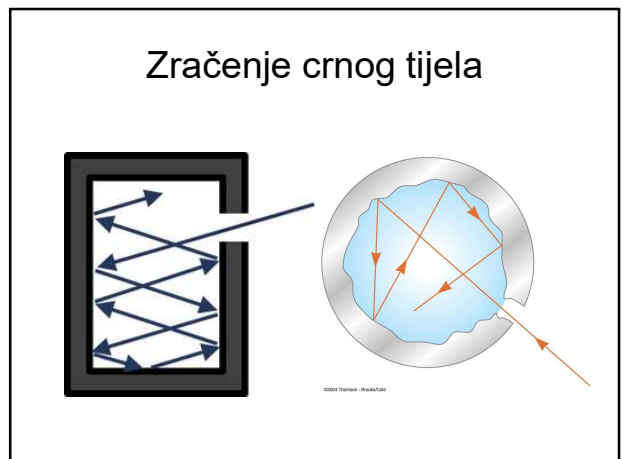
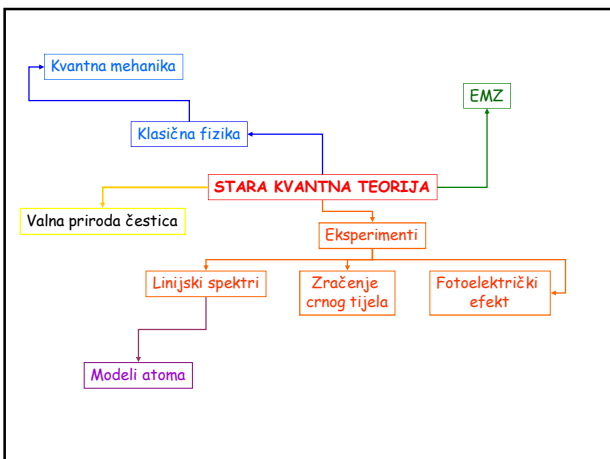



### Elektromagnetsko zračenje


$$\lambda = \frac{c}{\nu}$$

$$\tilde{\nu} = \frac{1}{\lambda}$$

$$\nu = c \tilde{\nu}$$




**Jožef Stefan**  
1835 – 1893

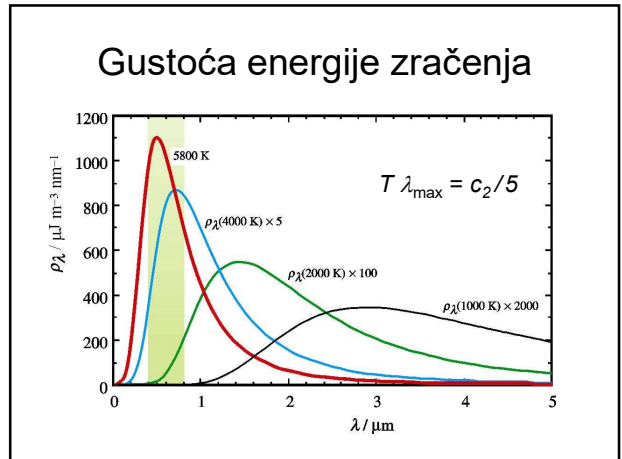


**Ludwig Eduard Boltzmann**  
1844 – 1906

$M = \sigma T^4$

Stefan – Boltzmannov zakon

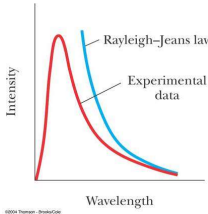
$M$  = egzitancija - omjer ukupne emitirane snage s djelića površine i ploštine te površine, tj. gustoća toka energije iz izvora



### Ultraljubičasta katastrofa

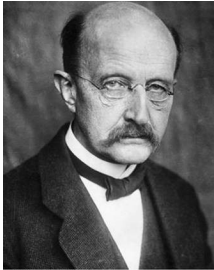
- Rayleigh-Jeans

$\Rightarrow \rho_\lambda = 8\pi k_B T / \lambda^4$

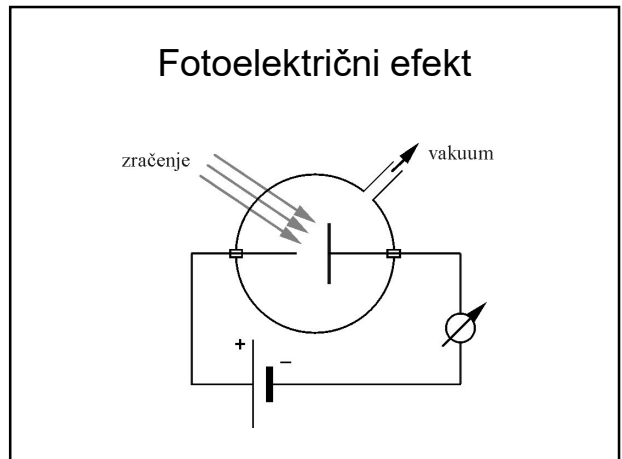
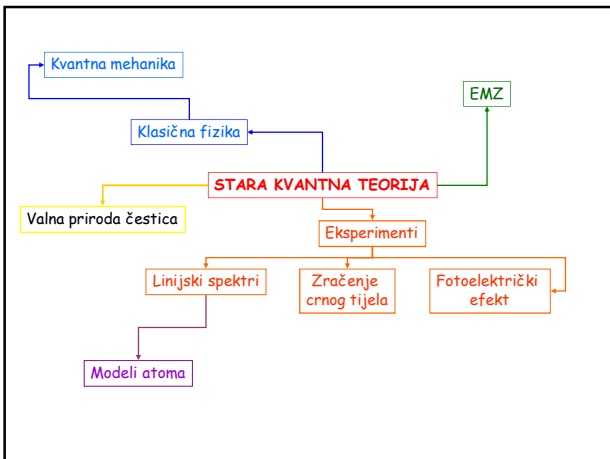


