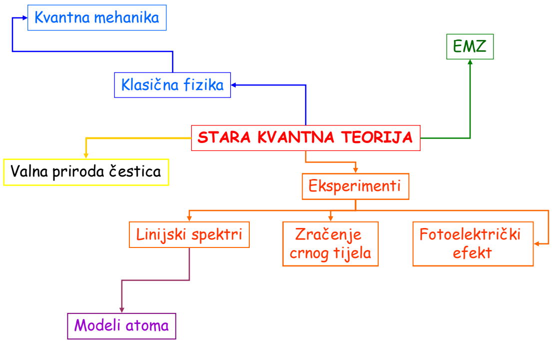
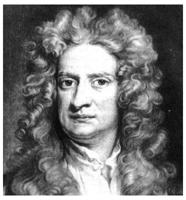


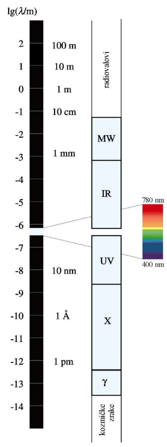


Sir Isaac Newton (1642-1727)

Christian Huygens (1629 –1695)

James Clerk Maxwell (1831 - 1879)

Područja zračenja

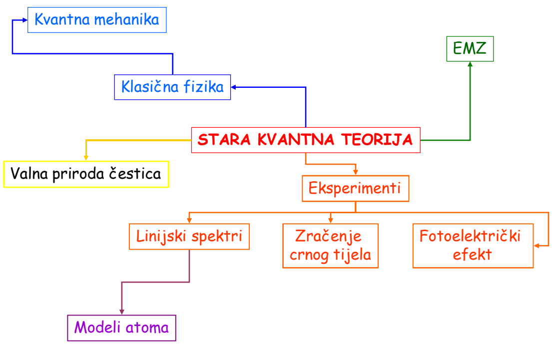


Elektromagnetsko zračenje

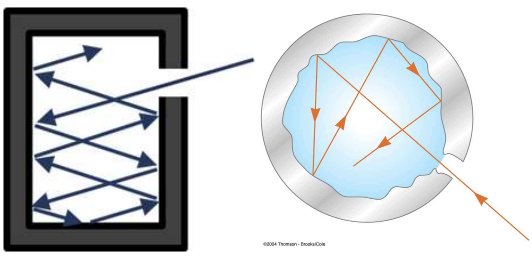
$$\lambda = \frac{c}{\nu}$$

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

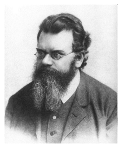
$$\nu = c\tilde{\nu}$$



Zračenje crnog tijela



Jožef Stefan
1835 – 1893



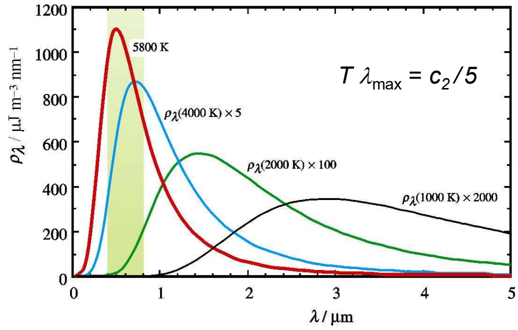
Ludwig Eduard Boltzmann
1844 – 1906

$$M = \sigma T^4$$

Stefan – Boltzmannov zakon

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

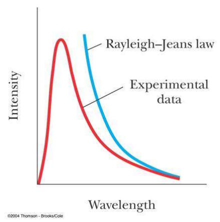
Gustoća energije zračenja



Ultraljubičasta katastrofa

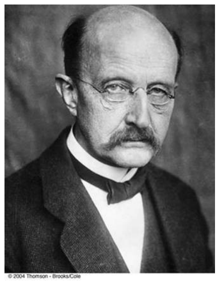
- Rayleigh-Jeans

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



Max Planck

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



