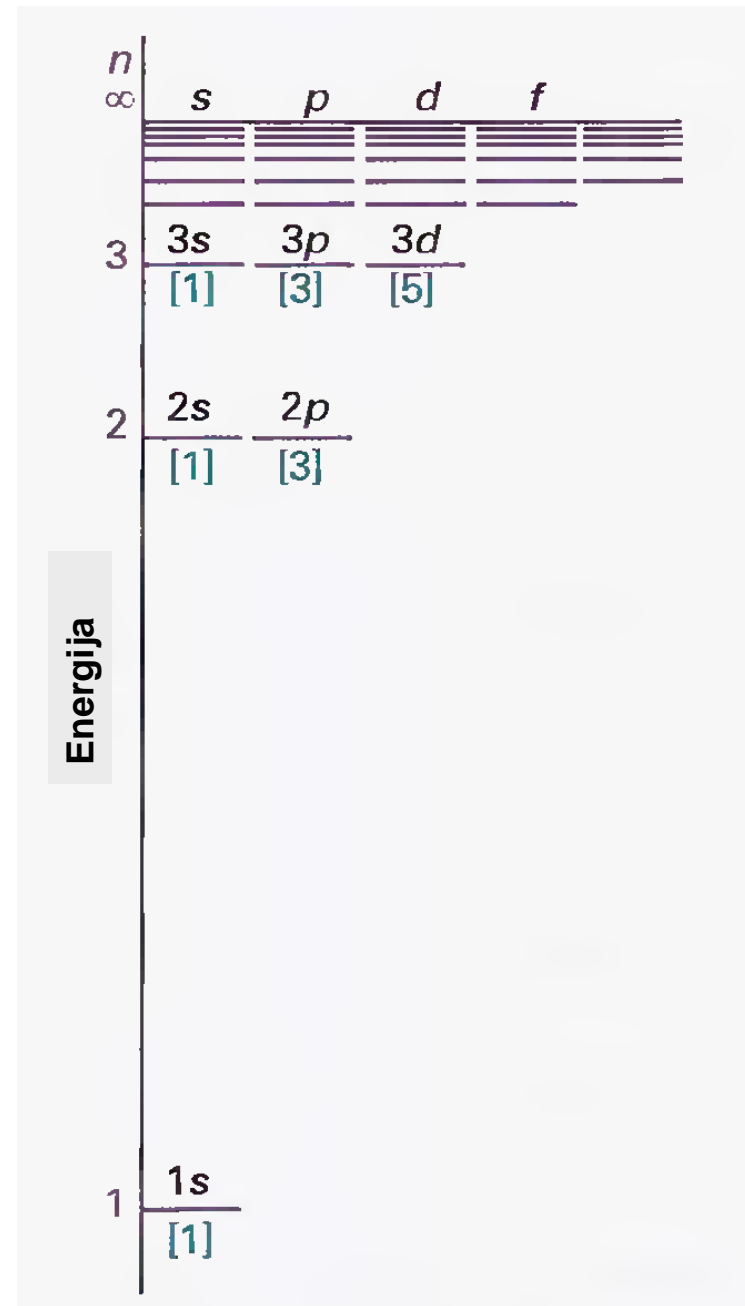


# Radijalne gustoće vjerojatnosti



# Energija

$$E_e = -hcZ^2 R_{\infty} \frac{\mu}{m_e} \cdot \frac{1}{n^2}$$

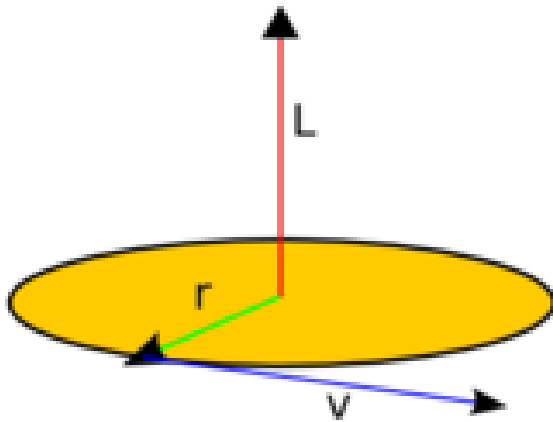


# Energija

- za jednoelektronske atome ovisi samo o  $n$
- s povećanjem  $n$  – energetske nivoe su sve bliže  $\Rightarrow$  kontinuum
- energija ionizacije  $E_i$
- negativan predznak  $E \Rightarrow$  atomi imaju nižu energiju nego elektroni i jezgra na beskonačnoj udaljenosti
- $n = 1 \Rightarrow$  osnovno stanje najniže energije
- energija ovisi i o naboju jezgre  $Z$