### Max Planck

- 1900. jednačba koja zadovoljavajuće opisuje eksperimentalne podatke, a kasnije i izveo uvodeći pojam kvanta
- 1918. Nobelova nagrada za fiziku



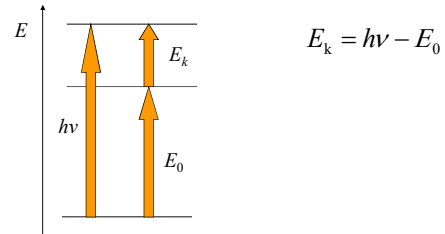
10



## Eksperimentalne činjenice

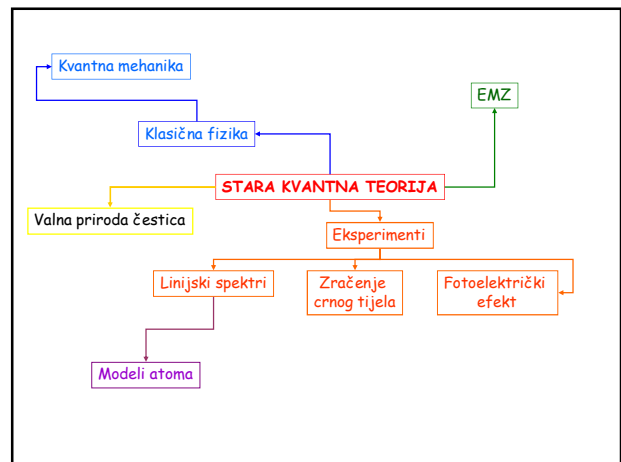
1. Električna struja proporcionalna je intenzitetu zračenja.
2. Kinetička energija elektrona neovisna je o intenzitetu zračenja.
3. Maksimalna kinetička energija elektrona raste s frekvencijom zračenja.
4. Zračenje većih valnih duljina od neke granične više ne uzrokuje fotoefekt.

## Fotoelektrični efekt

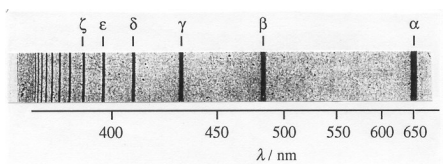


## Eksperimentalne činjenice

1. Električna struja proporcionalna je intenzitetu zračenja.  
Veći intenzitet → veći broj fotona → veći broj izbačenih elektrona → veća struja.
2. Kinetička energija elektrona neovisna je o intenzitetu zračenja.  
Kinetička energija fotoelektrona ne ovisi o broju upadnih fotona.
3. Maksimalna kinetička energija elektrona raste s frekvencijom zračenja.  
Kinetička energija fotoelektrona proporcionalna je energiji, odnosno frekvenciji upadnih fotona.
4. Zračenje većih valnih duljina od neke granične više ne uzrokuje fotoefekt.  
Izlazni rad ovisi samo o tome koliko su elektroni čvrsto vezani u samom metalu, a to ovisi o prirodi metala.



## Linijski spektri – spektar atoma vodika



Balmerova serija linija u spektru atoma vodika



## Linijski spektri – spektar atoma vodika

"If you understand hydrogen, you understand all that can be understood."  
Victor Weisskopf

$$\lambda / \text{Å} = 3546,6 \frac{n^2}{n^2 - 4} \quad (n = 3, 4, 5, \dots, 11)$$

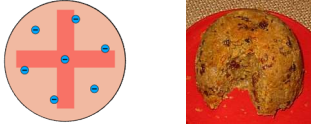
Balmerova serija

$$\tilde{\nu} = R_H \left( \frac{1}{(n')^2} - \frac{1}{(n'')^2} \right)$$

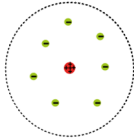
Rydbergova jednadžba

## modeli atoma

- J. J. Thomson (1904) "plum pudding" model

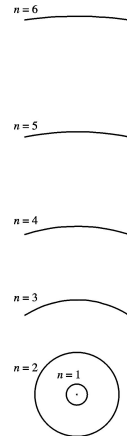


- H. Rutherford (1911)



## Bohrov model atoma

- Stacionarna stanja
- Kvantiziranost energije
- Pri prijelazu  $\Delta E = h\nu$
- Kvantiziranost kutne količine gibanja
- $L = n\hbar$



## Bohrov model atoma

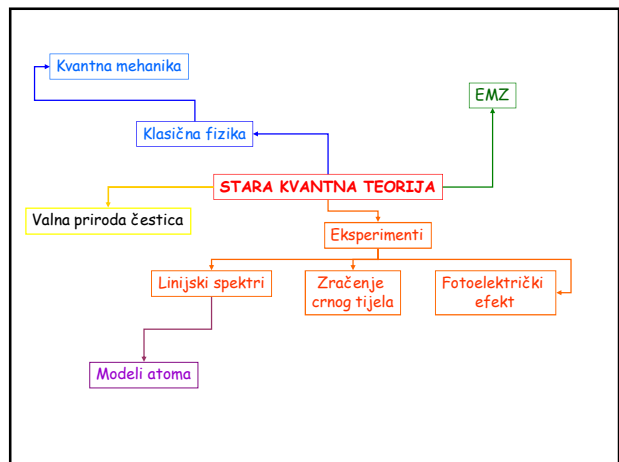
Izračunao:

- polumjere putanje elektrona  $r = \frac{n\hbar}{mv} = \frac{(4\pi\epsilon_0)\hbar^2}{me^2} n^2$

