Wstęp do Optyki i Fizyki Materii Skondensowanej

1100-3003

Atomy
Przejścia optyczne

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inżynieria nanostruktur

Równanie Schrödingera

Szczególne rozwiązania równania Schrödingera

$$i\hbar \frac{\partial}{\partial t}\, \psi(\vec{r},t) = -\frac{\hbar^2}{2m}\, \nabla^2 \psi(\vec{r},t) + V(\vec{r},t)\psi(\vec{r},t)$$

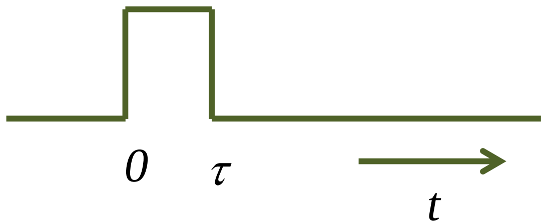
Potencjał niezależny od czasu

$$H_0 = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + U(x) \qquad \psi(x,t) = A\varphi(x)e^{-iEt/\hbar}$$

Potencjał ~~nie~~zależny od czasu $\quad H = H_0 + V(t)$

Najprostszy przypadek:

$$V(t) = \begin{cases} W(t) & \text{dla } 0 \le t \le \tau \\ 0 & \text{dla } t < 0 \text{ i } t > \tau \end{cases}$$



Atomy

Atom wodoru

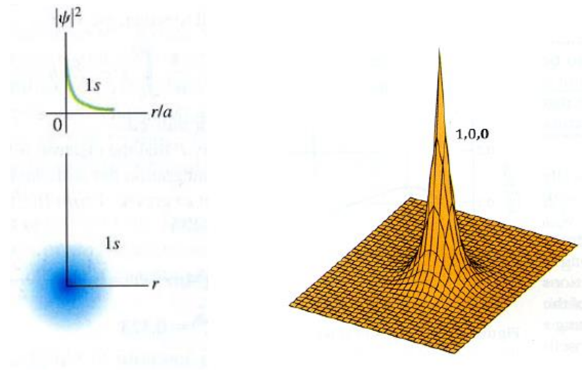
Eigenstates (stany własne) of L :

$$\psi_{1s} = \frac{1}{\sqrt{\pi a^3}} \exp(-\frac{r}{a})$$

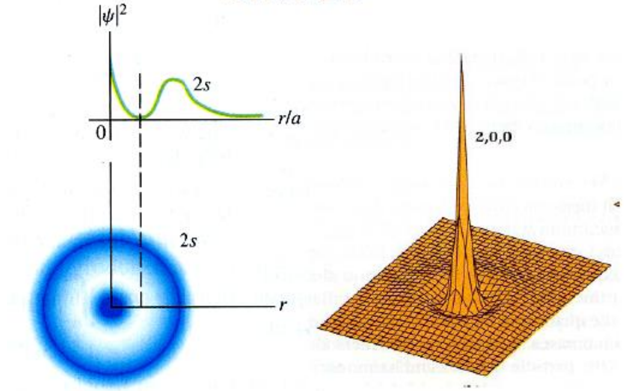
$$\psi_{2s} = \frac{1}{4\sqrt{2\pi a^3}} (2 - \frac{r}{a}) \exp(-\frac{r}{2a})$$

$$\psi_{2po} = \frac{1}{4\sqrt{2\pi a^3}} \frac{r}{a} \exp(-\frac{r}{2a}) \cos\theta$$

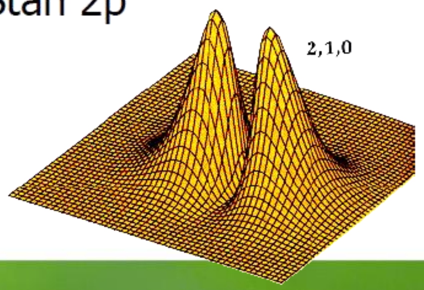
$$\psi_{2p\pm} = \frac{1}{8\sqrt{\pi a^3}} \frac{r}{a} \exp(-\frac{r}{2a}) \sin\theta \exp(\pm i\varphi)$$