$$E_e = -hcZ^2 R_\infty \frac{\mu}{m_e} \cdot \frac{1}{n^2}$$

# Kutna količina gibanja



$$\vec{L} = \vec{r} \times m\vec{v}$$

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

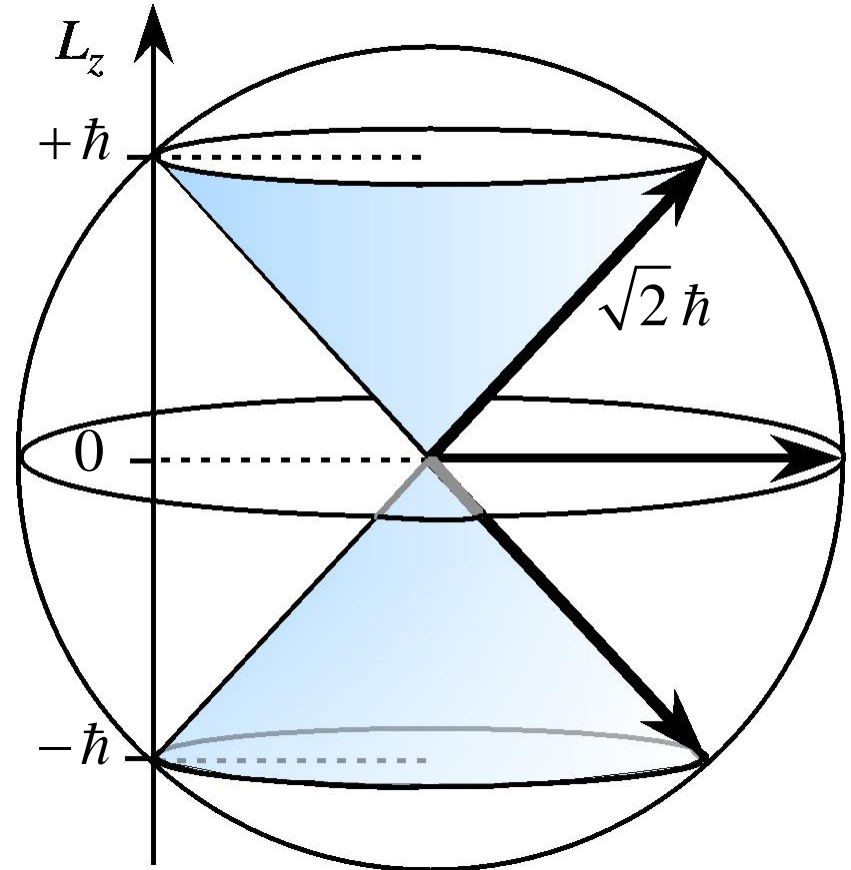
# Prostorna kvantizacija

z-komponenta kutne količine gibanja

$$l = 1$$

$$m_l = 0, -1, +1$$

$$L_z = m_l \hbar$$



# Spin

- 1925. Goudsmit & Uhlenbeck