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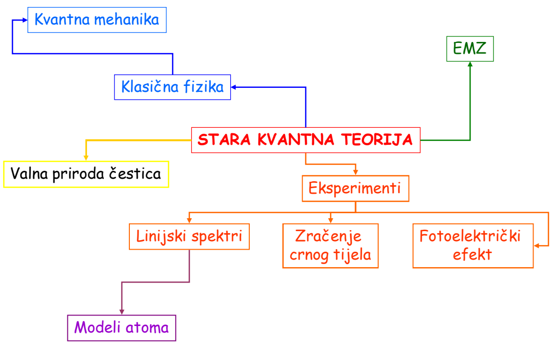
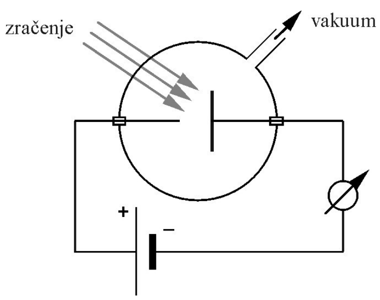


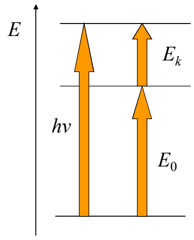
Fotoelektrični efekt



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.

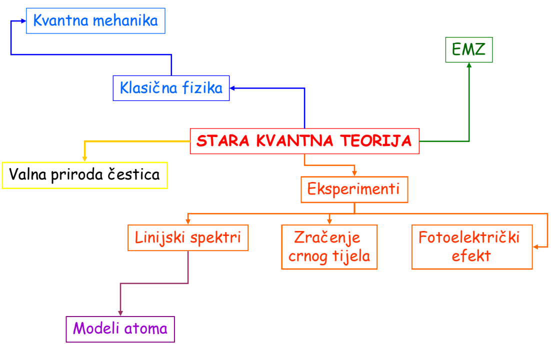
Fotoelektrični efekt



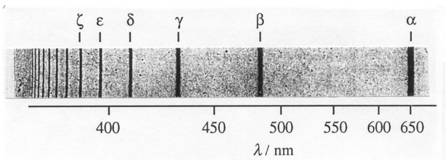
$$E_k = h\nu - E_0$$

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

$$\lambda / \mathring{A} = 3546,6 \frac{n^2}{n^2 - 4} \quad (n = 3, 4, 5, ..., 11)$$

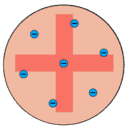
Balmerova serija

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

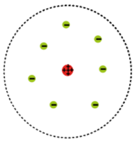
Rydbergova jednadžba

modeli atoma

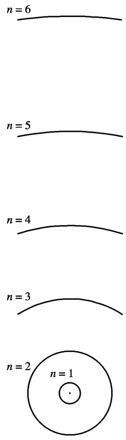
- J. J. Thomson (1904) “plum pudding” model




- H. Rutherford (1911)



Bohrov model atoma

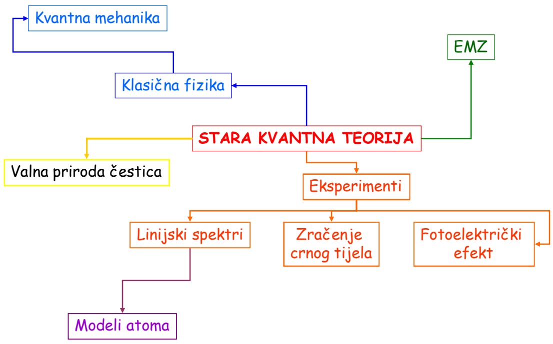


- Stacionarna stanja
- Kvantiziranost energije
- Pri prijelazu $\Delta E = h\nu$
- Kvantiziranost kutne količine gibanja
- $L = n\hbar$

Bohrov model atoma

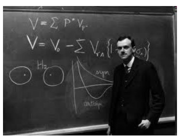
Izračunao:

- polumjere putanje elektrona $$r = \frac{n\hbar}{mv} = \frac{(4\pi\varepsilon_0)\hbar^2}{me^2} n^2$$
- brzine $$v = \frac{1}{4\pi\varepsilon_0}\frac{e^2}{\hbar n}$$
- ukupne energije stacionarnih stanja $$E = -\frac{hcR_\infty}{n^2}$$
- valne duljine linija u spektru atoma vodika



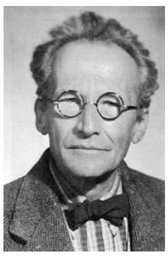
kvantna mehanika

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"



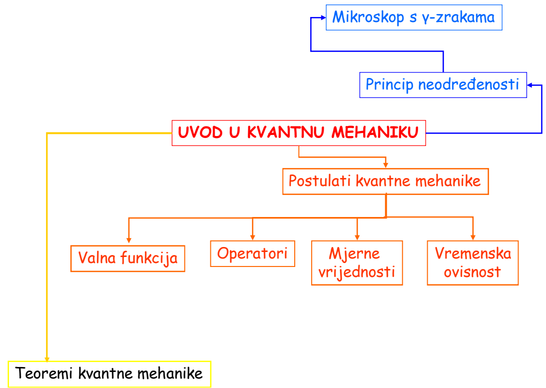
Erwin Schrödinger (1887 – 1961)

* 1987 Beč

1920 Stuttgart
1921 Wroclaw
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)

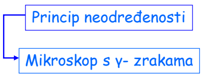
* 1901 Würzburg

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

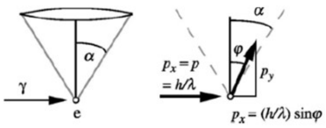


Werner Heisenberg, 1927.

- nije moguće istovremeno odrediti koordinatu, x , i konjugiranu količinu gibanja neke čestice do proizvoljne točnosti

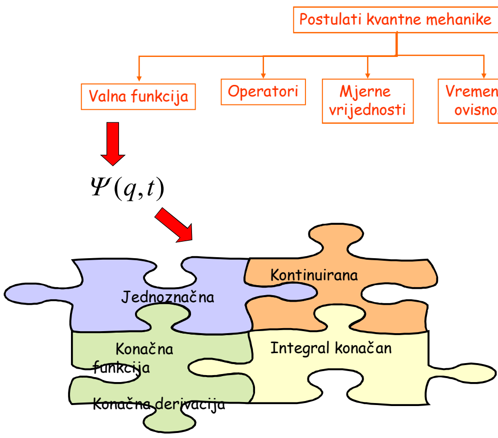
$$\Delta x \cdot \Delta p_x \approx h$$

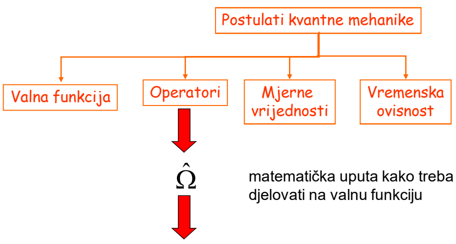
Werner Heisenberg



Crtež 2.1. Mikroskop s γ-zrakama.

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

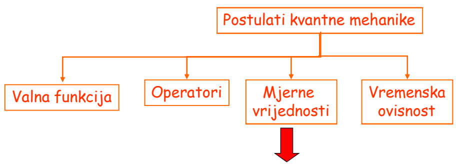




$\hat{\Omega}$ matematička uputa kako treba djelovati na valnu funkciju

Tablica 2.1 Osnovni kvantnomehanički operatori u koordinatnoj reprezentaciji.