- brzine  $v = \frac{1}{4\pi\epsilon_0} \frac{e^2}{\hbar n}$

- ukupne energije stacionarnih stanja  $E = -\frac{hcR_\infty}{n^2}$

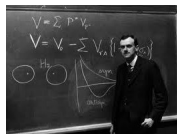
- valne duljine linija u spektru atoma vodika



## kvantna mehanika

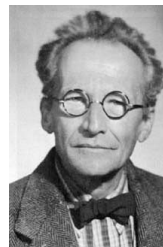


Erwin Schrödinger (1887 – 1961)



Paul Adrien Maurice Dirac (1902 – 1984)

The Nobel Prize in Physics 1933  
"for the discovery of new productive forms of atomic theory"



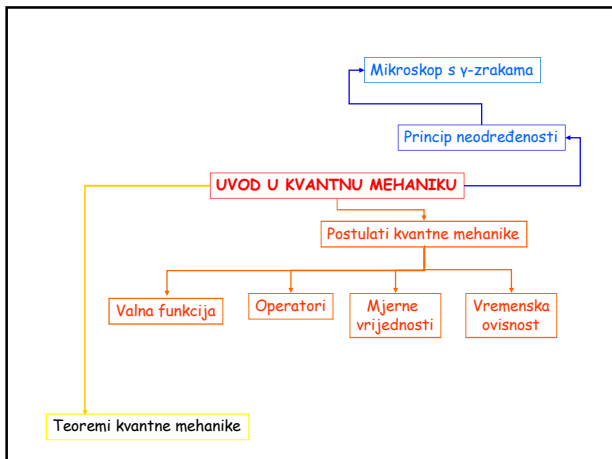
Erwin Schrödinger (1887 – 1961)

\* 1987 Beč

1920 Stuttgart  
1921 Wrocław  
1921 – 1927 Zürich  
1927 – 1933 Berlin  
1933 – 1936 Oxford  
1936 – 1938 Graz  
1940 – 1955 Dublin  
1956 – 1961 Beč

1933 Nobelova nagrada s P.A.M. Diracom


† Beč, pok. Alpbach



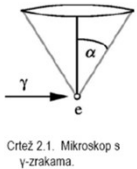

**Werner Heisenberg (1901 – 1976)**  
 \* 1901 Würzburg  
 1923 doktorirao kod A. Sommerfelda (München)  
 1924 – 1927 kod M. Borna (Göttingen) i N. Bohra (Kopenhagen)  
 1927 – 1941 Leipzig  
 1941 – 1945 KWI Berlin  
 1946 – 1948 KWI/MPI Göttingen  
 1958 – 1966 MPI i Uni München  
 1932 Nobelova nagrada (matrična mehanika)  
 † 1976 München  
 Doktorand Ivan Supek

**Princip neodređenosti**  
**Mikroskop s γ-zrakama**


Werner Heisenberg, 1927.  
 • nije moguće istovremeno odrediti koordinatu,  $x$ , i konjugiranu količinu gibanja neke čestice do proizvoljne točnosti



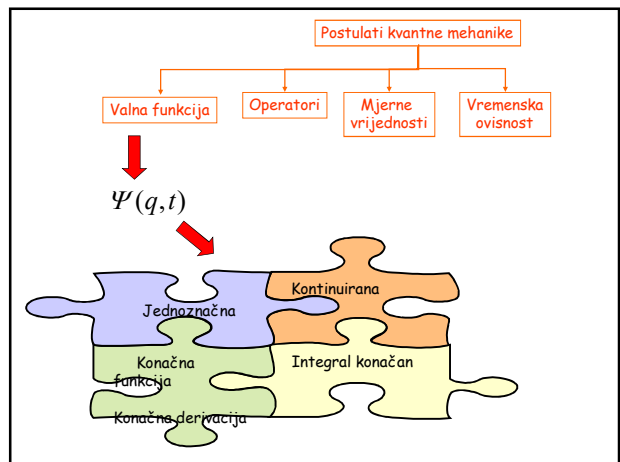
Werner Heisenberg

$$\Delta x \cdot \Delta p_x \approx h$$


Crtež 2.1. Mikroskop s γ-zrakama.



Crtež 2.2. Komponente količine gibanja fotona prije (lijevo) i poslije sudara s elektronom.



**Postulati kvantne mehanike**

Valna funkcija    Operatori    Mjerne vrijednosti    Vremenska ovisnost

↓

$\hat{\Omega}$     matematička uputa kako treba djelovati na valnu funkciju

Tablica 2.1 Osnovni kvantnomehanički operatori u koordinatnoj reprezentaciji.

Naziv	Veličina	Simbol	Kvantnomehanički operator
koordinata		$x$	$\hat{x} = x \cdot$
količina gibanja, impuls		$p_x$	$\hat{p}_x = -i\hbar \frac{\partial}{\partial x}$

