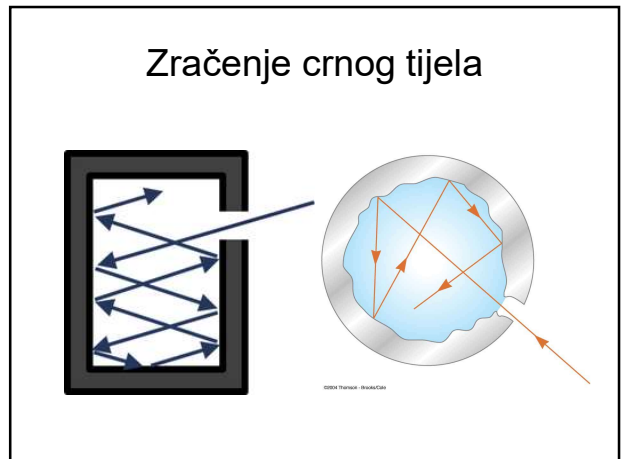
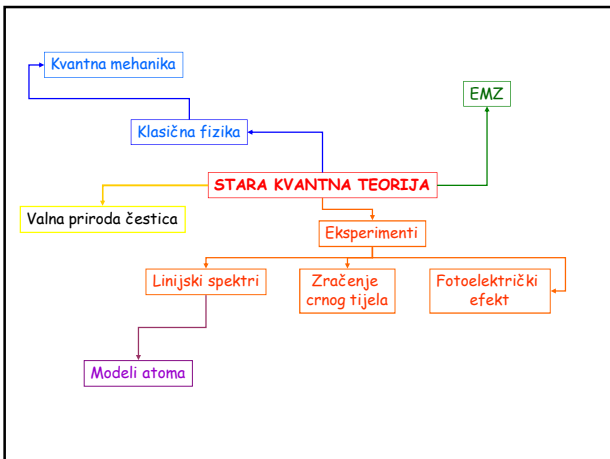



Elektromagnetsko zračenje


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

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

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




Jožef Stefan
1835 – 1893

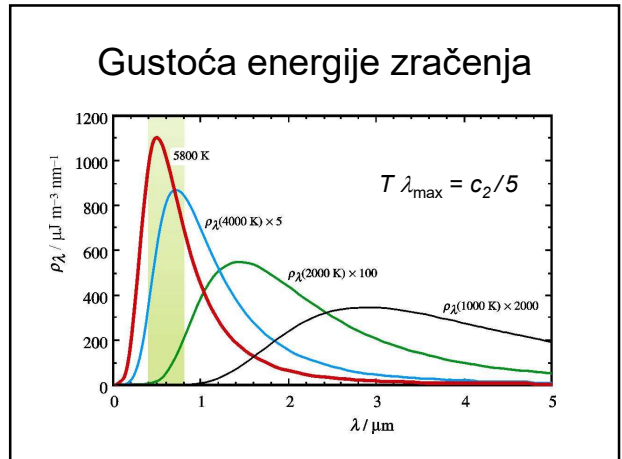


Ludwig Eduard Boltzmann
1844 – 1906

$M = \sigma T^4$

Stefan – Boltzmannov zakon

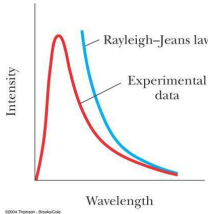
M = egzitancija - omjer ukupne emitirane snage s djelića površine i ploštine te površine, tj. gustoća toka energije iz izvora



