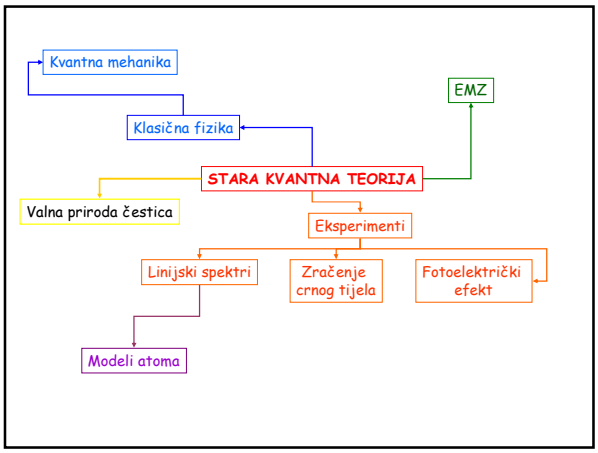
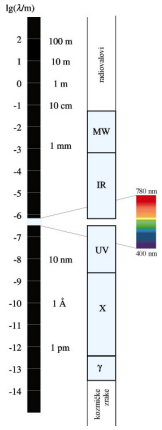


Sir Isaac Newton (1642-1727)

Christian Huygens (1629 –1695)

James Clerk Maxwell (1831 - 1879)

Područja zračenja

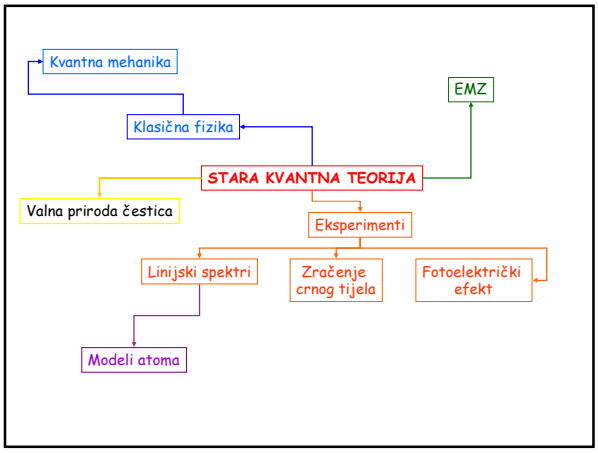


Elektromagnetsko zračenje

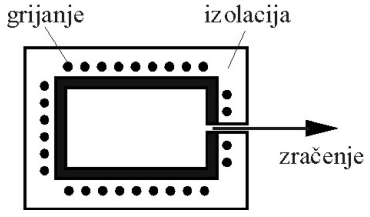
$$\lambda = \frac{c}{\nu}$$

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

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



Zračenje crnog tijela



Jožef Stefan

1835 –1893

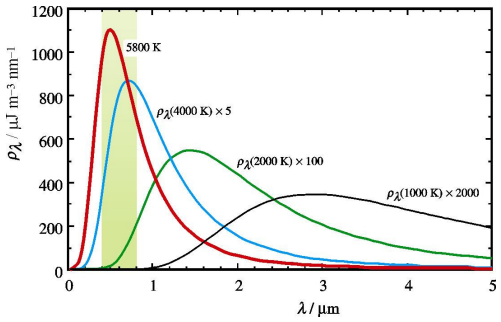
Ludwig Eduard Boltzmann

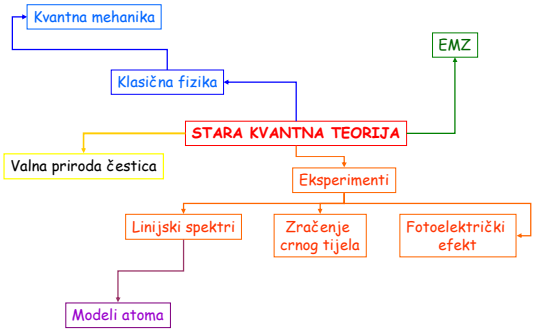
1844 –1906

$M = \sigma T^4$

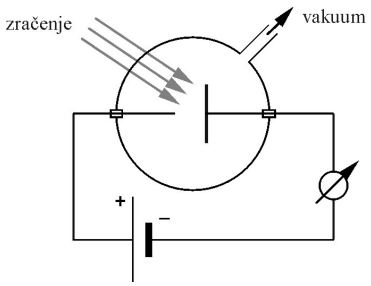
Stefan – Boltzmannov zakon

Gustoća energije zračenja





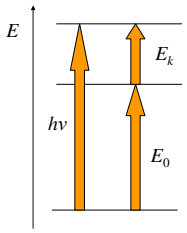
Fotoelektrični efekt



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.