**Postulati kvantne mehanike**

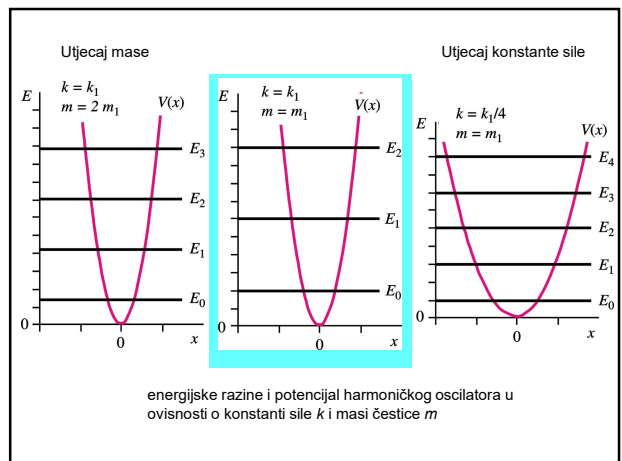
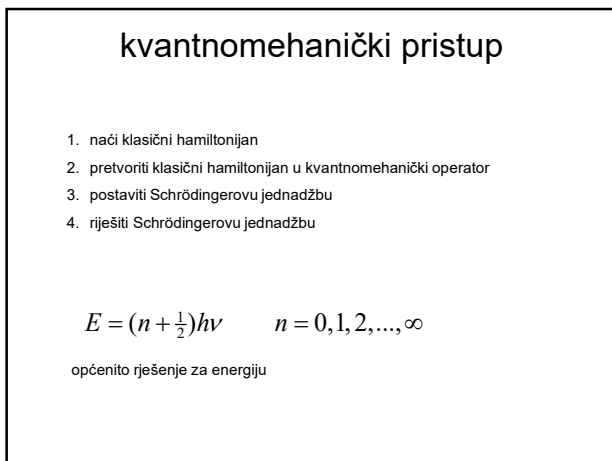
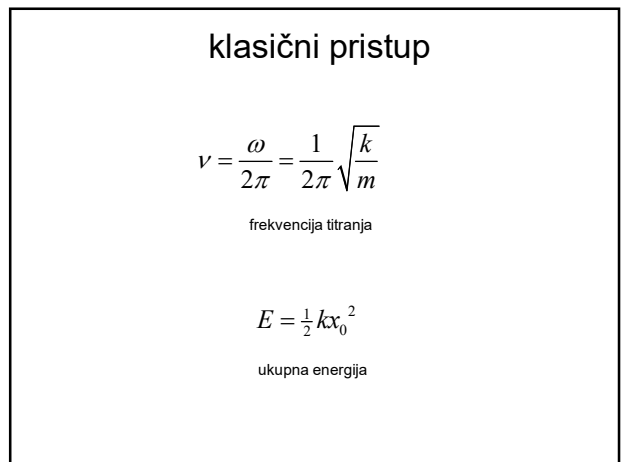
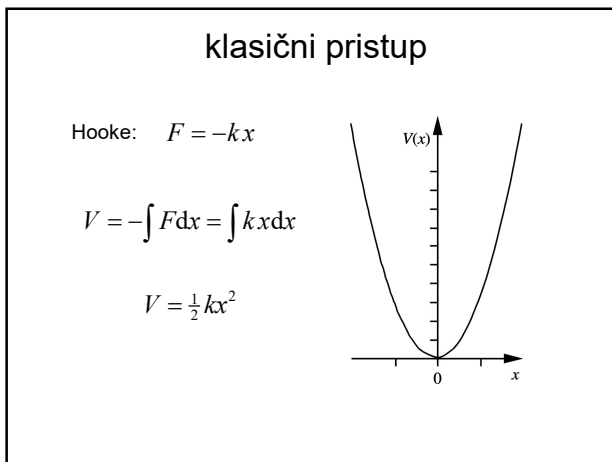
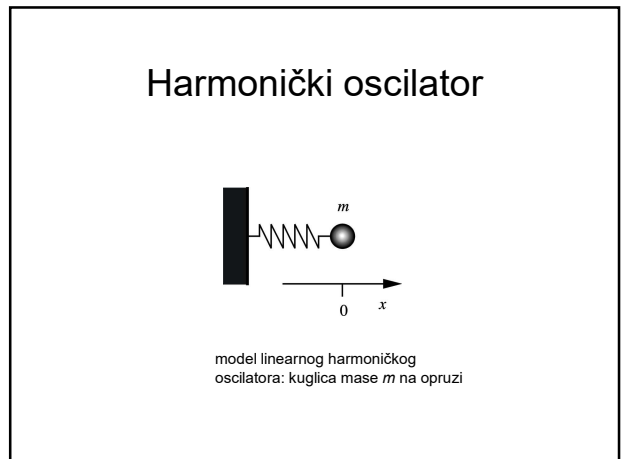
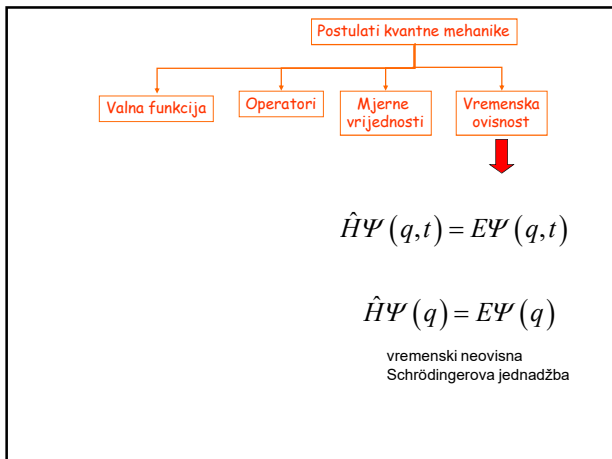
Valna funkcija    Operatori    Mjerne vrijednosti    Vremenska ovisnost