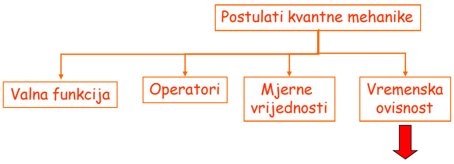
Veličina		Kvantnomehanički
Naziv	Simbol	operator
koordinata	x	$\hat{x} = x\cdot$
količina gibanja, impuls	p_x	$\hat{p}_x = -i\hbar\frac{\partial}{\partial x}$



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

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

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

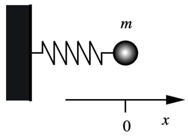


$$\hat{H}\Psi(q,t) = E\Psi(q,t)$$

$$\hat{H}\Psi(q) = E\Psi(q)$$

vremenski neovisna Schrödingerova jednadžba

Harmonički oscilator



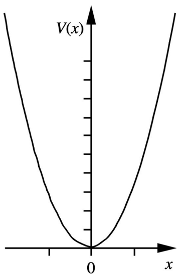
model linearnog harmoničkog oscilatora: kuglica mase *m* na opruzi

klasični pristup

Hooke: $F = -kx$

$$V = -\int F\mathrm{d}x = \int kx\mathrm{d}x$$

$$V = \tfrac{1}{2}kx^2$$



klasični pristup

$$\nu = \frac{\omega}{2\pi} = \frac{1}{2\pi}\sqrt{\frac{k}{m}}$$

frekvencija titranja

$$E = \tfrac{1}{2}kx_0^{\,2}$$

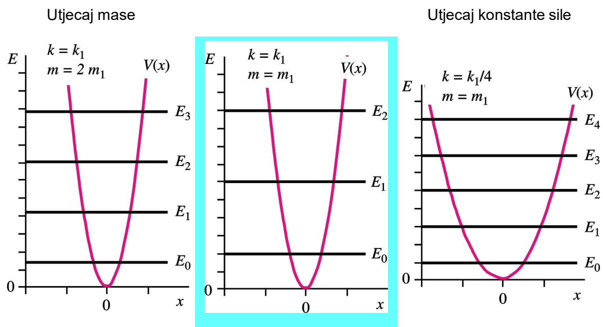
ukupna energija

kvantnomehanički pristup

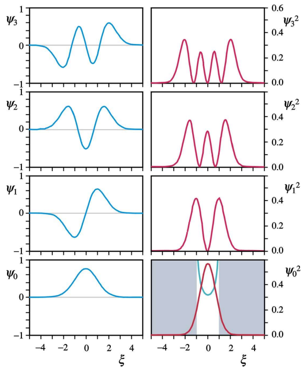
1. naći klasični hamiltonijan
2. pretvoriti klasični hamiltonijan u kvantnomehanički operator
3. postaviti Schrödingerovu jednadžbu
4. riješiti Schrödingerovu jednadžbu

$$E = (n + \tfrac{1}{2})h\nu \qquad n = 0, 1, 2, \ldots, \infty$$

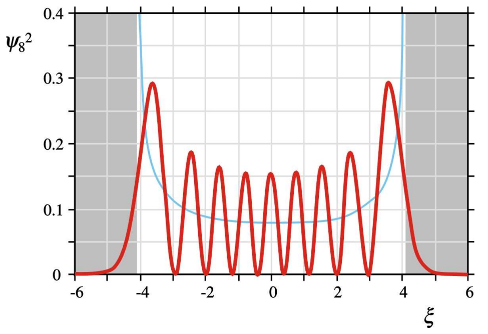
općenito rješenje za energiju



energijske razine i potencijal harmoničkog oscilatora u ovisnosti o konstanti sile *k* i masi čestice *m*

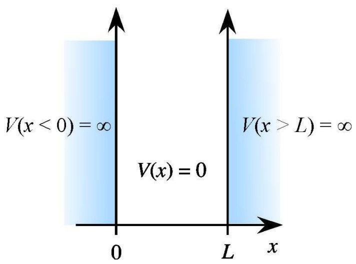


Valne funkcije i njihovi kvadrati za prve četiri razine harmoničkog oscilatora

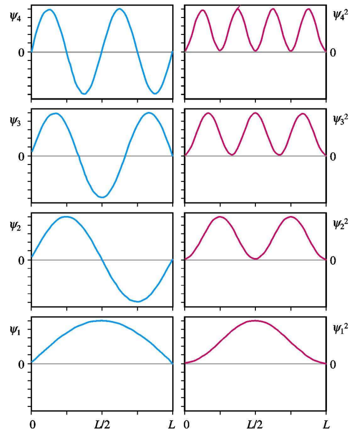


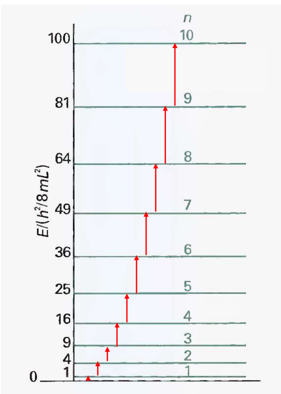
kvantnomehanička i klasična vjerojatnost nalaženja čestice za *n* = 8 razinu