- klasična slika: vlastita kutna količina gibanja elektrona



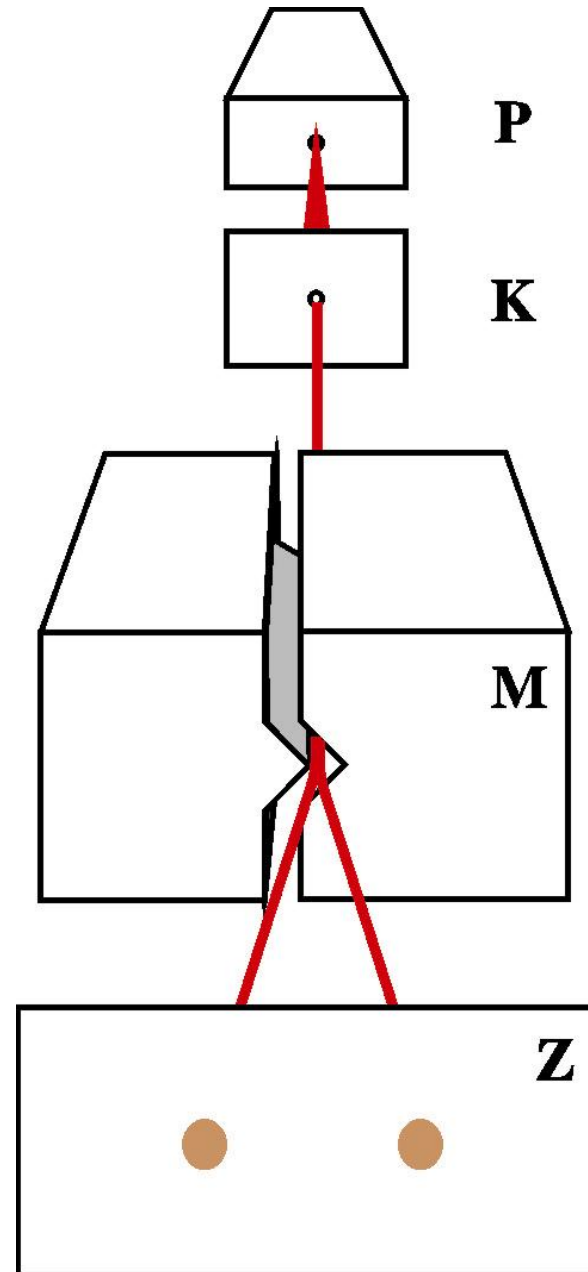
- kutna količina gibanja spina

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

-  $s$  - kvantni broj spina  $s = 1/2$

# Stern i Gerlach 1921.

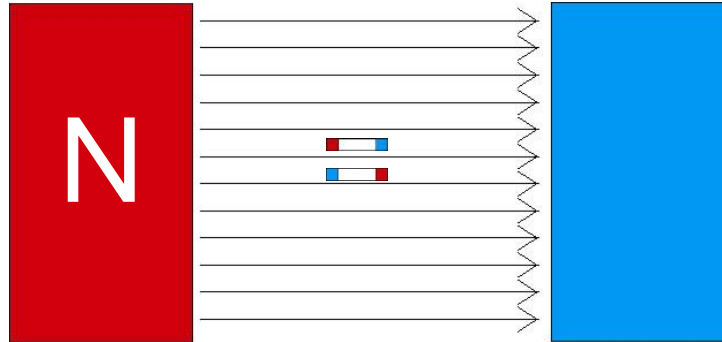
- uski snop atoma srebra kroz nehomogeno magnetsko polje



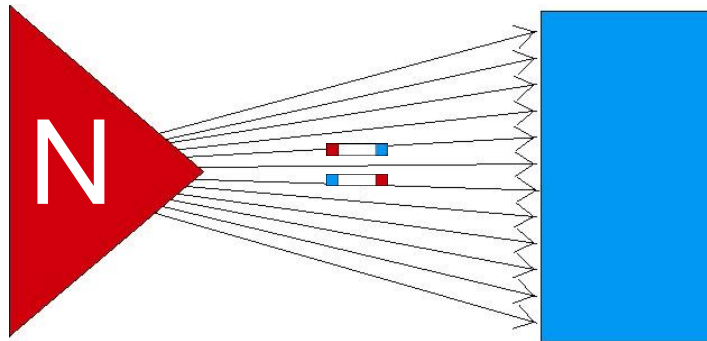
<http://www.youtube.com/watch?v=rg4Fnag4V-E>