Stan 2s



Stan 2p



Atomy

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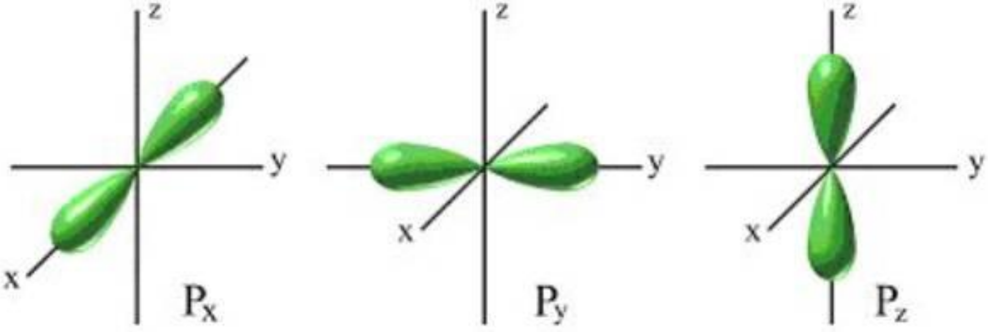
Real functions (funkcje rzeczywiste):

$$\psi_{1s} = \frac{1}{\sqrt{\pi a^3}} \exp(-\frac{r}{a})$$

$$\psi_{2px} = \frac{1}{4\sqrt{2\pi a^3}} \frac{x}{a} \exp(-\frac{r}{2a}) = \frac{1}{\sqrt{2}} \left(\psi_{2p+1} + \psi_{2p-1}\right)$$

$$\psi_{2py} = \frac{1}{4\sqrt{2\pi a^3}} \frac{y}{a} \exp(-\frac{r}{2a}) = \frac{1}{\sqrt{2}} \left(\psi_{2p+1} - \psi_{2p-1}\right)$$

$$\psi_{2pz} = \frac{1}{4\sqrt{2\pi a^3}} \frac{z}{a} \exp(-\frac{r}{2a}) = \psi_{2p0}$$



Atomy

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Spherical harmonics (harmoniki sferyczne) Y_{lm}:

$$\Psi_{nlm}(r,\theta,\varphi) = R_{nl}(r) Y_{lm}(\theta,\varphi)$$

$$R_{20}(r) = \left(\frac{Z}{2a}\right)^{3/2} 2 \left(1 - \frac{Zr}{2a}\right) \exp\left(-\frac{Zr}{2a}\right)$$

$$R_{21}(r) = \left(\frac{Z}{2a}\right)^{3/2} \frac{2}{\sqrt{3}} \left(\frac{Zr}{2a}\right) \exp\left(-\frac{Zr}{2a}\right)$$

$$Y_{00}(\theta,\varphi) = \sqrt{\frac{1}{4\pi}}$$

$$Y_{10}(\theta,\varphi) = \sqrt{\frac{3}{4\pi}} \cos(\theta)$$

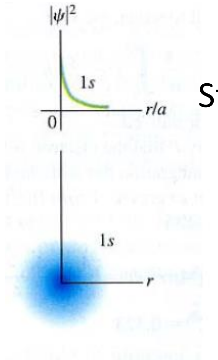
$$Y_{1\pm1}(\theta,\varphi) = \sqrt{\frac{3}{8\pi}} \sin(\theta) \exp(\pm i\varphi)$$

Atomy

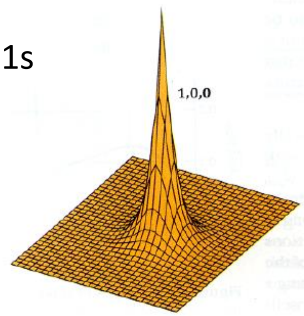
Eigenstate:

E.g. hydrogen wavefunction

$$\Psi = R_{n,l}(r)\Theta_{l,m}(\theta)\Phi_m(\phi)$$



Stan 1s



$$R_{n,l}(r) = \sqrt{\frac{(n-l+1)!}{2n(n+l)!}}\left(\frac{2Z}{na_0}\right)^{3/2} e^{-\rho/2}\rho^l G_{n-l-1}^{2l+1}(\rho)$$

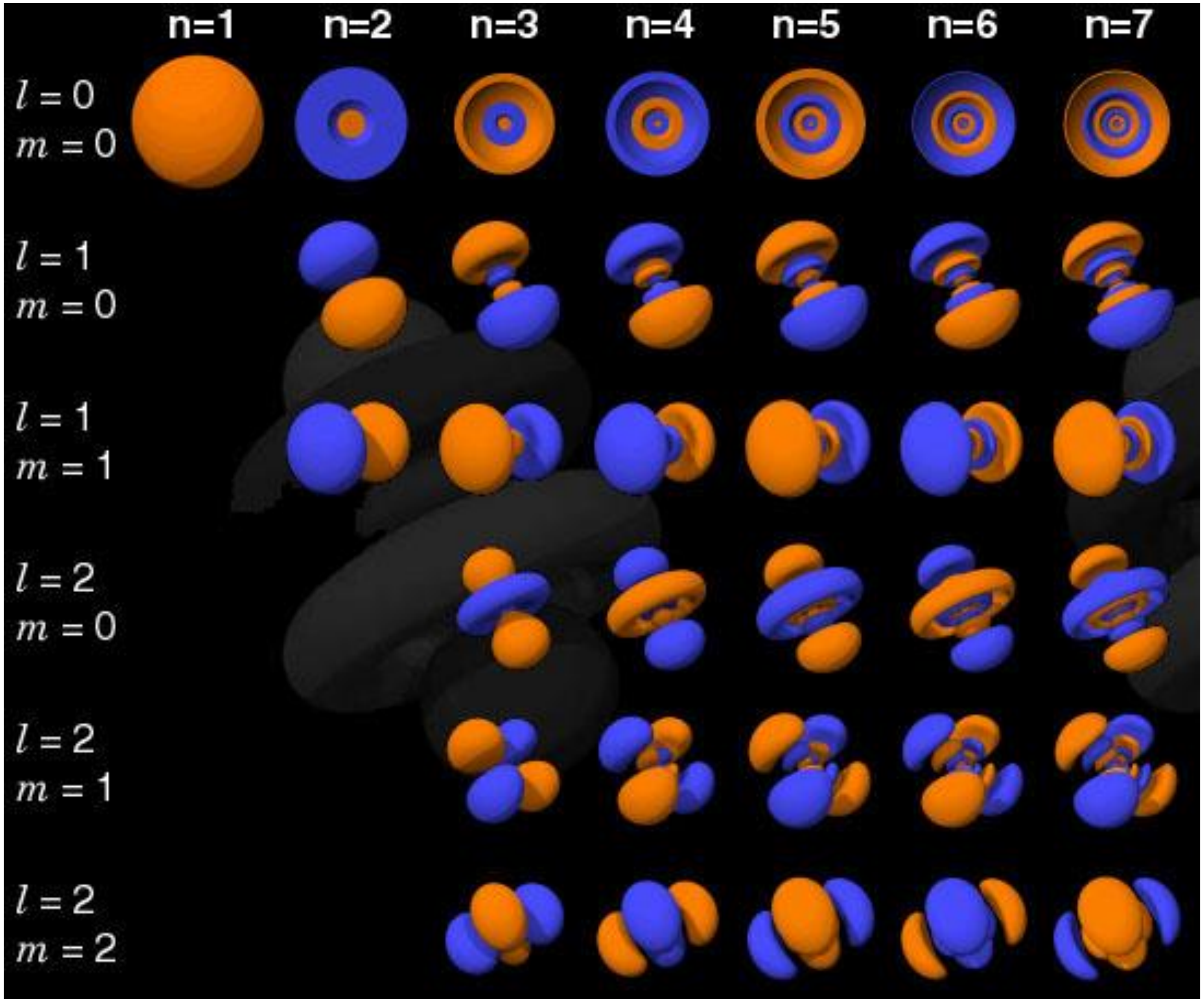
$$\Theta_{l,m}(\theta) = (-1)^m\sqrt{\frac{2l+1}{2\pi}\frac{(l-m)!}{(l+m)!}}P_l^m(\cos\theta)$$