Čestica u kutiji



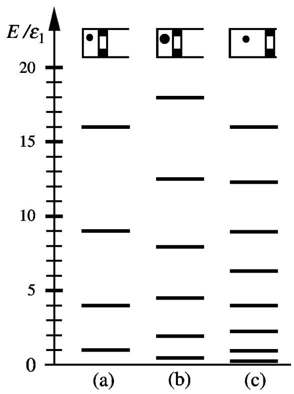
Potencijal za česticu u 1-D kutiji





$$E = \frac{h^2}{8\,m\,L^2}n^2 \;(n = 1, 2, \ldots \infty)$$

$$\Delta E = E_{n+1} - E_n = \frac{h^2}{8mL^2}(2n+1)$$

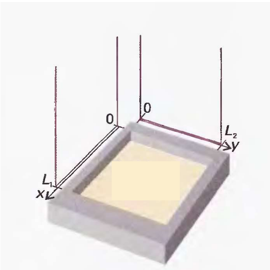


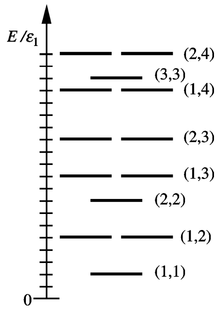
Energijske razine za česticu u 1-D kutiji za različite mase čestice i duljine kutije:
(a) $m = m_1$; $L = L_1$
(b) $m = 2m_1$; $L = L_1$
(c) $m = m_1$; $L = 2L_1$

Dvodimenzionalni prostor

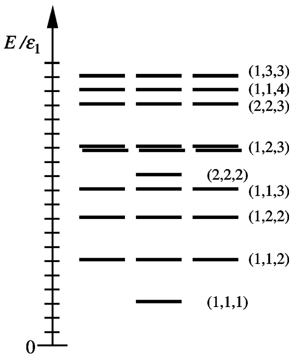
Jednadžbu treba separirati na dvije; svaka ovisi samo o jednoj koordinati

$$E(n_x, n_y) = \frac{h^2}{8\,m\,L^2}(n_x^{\;2} + n_y^{\;2})$$

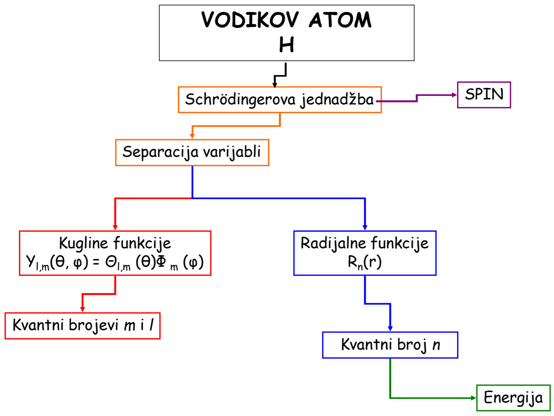




Energijske razine za česticu u 2-D kutiji



Energijske razine za česticu u 3-D kutiji



Elektronska struktura atoma

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

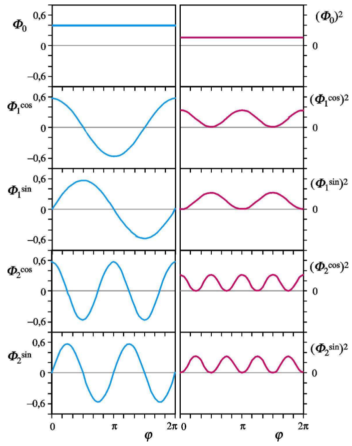
kvantni brojevi:
magnetski kvantni broj *m*
azimutni kvantni broj *l*
glavni kvantni broj *n*