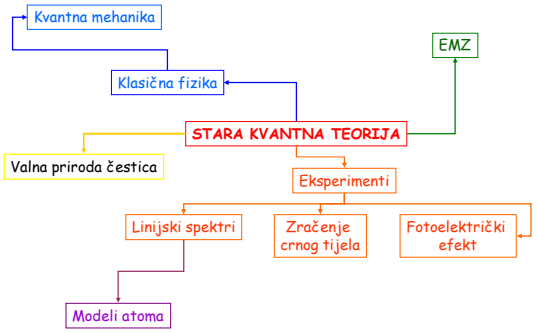
Fotoelektrični efekt



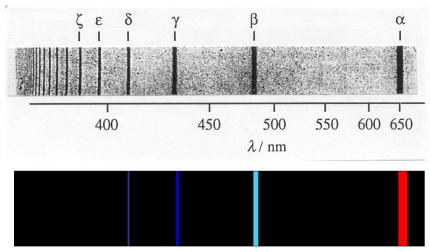
$E_k = h\nu - E_0$

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.

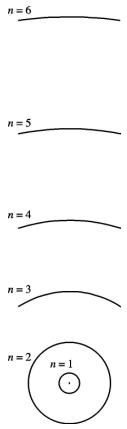


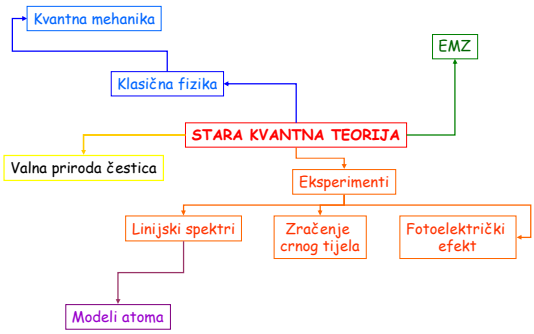
Linijski spektri
Balmerova serija



Bohrov model atoma

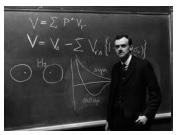
- Stacionarna stanja
- Pri prijelazu $\Delta E = h\nu$
- Kvantiziranost $L = n\hbar$





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"

Mikroskop s γ-zrakama

Princip neodređenosti

UVOD U KVANTNU MEHANIKU

Postulati kvantne mehanike

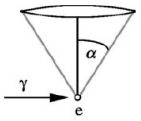
Valna funkcija | Operatori | Mjerne vrijednosti | Vremenska ovisnost

Teoremi kvantne mehanike

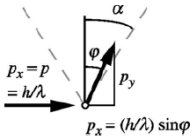
Princip neodređenosti

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

Mikroskop s γ- zrakama



Crtež 2.1. Mikroskop s γ-zrakama.

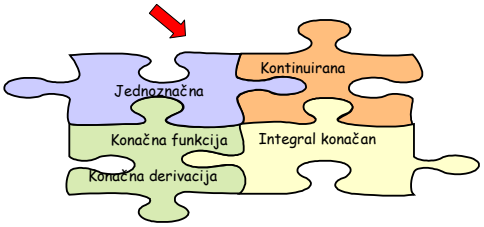


Crtež 2.2. Komponente količine gibanja fotona prije (lijevo) i poslije sudara s elektronom.