$$\Phi_m(\phi) = Ce^{im\phi}$$

Quantum numbers!

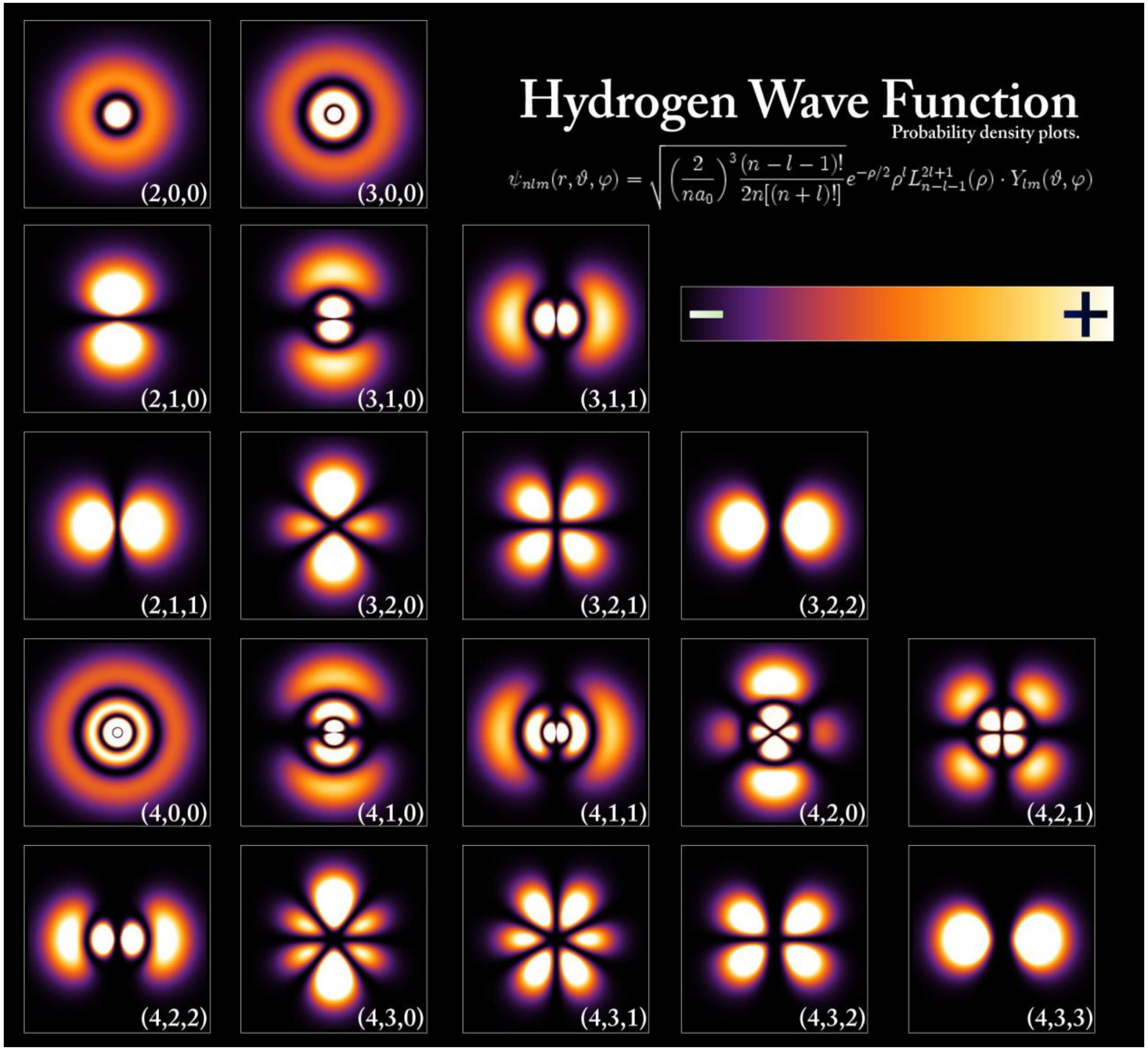
$$\Psi = R_{n,l}(r)\Theta_{l,m}(\theta)\Phi_m(\phi) = |n, l, m\rangle$$