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

Elektronska struktura atoma

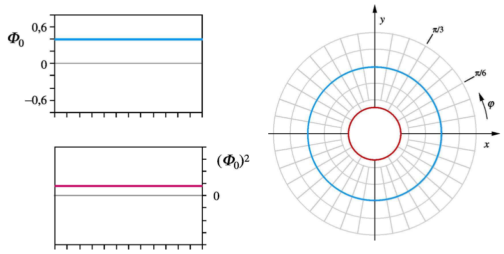
Valne funkcije koje su rješenja Schrödingerove jednadžbe imaju oblik:

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

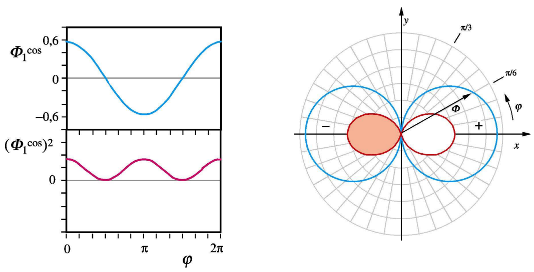


funkcije $\Phi_m(\varphi)$ i njihovi kvadrati za m = 0, ±1, ±2

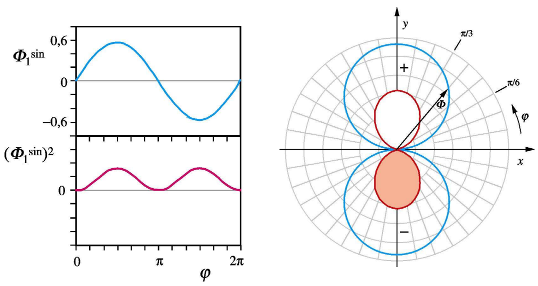
m = 0 $\Phi_0(\varphi) = \frac{1}{\sqrt{2\pi}}$



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

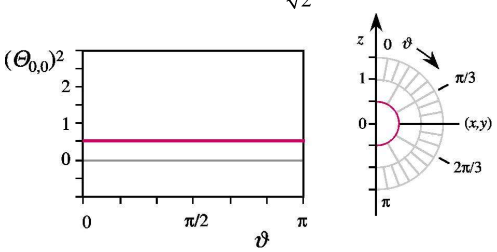


m = 1 $\Phi_1^{\sin} = \frac{1}{\sqrt{\pi}}\sin(\varphi)$



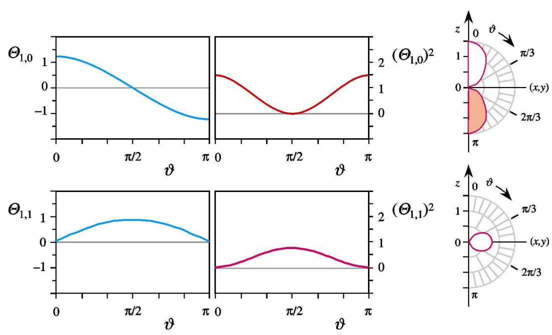
Rješenja Θ

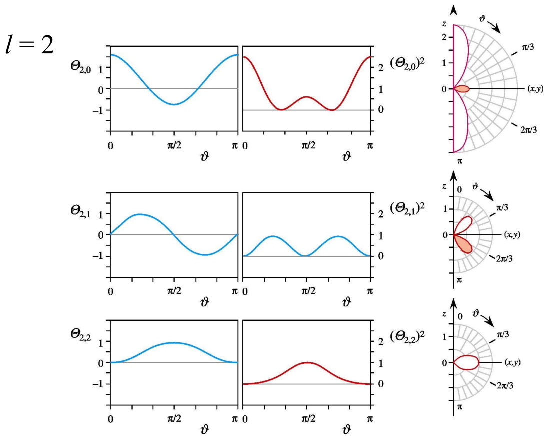
$l = 0 \quad m = 0 \qquad \Theta_{0,0} = \frac{1}{\sqrt{2}}$