Postulati kvantne mehanike

Valna funkcija | Operatori | Mjerne vrijednosti | Vremenska ovisnost

$\Psi(q,t)$



Postulati kvantne mehanike

Valna funkcija | Operatori | Mjerne vrijednosti | Vremenska ovisnost

$\hat{\Omega}$

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

Postulati kvantne mehanike

Valna funkcija | Operatori | Mjerne vrijednosti | Vremenska ovisnost

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

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

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

Postulati kvantne mehanike

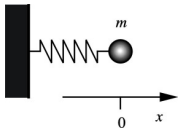
Valna funkcija | Operatori | Mjerne vrijednosti | Vremenska ovisnost

$$\hat{H}\Psi(q,t) = i\hbar\frac{\partial\Psi(q,t)}{\partial t}$$

Stacionarna stanja

$$\Psi^*(q,t)\Psi(q,t) = \Psi^*(q)\Psi(q)$$

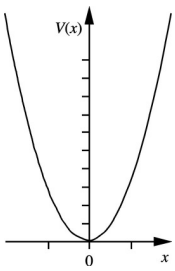
Harmonički oscilator



Hooke: $F = -k\,x$

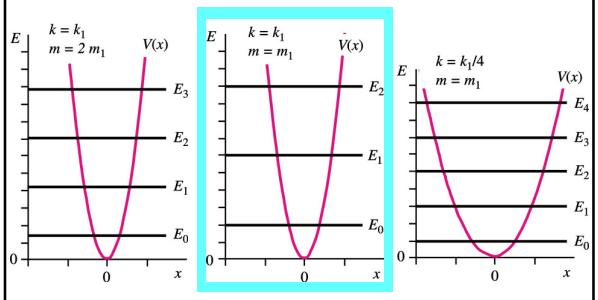
$$V = -\int F\mathrm{d}x = \int k\,x\mathrm{d}x$$