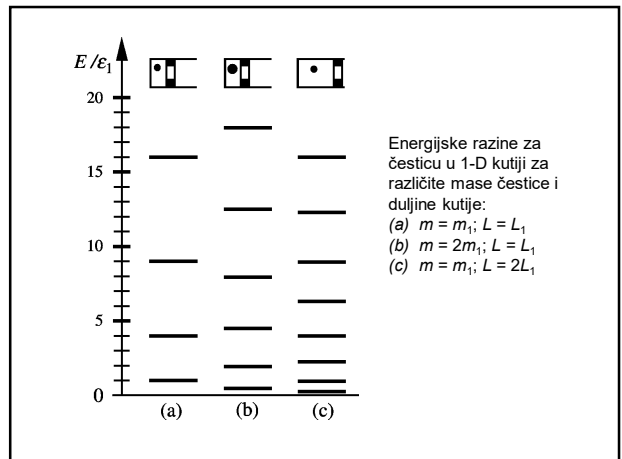
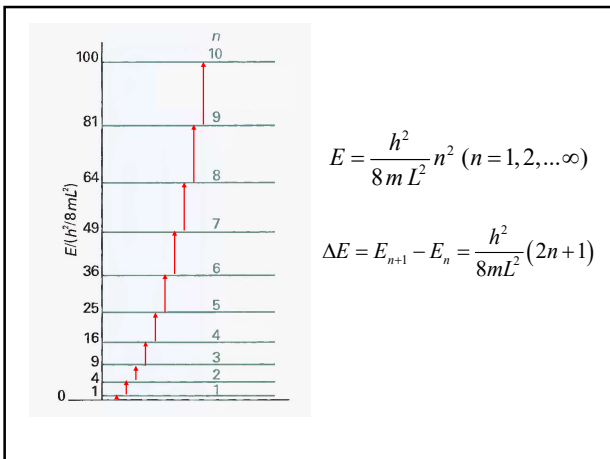
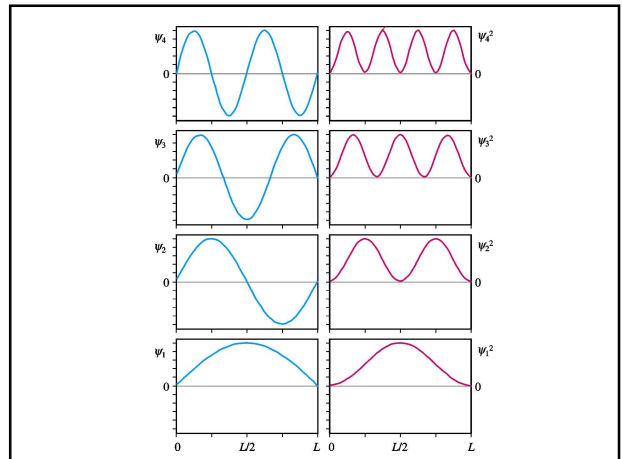
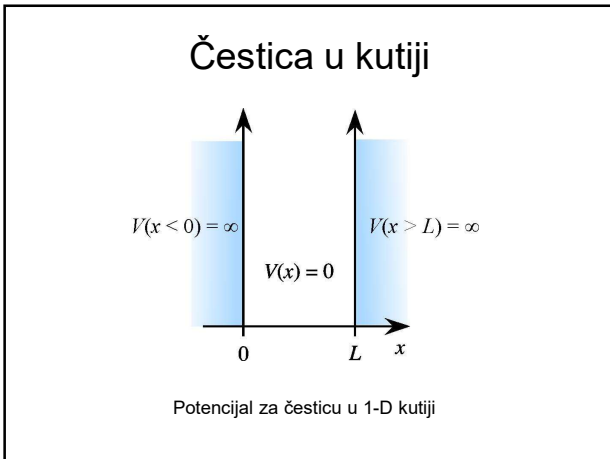
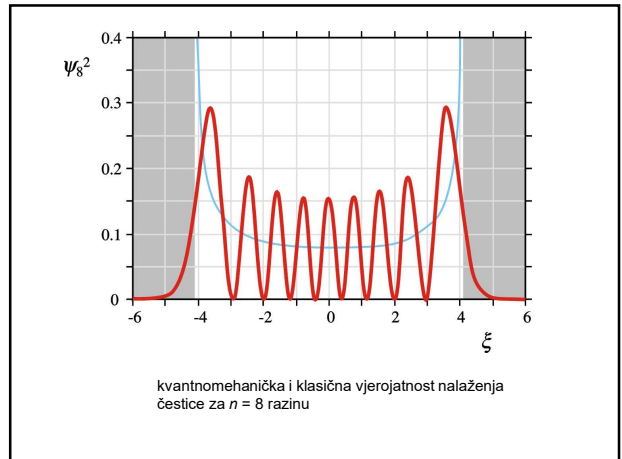
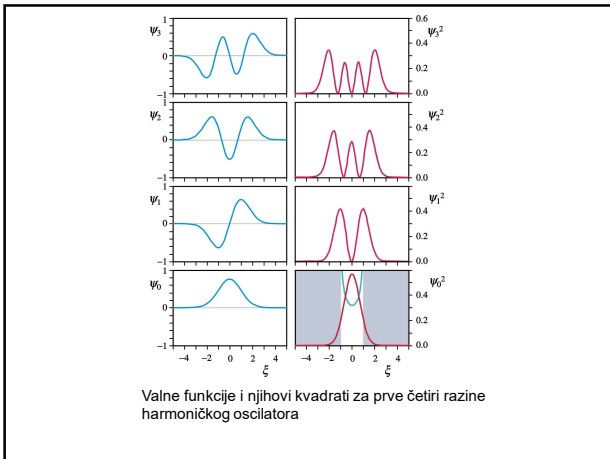
↓

jednadžba svojstvenih vrijednosti →  $\hat{\Omega}\varphi_i = \omega_i\varphi_i$

$$\langle \Omega \rangle = \frac{\int \Psi^* \hat{\Omega} \Psi d\tau}{\int \Psi^* \Psi d\tau}$$

$$\langle \Omega \rangle = \int \Psi^* \hat{\Omega} \Psi d\tau$$

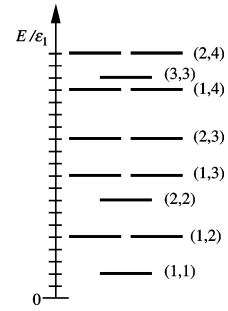
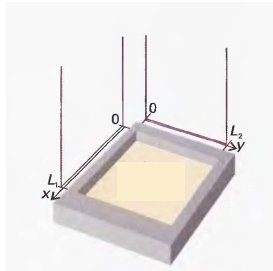