Ultraljubičasta katastrofa

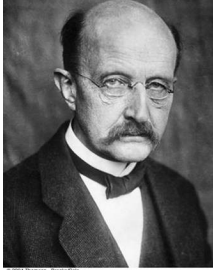
- Rayleigh-Jeans

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

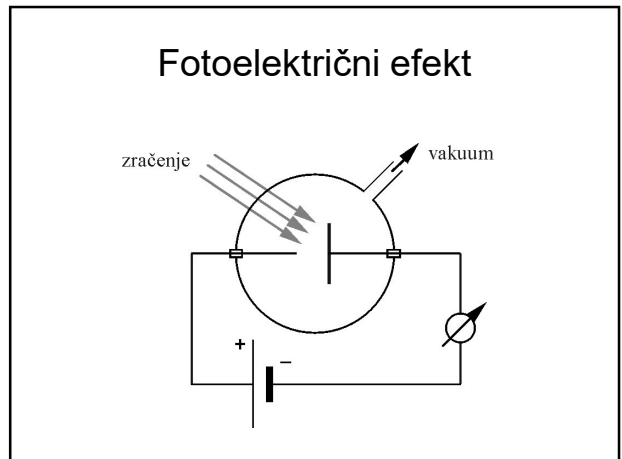
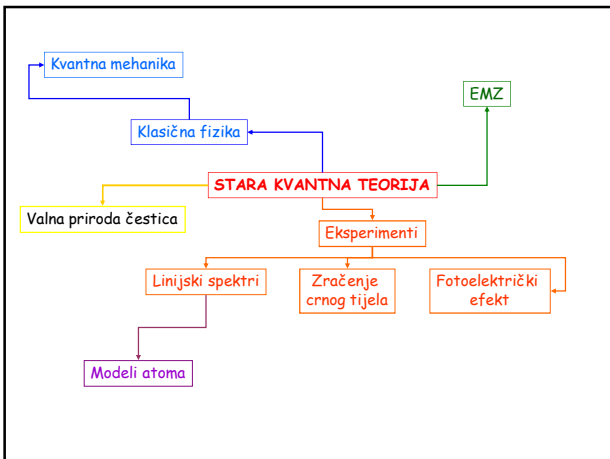


Max Planck

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



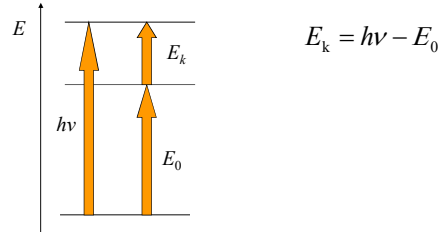
10



Eksperimentalne činjenice

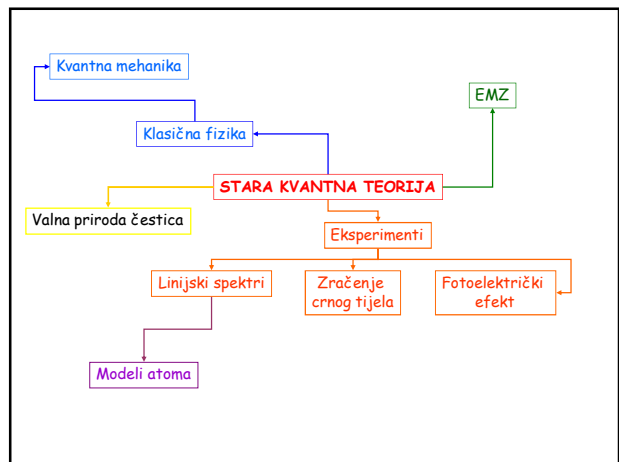
1. Električna struja proporcionalna je intenzitetu zračenja.
2. Kinetička energija elektrona neovisna je o intenzitetu zračenja.
3. Maksimalna kinetička energija elektrona raste s frekvencijom zračenja.
4. Zračenje većih valnih duljina od neke granične više ne uzrokuje fotoefekt.

Fotoelektrični efekt

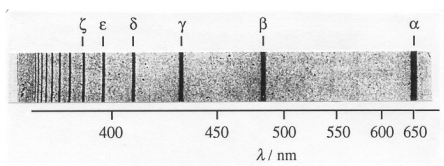


Eksperimentalne činjenice

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

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

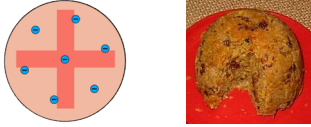
Balmerova serija

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

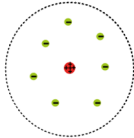
Rydbergova jednadžba

modeli atoma

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

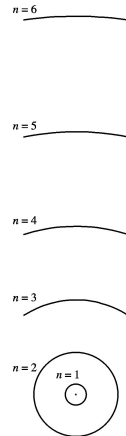


- H. Rutherford (1911)



Bohrov model atoma

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



Bohrov model atoma

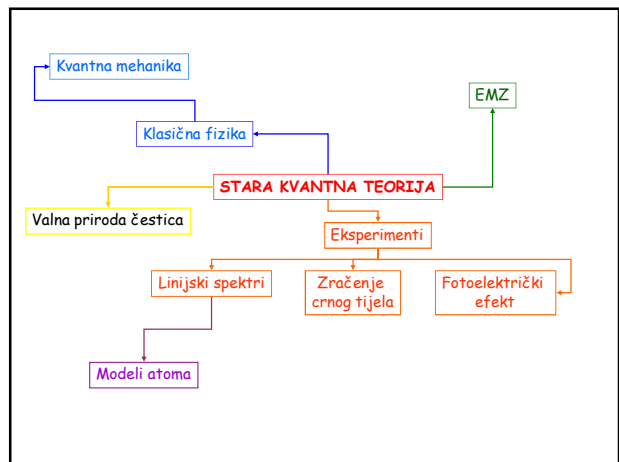
Izračunao:

- 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
$$E = -\frac{hcR_\infty}{n^2}$$

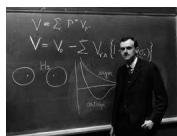
- valne duljine linija u spektru atoma vodika



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"



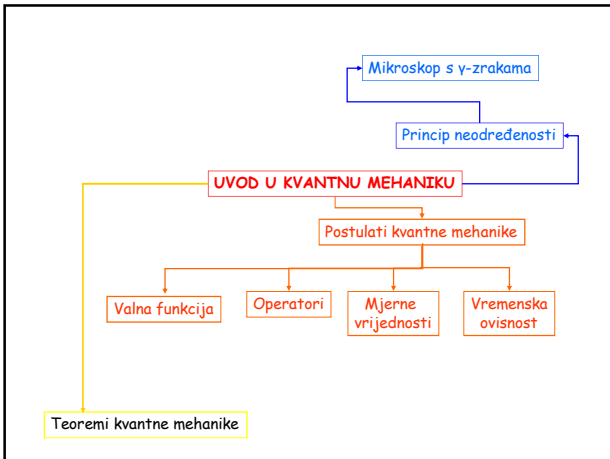

Erwin Schrödinger (1887 – 1961)

* 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

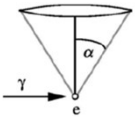
Princip neodređenosti
Mikroskop s γ-zrakama

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

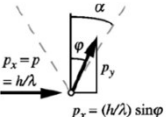


Werner Heisenberg

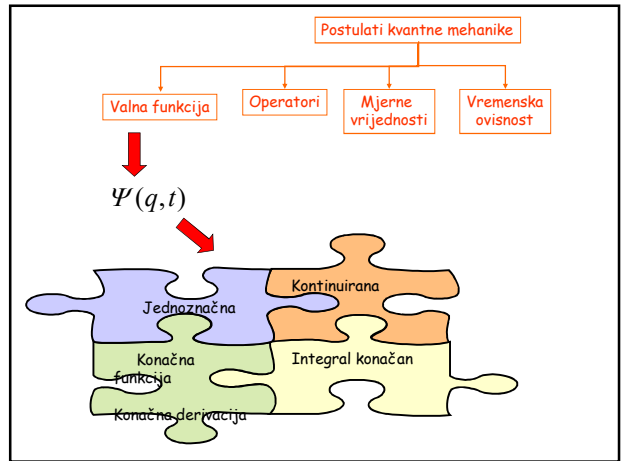
$\Delta x \cdot \Delta p_x \approx h$



Crtež 2.1. Mikroskop s γ-zrakama.



Crtež 2.2. Komponente količine gibanja fotona prije (lijevo) i poslije sudara s elektronom.
 $p_x = p = h/\lambda$
 $p_x = (h/\lambda) \sin \alpha$



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 | $\hat{p}_x = -i\hbar \frac{\partial}{\partial x}$ |