$m = 0 \qquad m = 1$

$l = 1 \qquad \Theta_{1,0} = \frac{\sqrt{6}}{2}\cos\vartheta \qquad \Theta_{1,1} = \frac{\sqrt{3}}{2}\sin\vartheta$





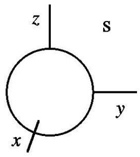
Kugline funkcije – ukupne valne funkcije

dobivene množenjem funkcija Φ_m i $\Theta_{l,m}$

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

$l = 0$

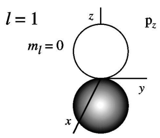
$m_l = 0$

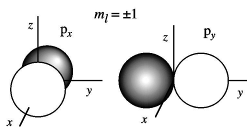


Kugline funkcije

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

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



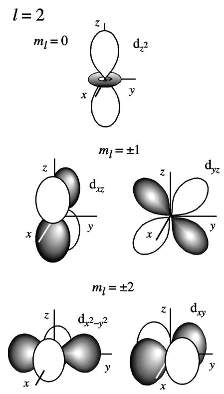


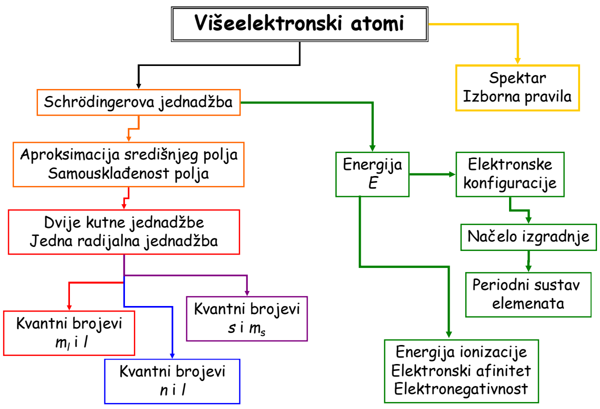
Kugline funkcije

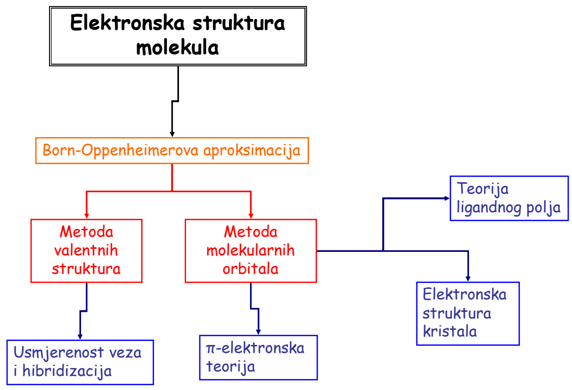
$$Y_{2,0} = \frac{1}{4}\sqrt{\frac{5}{\pi}}(3\cos^2\vartheta - 1)$$

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

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







Born-Opperheimerova aproksimacija

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

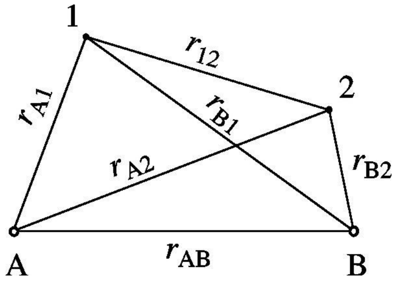
$$\left(\hat{T}_{\mathrm{e}} + V\right)\Psi_{\mathrm{e}} = E_{\mathrm{e}} \cdot \Psi_{\mathrm{e}}$$