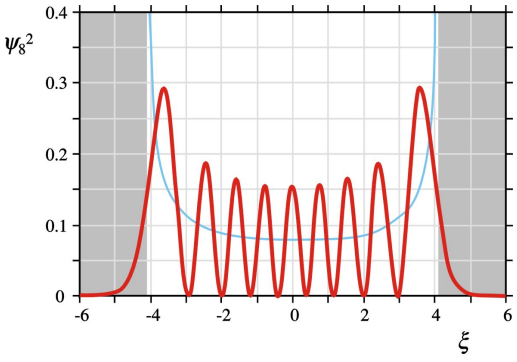
$$V = \tfrac{1}{2}kx^2$$



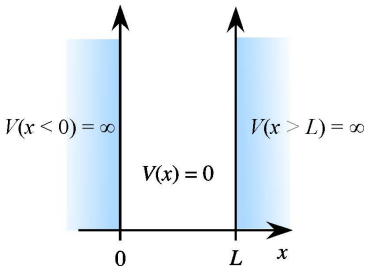
Utjecaj mase

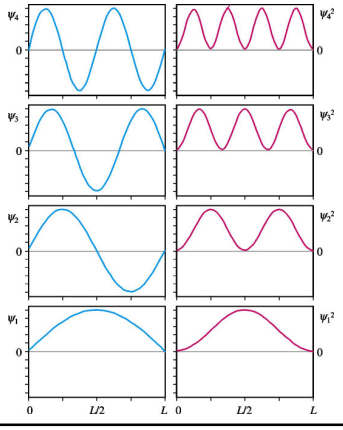
Utjecaj konstante sile

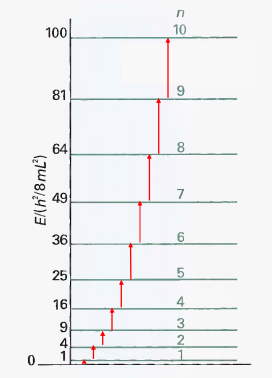




Čestica u kutiji

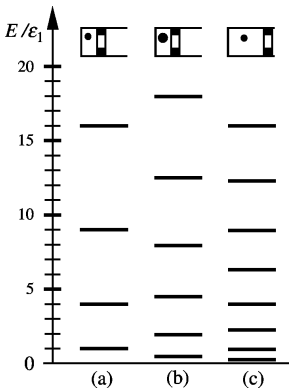


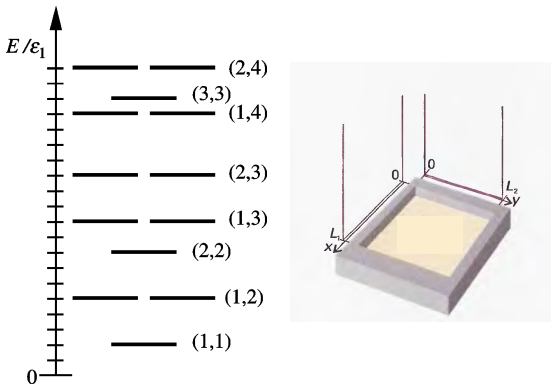


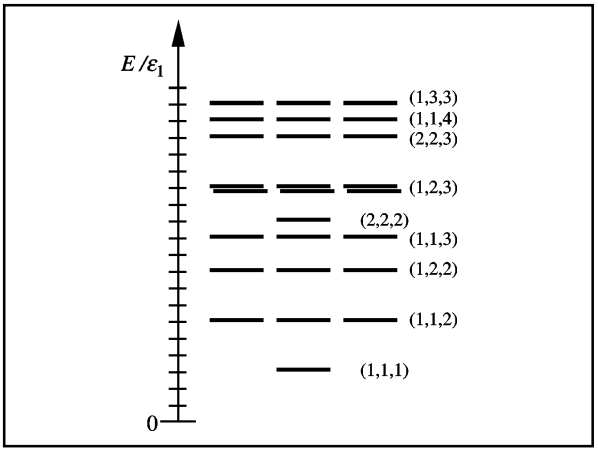


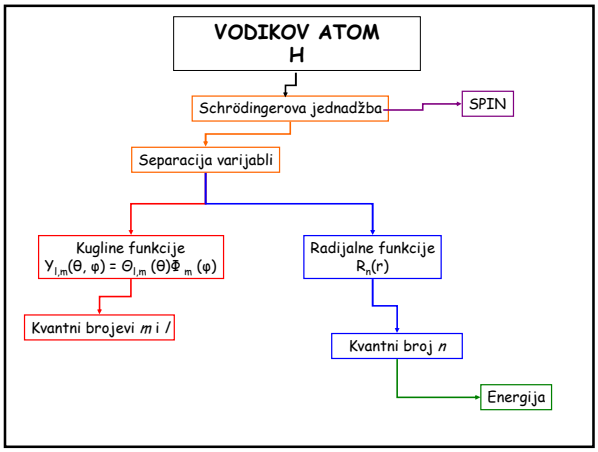
$$E = \frac{h^2}{8mL^2} n^2$$

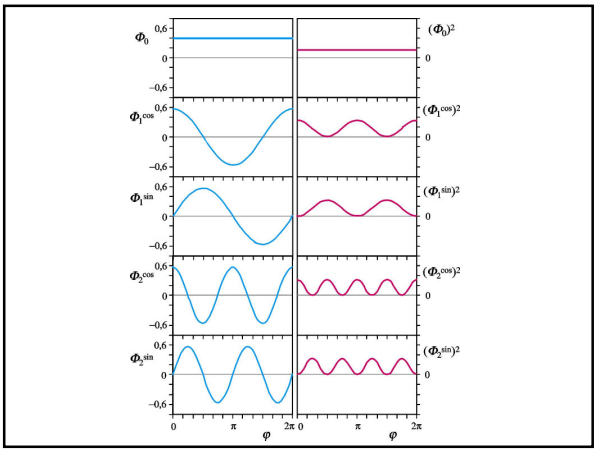
$$\Delta E = E_{n+1} - E_n = \frac{h^2}{8mL^2}(2n+1)$$







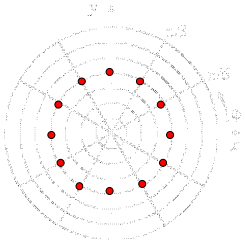




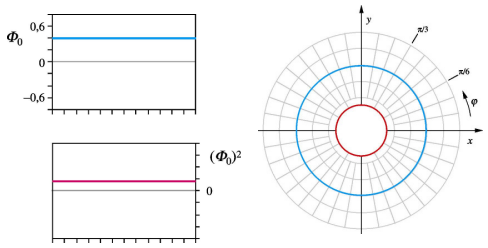
$$\Phi_m(\varphi) = \frac{1}{\sqrt{2\pi}} e^{im\varphi}$$