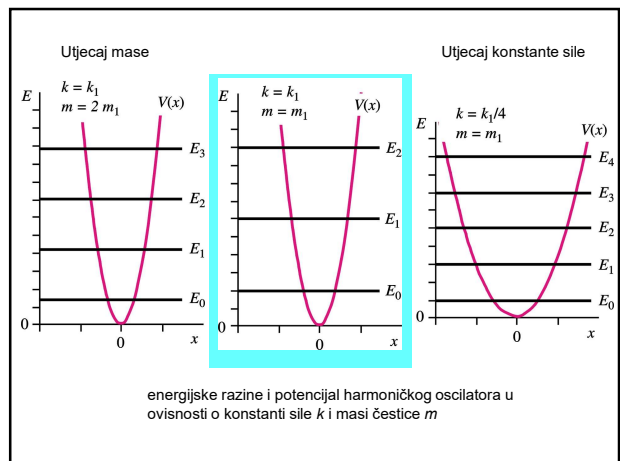
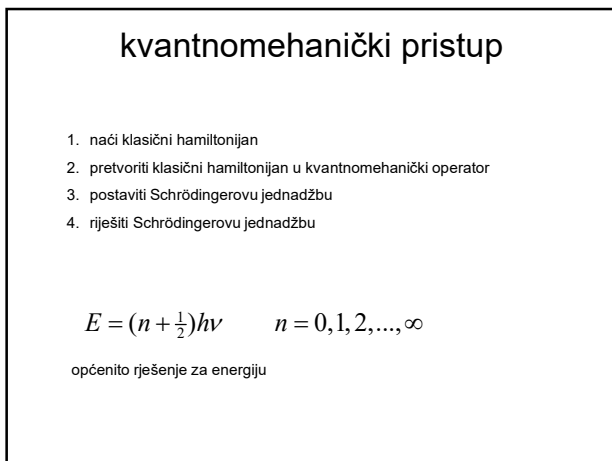
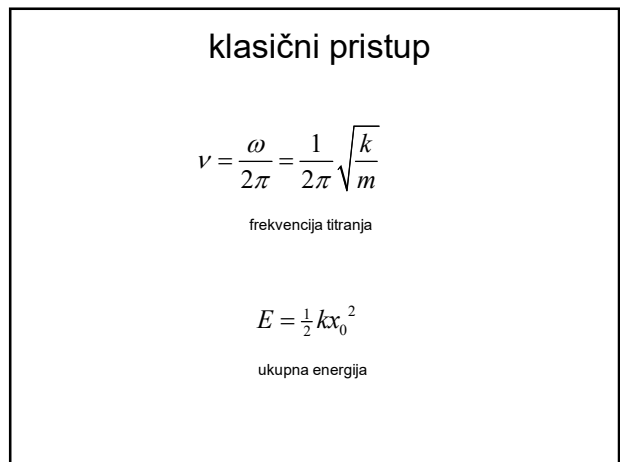
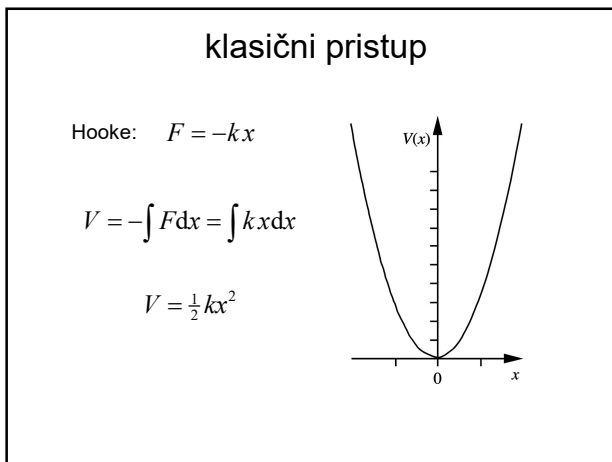
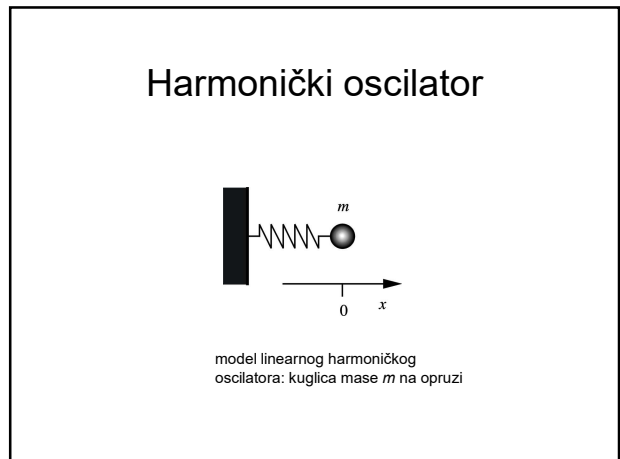
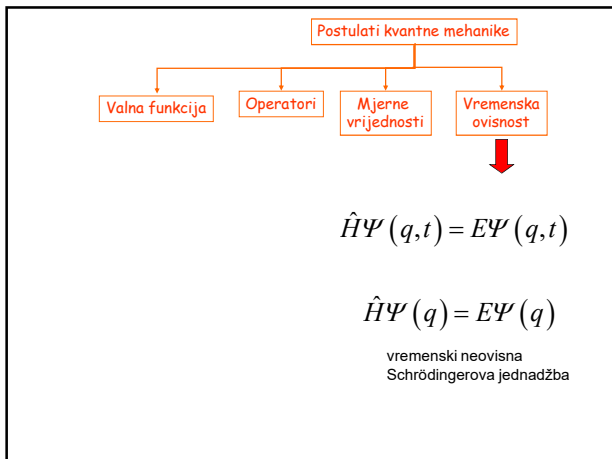
Postulati kvantne mehanike