# Eksperimentalna provjera prostorna kvantizacije

Homogeno  
polje



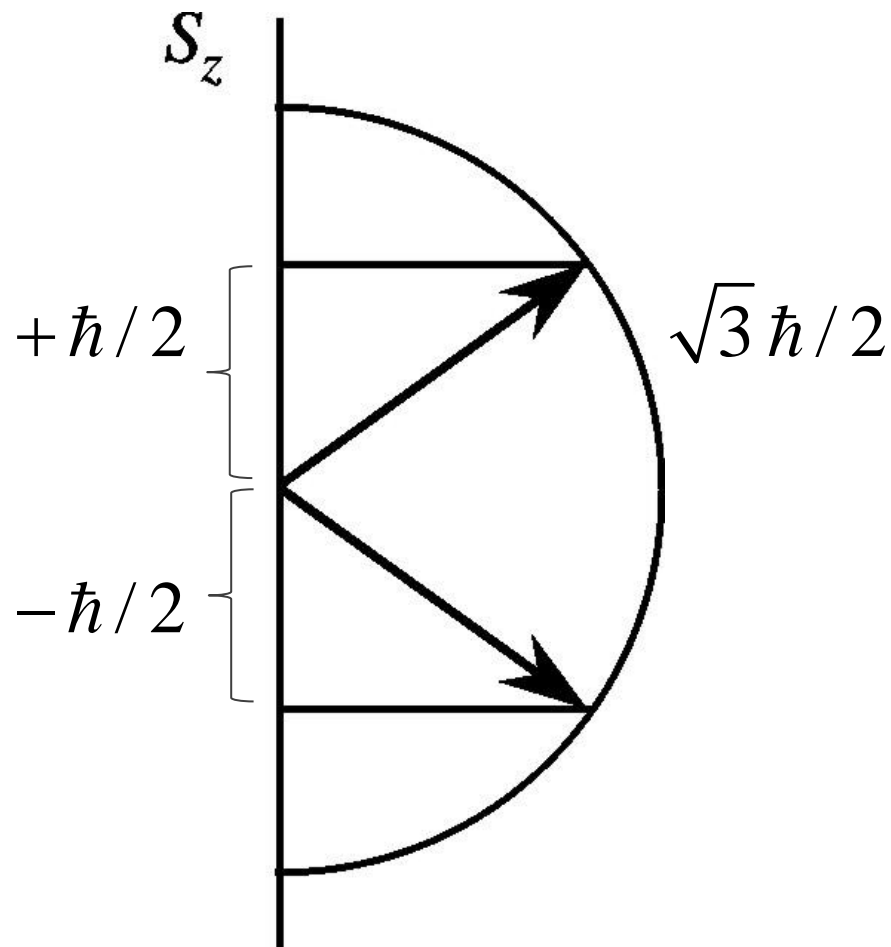
Nehomogeno  
polje





# Orijentacija u magnetskom polju

$$S_z = m_s \hbar$$



# Usporedba Bohrovog modela i rezultata Schrödingerove teorije:

- jednake energije  $E$
- kutne količine gibanja kvantizirane – no razlikuju se
  - z-komponenta kutne količine gibanja  $L_z$  kvantizirana kod Schrödingerove teorije
- egzaktna kružna putanja zamijenjena manje određenim opisom položaja elektrona
- stacionarna stanja u oba modela

## ***Jednoelektronski atom***

1. Kako se rješava Schrödingerova jednačba za atom vodika?
2. Zašto se uvode polarne koordinate?
3. Definirajte polarne koordinate.
4. Kako glasi element prostora u polarnim koordinatama?
5. Koliko kvantnih brojeva dobivamo rješavanjem Schrödingerove jednačbe?
6. O kojim kvantnim brojevima ovisi energija?
7. Kolika je degeneracija razine  $s$  kvantnim brojem  $n$ ?
8. Koje je značenje sporednog kvantnog broja?
9. Koje je značenje magnetskog kvantnog broja?

## Atomske orbitale

1. Kako izgleda  $\sin\varphi$  u polarnom dijagramu?
2. Što su kugline funkcije i kako izgledaju?
3. U čemu je najbitnija razlika s- i svih ostalih orbitala?
4. Kakav je odnos potencijalne, kinetičke i ukupne energije kod atoma vodika?
5. Po čemu se razlikuju rezultati Bohrova i Schrödingerova modela atoma?
6. Što se ne može objasniti Schrödingerovim modelom atoma?
7. Gdje je najveća elektronska gustoća u osnovnom stanju atoma vodika?
8. Gdje je najveća radijalna gustoća vjerojatnosti za osnovno stanje atoma vodika?
- 9 Opišite Stern-Gerlachov pokus.
10. Što dokazuje Stern-Gerlachov pokus?
11. Kakav bi bio rezultat pokusa da nema prostorne kvantizacije?

## Spin

1. Kako se objašnjava spin?
2. Koja je posljedica postojanja elektronskog spina?
3. Koji su kvantni brojevi vezani uz spin?