$m = 0$

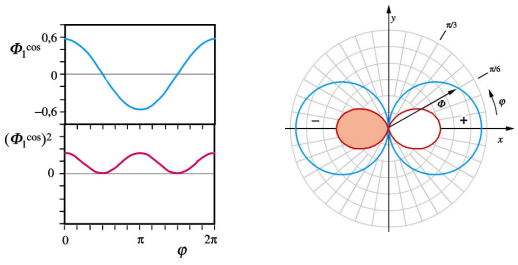
$$\Phi_m(\varphi) = \frac{1}{\sqrt{2\pi}}$$



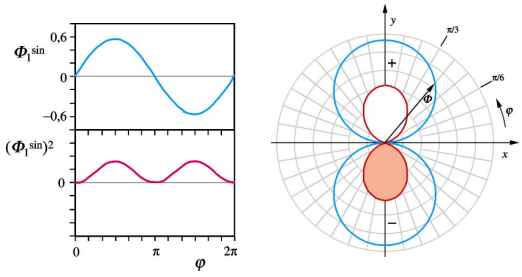
$m = 0$ $\quad \Phi_0(\varphi) = \frac{1}{\sqrt{2\pi}}$



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

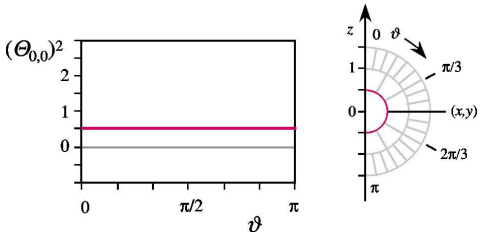


$m = 1$ $\quad \Phi_1^{\sin} = \frac{1}{\sqrt{\pi}}\sin(\varphi)$

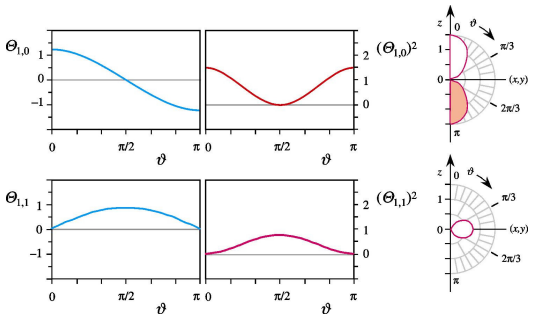


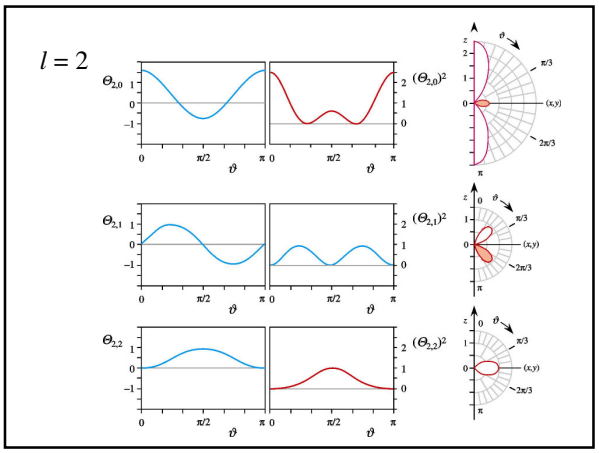
Rješenja Θ

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



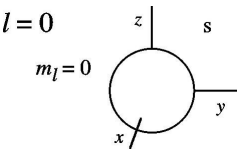
$l = 1$ $\quad \Theta_{1,0} = \frac{\sqrt{6}}{2}\cos\vartheta$ $\quad \Theta_{1,1} = \frac{\sqrt{3}}{2}\sin\vartheta$