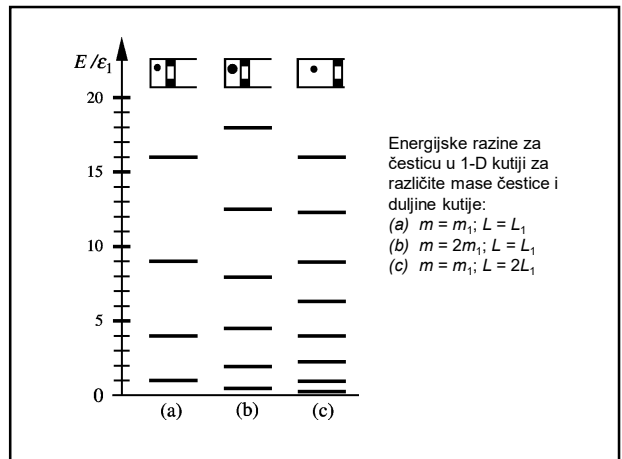
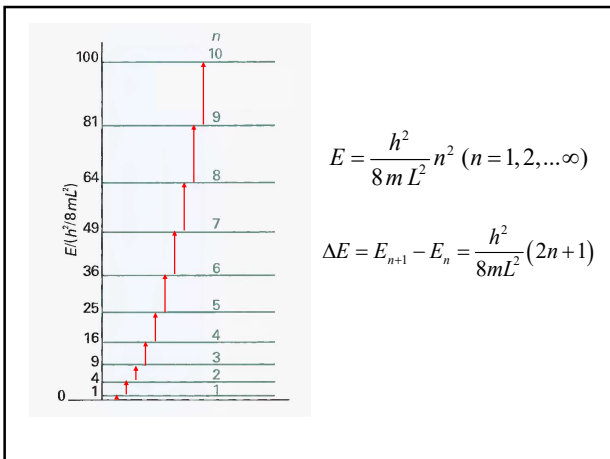
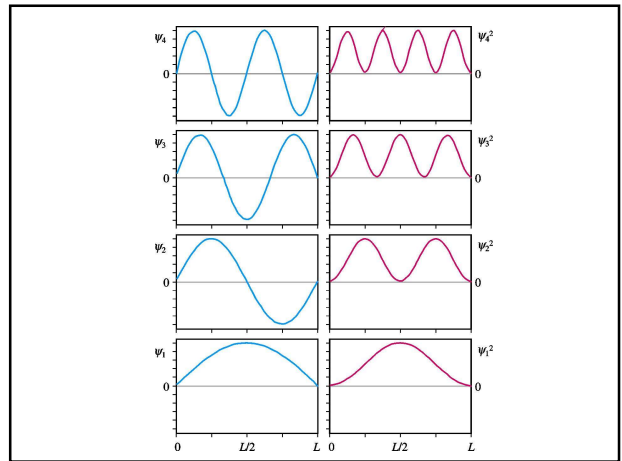
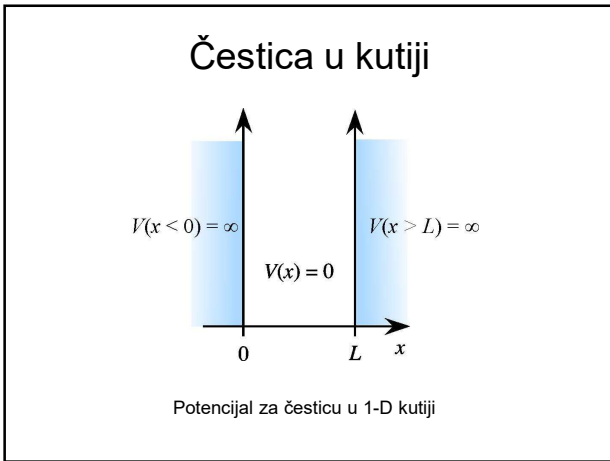
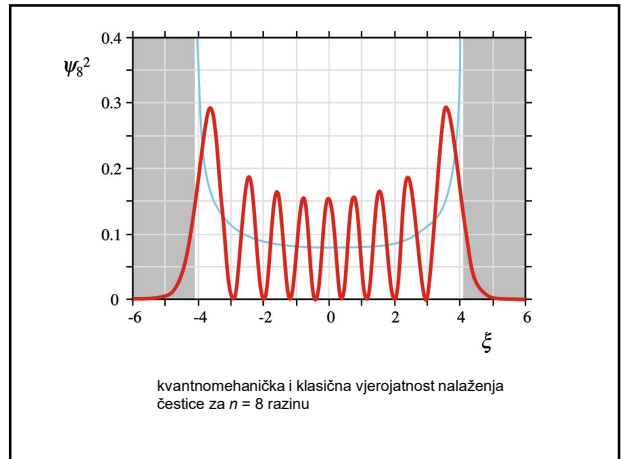
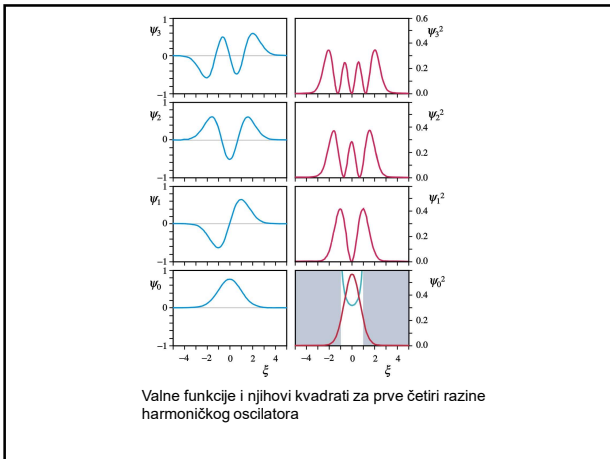
Valna funkcija Operatori Mjerne vrijednosti Vremenska ovisnost