Atomy



http://chemistry.stackexchange.com

Atomy



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Perturbation theory (rachunek zaburzeń)

Time-independent perturbation theory (rach. zab. bez czasu)

rach.zab.bez.czas.

$$\hat{H} = \hat{H}_0 + \lambda \hat{H}'$$ ← **perturbation**

↑

Known solutions of unperturbed Hamiltonian $\hat{H}_0 \psi_n^{(0)} = E_n^{(0)} \psi_n^{(0)}$

We are looking for the function ψ_n: $(\hat{H}_0 + \lambda \hat{H}')\psi_n = E_n \psi_n$

we can write E_n and ψ_n as power series in λ::

$$\psi_n = \psi_n^{(0)} + \lambda \psi_n^{(1)} + \lambda^2 \psi_n^{(2)} + \ldots$$
$$E_n = E_n^0 + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \ldots$$

Thus:

$$(\hat{H}_0 + \lambda \hat{H}')(\psi_n^{(0)} + \lambda \psi_n^{(1)} + \lambda^2 \psi_n^{(2)} + \ldots) = (E_n^0 + \lambda E^{(1)} + \lambda^2 E_n^{(2)} + \ldots)(\psi_n^{(0)} + \lambda \psi_n^{(1)} + \lambda^2 \psi_n^{(2)} + \ldots)$$

comparing coefficients of each power of λ

$$\hat{H}_0 \psi^{(0)} = E_n^{(0)} \psi_n^{(0)}$$
$$\hat{H}_0 \psi_n^{(1)} + \hat{H}' \psi_n^0 = E_n^{(0)} \psi_n^{(1)} + E_n^{(1)} \psi_n^0$$
$$\hat{H}_0 \psi_n^{(2)} + \hat{H}' \psi_n^{(1)} = E_n^{(0)} \psi_n^{(2)} + E_n^{(1)} \psi_n^{(1)} + E_n^{(2)} \psi_n^{(0)}$$

http://pl.wikibooks.org/wiki/Mechanika_kwantowa/Rachunek_zaburzeń_dla_równania_Schrödingera_niezależnego_od_czasu

Perturbation theory (rachunek zaburzeń)

Time-independent perturbation theory

Eigenfunction

$$E_n = E_0 + \lambda E_n^{'} = E_0 + \lambda H_{nn}^{'}$$

$$\psi_n = \psi_n^{(0)} + \lambda \psi_n^{(1)} = \psi_n^{(0)} + \lambda \sum_{k,k\neq n} \frac{\hat{H}_{kn}^{'}}{E_n^{(0)} - E_k^{(0)}} \psi_k^0$$

a solution exists only when its determinant : $\det\left(\lambda H' - \hat{I}E\right) = 0$