Kugline funkcije

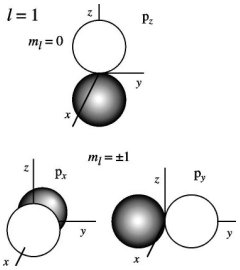
$$Y_{0,0} = \frac{1}{2\sqrt{\pi}}$$



Kugline funkcije

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

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

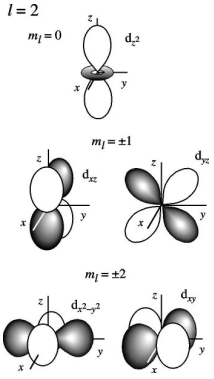


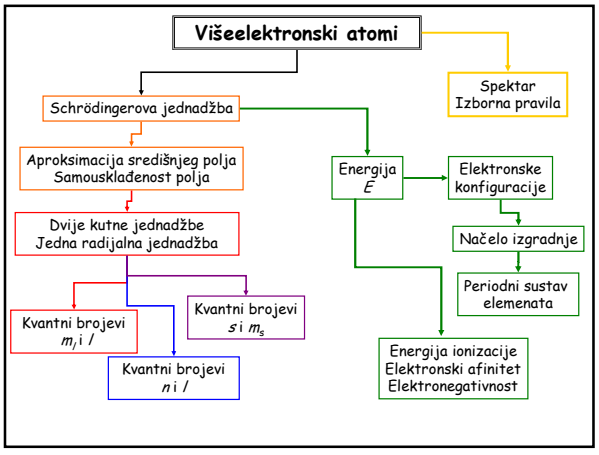
Kugline funkcije

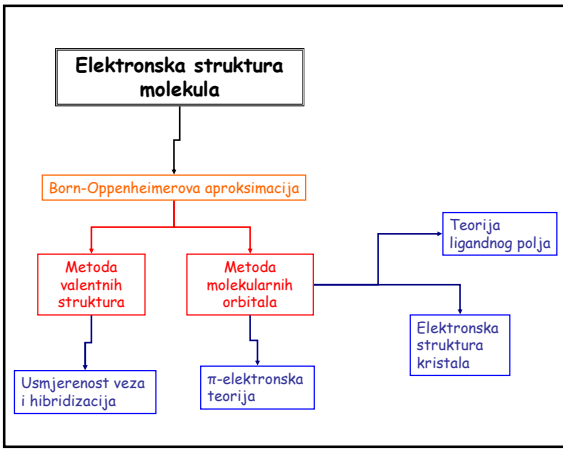
$$Y_{2,0} = \frac{1}{4}\sqrt{\frac{5}{\pi}}(3\cos^2\vartheta - 1)$$

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

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







Born-Opperheimerova aproksimacija

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

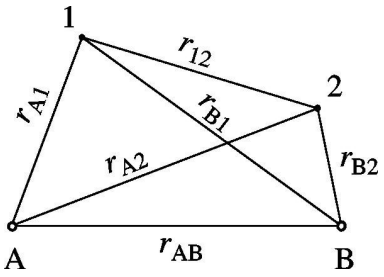
$$\left(\hat{T}_e + V\right)\Psi_e = E_e \cdot \Psi_e$$

ELEKTRONSKA GIBANJA UZ STALNI POLOŽAJ JEZGRE

$$\left(\hat{T}_N + E_e\right)\Psi_N = E \cdot \Psi_N$$

GIBANJE JEZGRA POD UTJECAJEM POTENCIJALA E_e

Metoda valentnih struktura



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

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

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

Hibridizacija

Pauling & Slater

- funkcije se miješaju i nastaju nove funkcije – hibridne orbitale

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

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

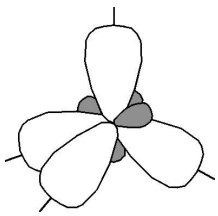
$$\sum_{j=1}^{n} {c_{ij}}^2 = 1$$

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

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

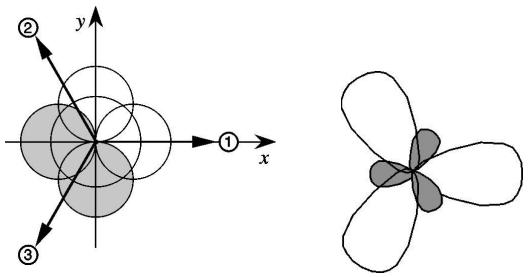
sp^3

CH_4

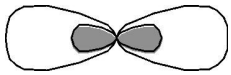


sp^2

$CH_2 = CH_2$



sp



CH ≡ CH

Metoda molekularnih orbitala

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