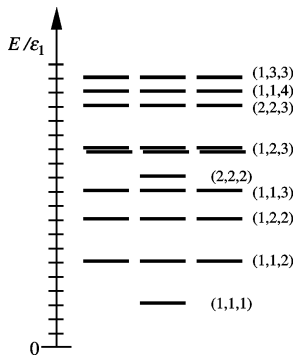
### Dvodimenzionalni prostor

Jednadžbu treba separirati na dvije; svaka ovisi samo o jednoj koordinati

$$E(n_x, n_y) = \frac{\hbar^2}{8mL^2} (n_x^2 + n_y^2)$$



Energijske razine za česticu u 2-D kutiji



Energijske razine za česticu u 3-D kutiji

### VODIKOV ATOM

H

Schrödingerova jednadžba

SPIN

Separacija varijabli

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

Kvantni brojevi  $m$  i  $l$

Radijalne funkcije  
 $R_n(r)$

Kvantni broj  $n$

Energija

### Elektronska struktura atoma

Za opisivanje položaja dviju čestica (jezgre i elektrona) u trodimenzijskom prostoru potrebno je 6 koordinata – složenija Schrödingerova jednadžba - separacija

kvantni brojevi:  
magnetski kvantni broj  $m$   
azimutni kvantni broj  $l$   
glavni kvantni broj  $n$

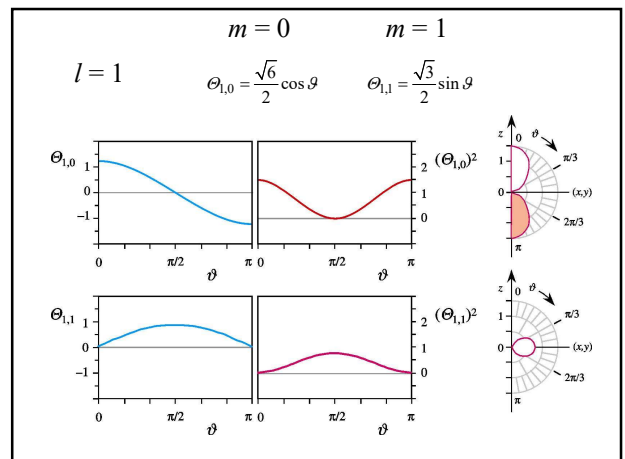
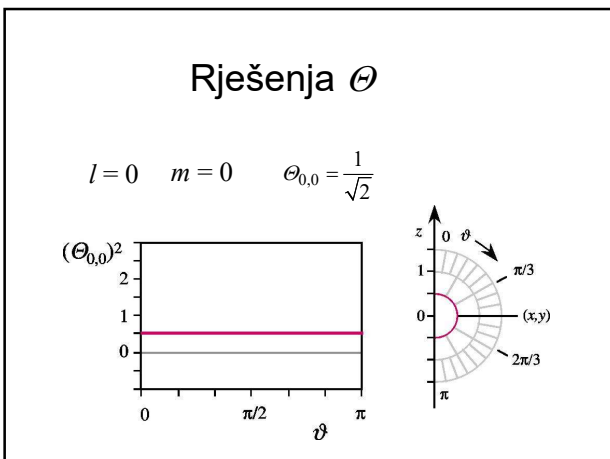
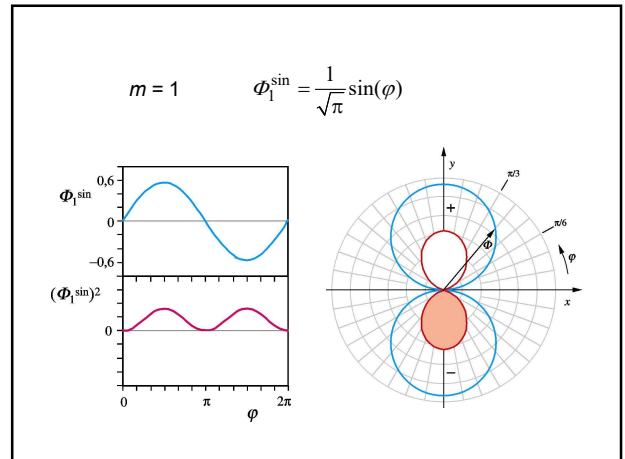
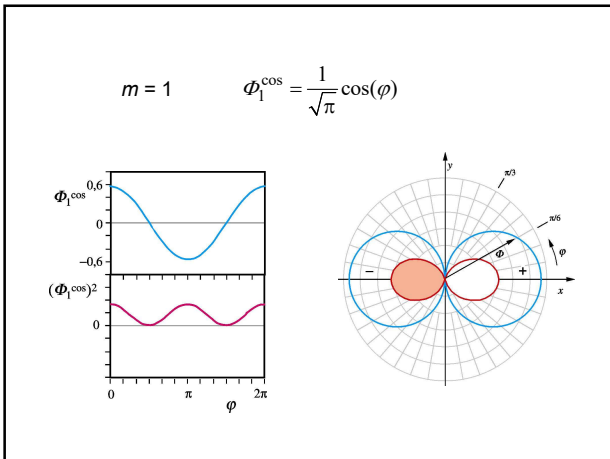
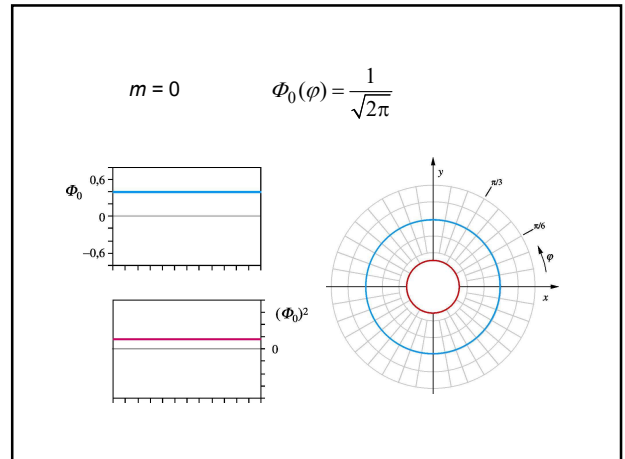
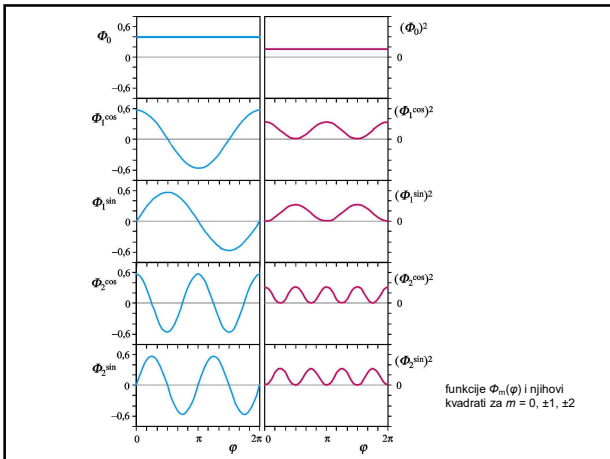
$$E = -hcZ^2 R_\infty \frac{\mu}{m_e L^2} \frac{1}{n^2}$$