ELEKTRONSKA GIBANJA UZ STALNI POLOŽAJ JEZGRE

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

GIBANJE JEZGRA POD UTJECAJEM POTENCIJALA E_e

Metoda valentnih struktura



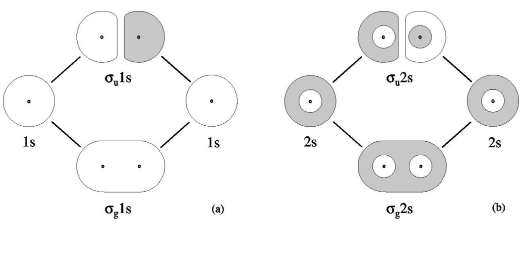
$$\hat{H} = \hat{T}_1 + \hat{T}_2 + \frac{e^2}{4\pi\varepsilon_0}\left(-\frac{1}{r_{\mathrm{A1}}} - \frac{1}{r_{\mathrm{B1}}} - \frac{1}{r_{\mathrm{A2}}} - \frac{1}{r_{\mathrm{B2}}} + \frac{1}{r_{12}} + \frac{1}{r_{\mathrm{AB}}}\right) =$$

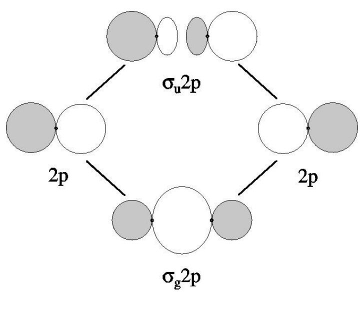
$$= \left(\hat{T}_1 - \frac{e^2}{4\pi\varepsilon_0 r_{\mathrm{A1}}}\right) + \left(\hat{T}_2 - \frac{e^2}{4\pi\varepsilon_0 r_{\mathrm{B2}}}\right) +$$

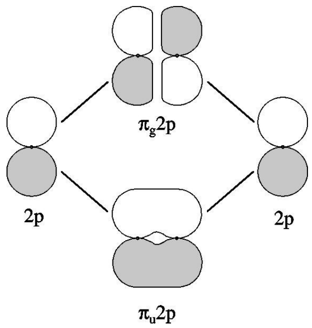
$$+ \frac{e^2}{4\pi\varepsilon_0}\left(-\frac{1}{r_{\mathrm{B1}}} - \frac{1}{r_{\mathrm{A2}}} + \frac{1}{r_{12}} + \frac{1}{r_{\mathrm{AB}}}\right) = \hat{H}_{\mathrm{A1}} + \hat{H}_{\mathrm{B2}} + \hat{H}'$$

Metoda molekularnih orbitala

$$\hat{H} = \left[\hat{T}_1 - \frac{e^2}{4\pi\varepsilon_0}\left(\frac{1}{r_{\mathrm{A1}}} + \frac{1}{r_{\mathrm{B1}}}\right)\right] + \left[\hat{T}_2 - \frac{e^2}{4\pi\varepsilon_0}\left(\frac{1}{r_{\mathrm{A2}}} + \frac{1}{r_{\mathrm{B2}}}\right)\right] + \frac{e^2}{4\pi\varepsilon_0}\left(\frac{1}{r_{12}} + \frac{1}{r_{\mathrm{AB}}}\right)$$







Hibridizacija

Pauling & Slater

- funkcije se miješaju i nastaju nove funkcije – hibridne orbitale

-s i p hibridne orbitale su ekvivalentne,
imaju maksimume u različitim smjerovima

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

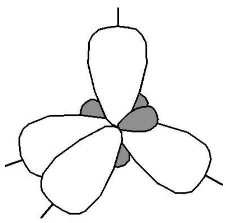
$$\sum_{j=1}^{n} c_{ij}^{\;2} = 1$$

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

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

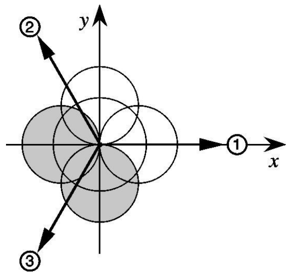
sp^3

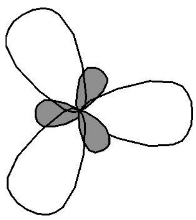
CH_4



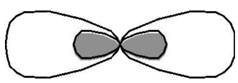
sp^2

$CH_2 = CH_2$





sp



CH ≡ CH