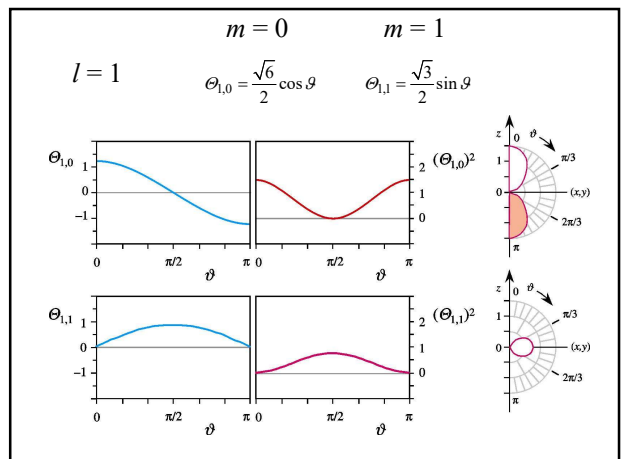
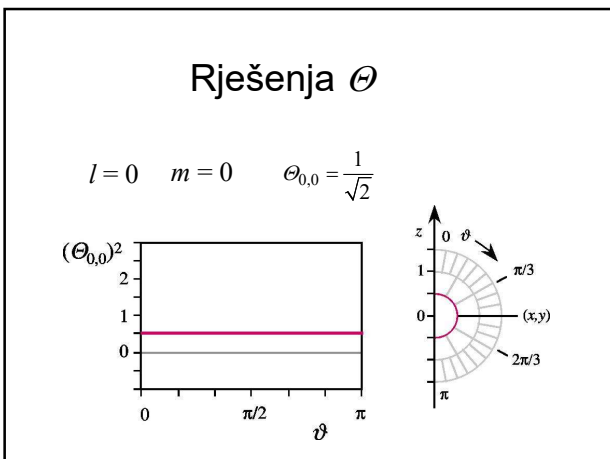
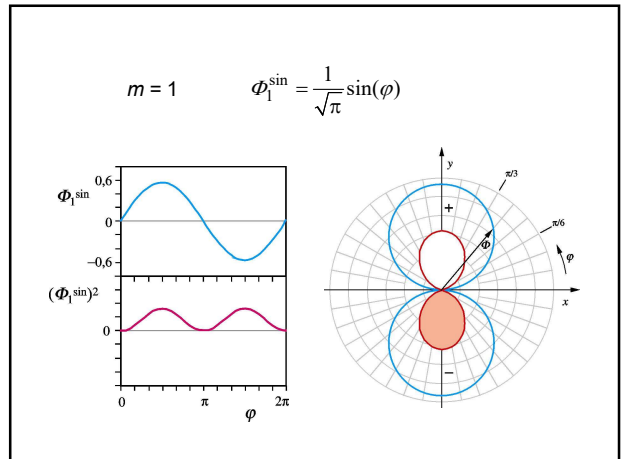
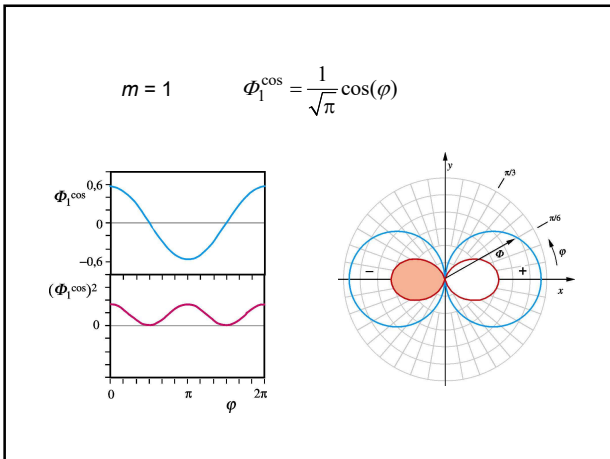
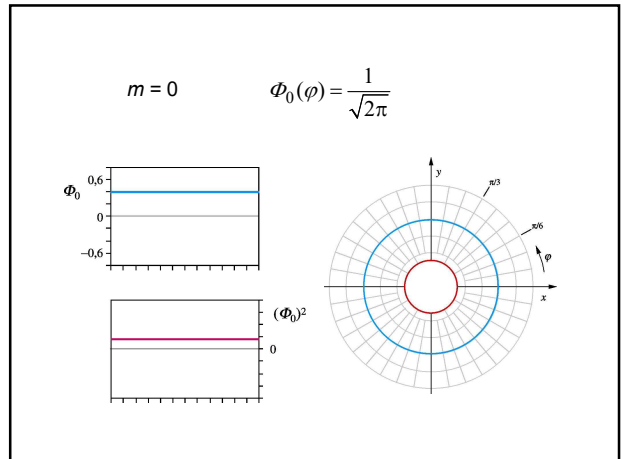
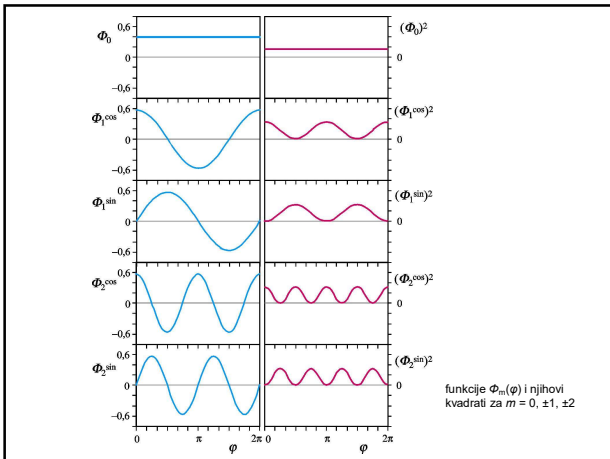
jednadžba svojstvenih vrijednosti $\rightarrow \hat{\Omega} \varphi_i = \omega_i \varphi_i$