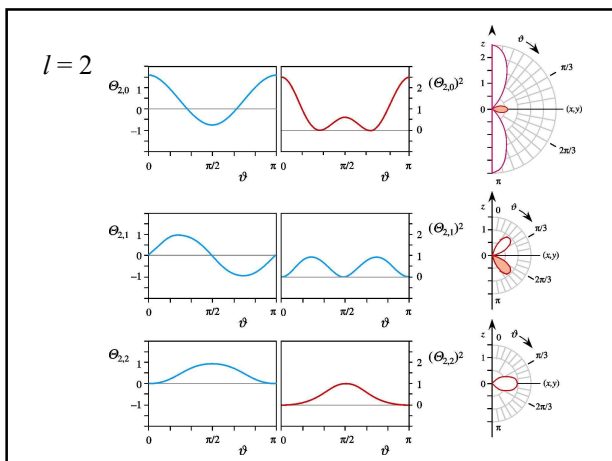
### Elektronska struktura atoma

Valne funkcije koje su rješenja Schrödingerove jednadžbe imaju oblik:

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







Kugline funkcije – ukupne valne funkcije  
dobivene množenjem funkcija  $\Phi_m$  i  $\Theta_{l,m}$

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

$l = 0$   
 $m_l = 0$

Kugline funkcije

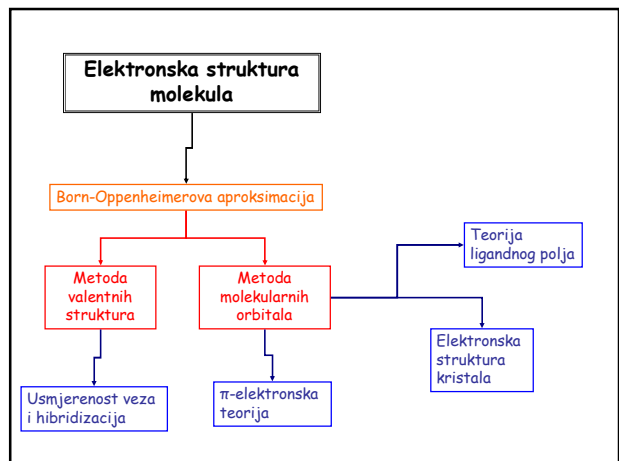
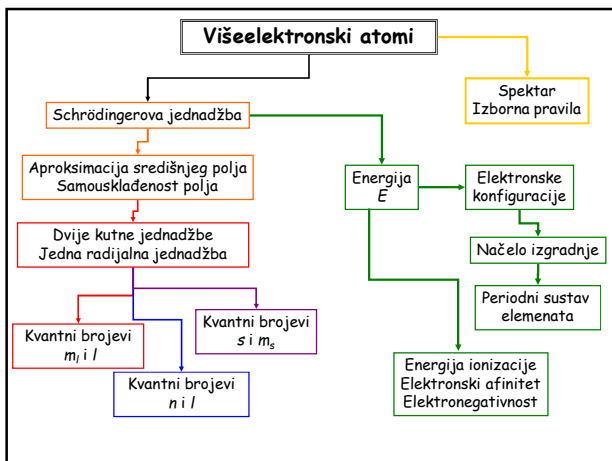
$$Y_{1,0} = \frac{1}{2}\sqrt{\frac{3}{\pi}} \cos \vartheta$$

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

Kugline funkcije

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

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

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


Born-Oppenheimerova aproksimacija

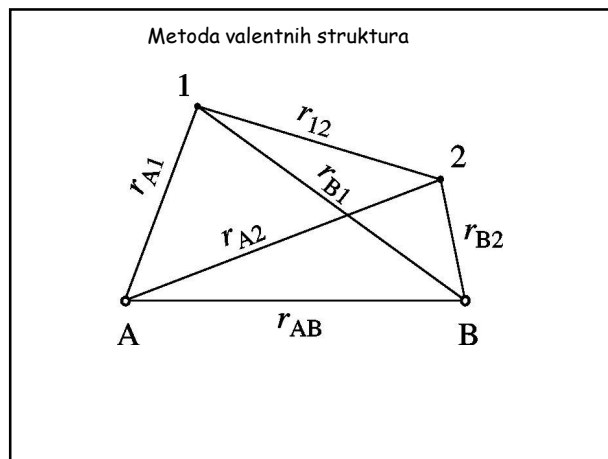
$$\Psi_{\text{uk}} = \Psi_{\text{N}} \cdot \Psi_{\text{e}}$$

$$(\hat{T}_{\text{e}} + V)\Psi_{\text{e}} = E_{\text{e}} \cdot \Psi_{\text{e}}$$

ELEKTRONSKA GIBANJA  
UZ STALNI POLOŽAJ  
JEZGRE

$$(\hat{T}_{\text{N}} + E_{\text{e}})\Psi_{\text{N}} = E \cdot \Psi_{\text{N}}$$

GIBANJE JEZGRA POD  
UTJECAJEM  
POTENCIJALA  $E_{\text{e}}$



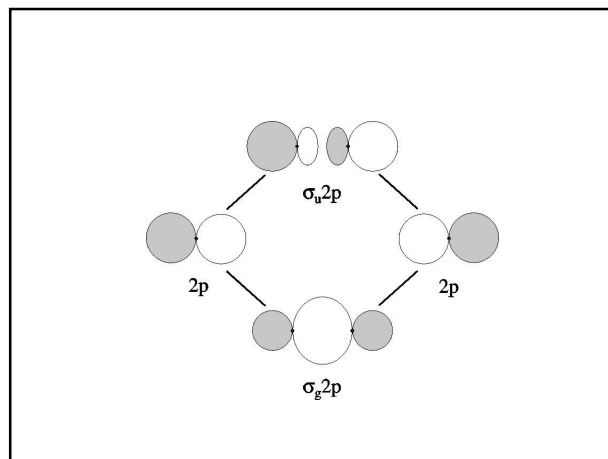
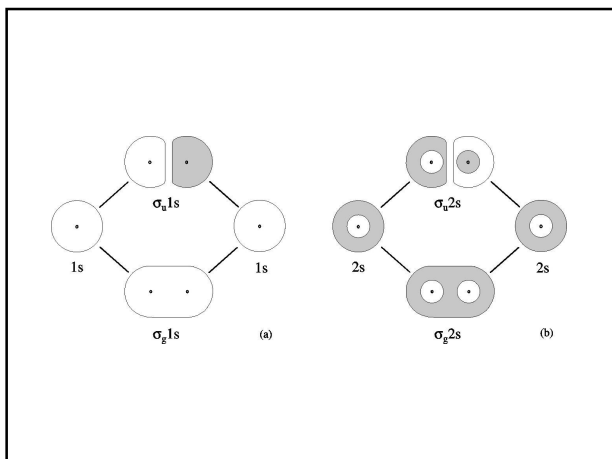
$$\hat{H} = \hat{T}_1 + \hat{T}_2 + \frac{e^2}{4\pi\epsilon_0} \left( -\frac{1}{r_{A1}} - \frac{1}{r_{B1}} - \frac{1}{r_{A2}} - \frac{1}{r_{B2}} + \frac{1}{r_{12}} + \frac{1}{r_{AB}} \right) =$$

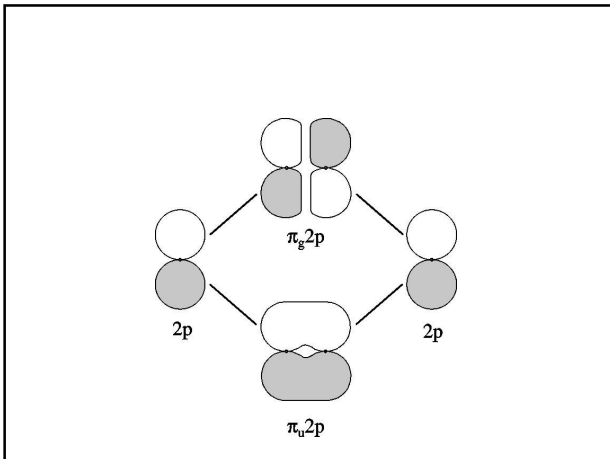
$$= \left( \hat{T}_1 - \frac{e^2}{4\pi\epsilon_0 r_{A1}} \right) + \left( \hat{T}_2 - \frac{e^2}{4\pi\epsilon_0 r_{B2}} \right) +$$

$$+ \frac{e^2}{4\pi\epsilon_0} \left( -\frac{1}{r_{B1}} - \frac{1}{r_{A2}} + \frac{1}{r_{12}} + \frac{1}{r_{AB}} \right) = \hat{H}_{A1} + \hat{H}_{B2} + \hat{H}'$$

Metoda molekularnih orbitala

$$\hat{H} = \left[ \hat{T}_1 - \frac{e^2}{4\pi\epsilon_0} \left( \frac{1}{r_{A1}} + \frac{1}{r_{B1}} \right) \right] + \left[ \hat{T}_2 - \frac{e^2}{4\pi\epsilon_0} \left( \frac{1}{r_{A2}} + \frac{1}{r_{B2}} \right) \right] + \frac{e^2}{4\pi\epsilon_0} \left( \frac{1}{r_{12}} + \frac{1}{r_{AB}} \right)$$





### Hibridizacija

Pauling & Slater

- funkcije se miješaju i nastaju nove funkcije - hibridne orbitale
- s i p hibridne orbitale su ekvivalentne, imaju maksimume u različitim smjerovima

$$\Psi_i = \sum_{j=1}^n c_{ij} \phi_j = c_{i1} \phi_1 + c_{i2} \phi_2 + \dots + c_{in} \phi_n$$

$$\sum_{j=1}^n c_{ij}^2 = 1$$

$$\sum_{i=1}^n c_{ij}^2 = 1$$

$$n = \frac{c_x^2 + c_y^2 + c_z^2}{c_s^2}$$