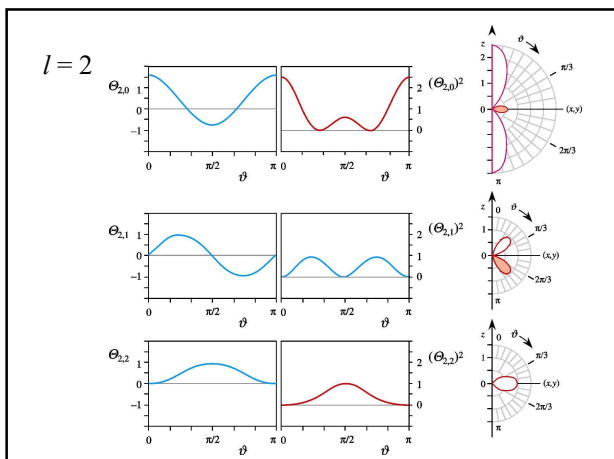
$$\langle \Omega \rangle = \frac{\int \Psi^* \hat{\Omega} \Psi d\tau}{\int \Psi^* \Psi d\tau}$$

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









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

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

$l = 0$
 $m_l = 0$

Kugline funkcije

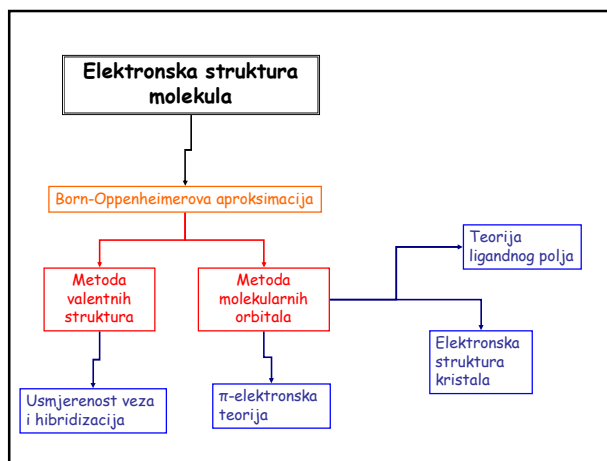
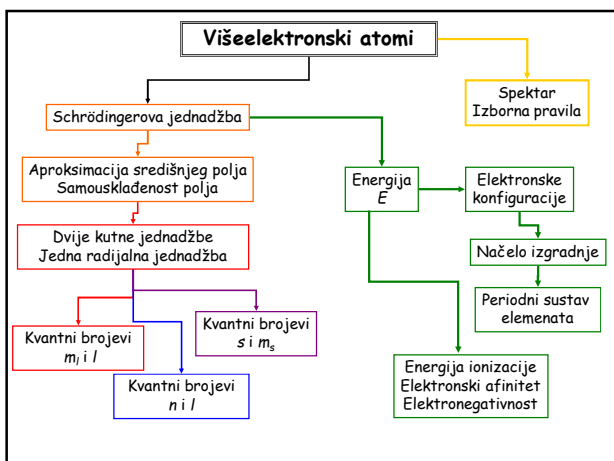
$$Y_{1,0} = \frac{1}{2}\sqrt{\frac{3}{\pi}} \cos \vartheta$$

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

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-Opperheimerova aproksimacija

$$\Psi_{uk} = \Psi_N \cdot \Psi_c$$

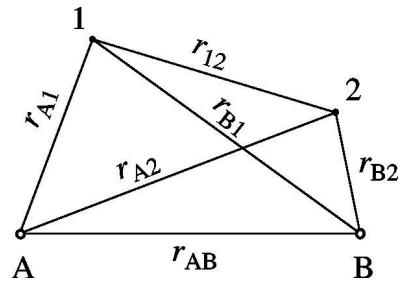
$$(\hat{T}_c + V)\Psi_c = E_c \cdot \Psi_c$$

ELEKTRONSKA GIBANJA
UZ STALNI POLOŽAJ
JEZGRE

$$(\hat{T}_N + E_c)\Psi_N = E \cdot \Psi_N$$

GIBANJE JEZGRA POD
UTJECAJEM
POTENCIJALA E_c

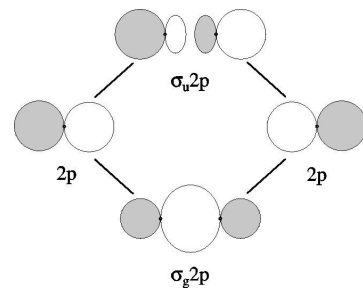
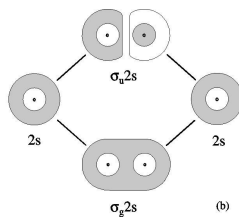
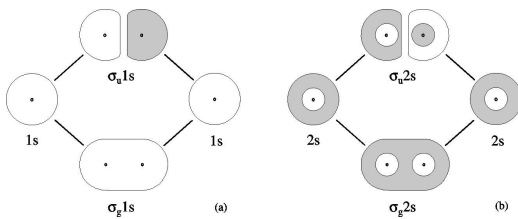
Metoda valentnih struktura

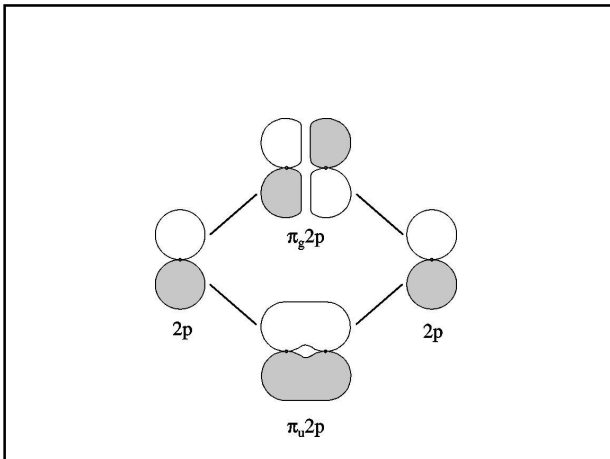


$$\begin{aligned} \hat{H} &= \hat{T}_1 + \hat{T}_2 + \frac{e^2}{4\pi\epsilon_0} \left(-\frac{1}{r_{A1}} - \frac{1}{r_{B1}} - \frac{1}{r_{A2}} - \frac{1}{r_{B2}} + \frac{1}{r_{12}} + \frac{1}{r_{AB}} \right) = \\ &= \left(\hat{T}_1 - \frac{e^2}{4\pi\epsilon_0 r_{A1}} \right) + \left(\hat{T}_2 - \frac{e^2}{4\pi\epsilon_0 r_{B2}} \right) + \\ &\quad + \frac{e^2}{4\pi\epsilon_0} \left(-\frac{1}{r_{B1}} - \frac{1}{r_{A2}} + \frac{1}{r_{12}} + \frac{1}{r_{AB}} \right) = \hat{H}_{A1} + \hat{H}_{B2} + \hat{H}' \end{aligned}$$

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

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

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

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

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