Perturbation

$$\widehat{H}_{ij}' = \langle \psi_i | \widehat{H}' | \psi_j \rangle$$

$$\begin{vmatrix} \lambda H_{11}' - E' & \lambda H_{12}' & \cdots & \lambda H_{1k}' \\ \lambda H_{21}' & \lambda H_{22}' - E' & \cdots & \lambda H_{2k}' \\ \vdots & \vdots & \ddots & \vdots \\ \lambda H_{k1}' & \lambda H_{k2}' & \cdots & \lambda H_{kk}' - E' \end{vmatrix} = 0$$

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Hydrogen-like atom

Alkali metal atoms (*wodoropodobne*):

perturbation theory $\hat{H} = \hat{H}_0 + \hat{H}'$:

$$\hat{H}_0 \psi_i = E_i \psi_i$$

perturbation $\hat{H}'_{ij} = \langle \psi_i | \hat{H}' | \psi_j \rangle$

the method: $\det\left|\hat{H}' - E\hat{I}\right| = 0$

a) $V(r) = -\frac{3e^2}{4\pi\varepsilon_0 r} + A\delta(r-a)$

b) $V(r) = \begin{cases} -\frac{Ze^2}{4\pi\varepsilon_0 r}; r \le b \\ -\frac{e^2}{4\pi\varepsilon_0 r}; r > b \end{cases}$

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a) $$V'(r) = A\delta(r-a)$$

b) $$V'(r) = \begin{cases} 0 \quad ; r \le b \\ -\dfrac{(Z-1)e^2}{4\pi\varepsilon_0 r} ; r > b \end{cases}$$

Pole elektryczne

Stark effect of hydrogen atom

electric field E

$$H' = \vec{p}\vec{E} = ezE_z$$

dipole moment p

Eigenfunctions of hydrogen atom for 2p state:

$$\psi_{200}, \psi_{21-1}, \psi_{210}, \psi_{211}$$

Perturbation $\hat{H}'_{ij} = \langle \psi_i | \hat{H}' | \psi_j \rangle$

$$\Psi_{nlm}(r,\theta,\varphi) = R_{nl}(r) Y_{lm}(\theta,\varphi)$$

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Pole elektryczne

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Exercises !

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Pole magnetyczne i spin

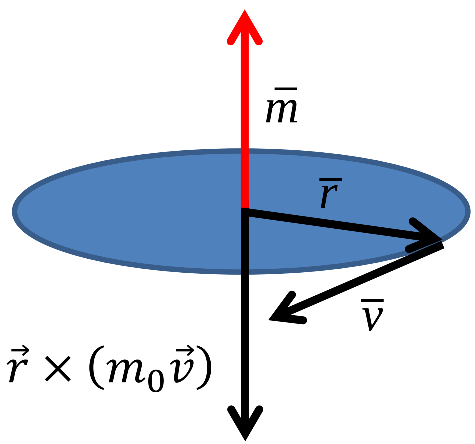
Pole magnetyczne:

$$H' = -\vec{m}\vec{B}$$

Here $\vec{m}$ is the magnetic moment

klasycznie:

$$|\vec{m}| = |I\vec{S}| = \frac{e}{T}\pi r^2 = \frac{e}{2\pi r/v}\pi r^2 = \frac{e}{2} r v \quad [\mathrm{Am}^2]$$

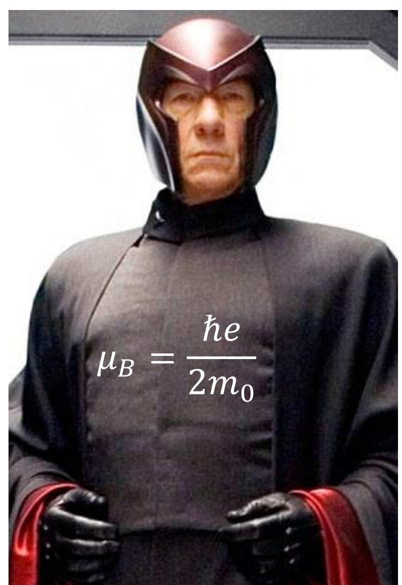


Stąd: $\vec{m} = -\frac{e}{2m_0}\vec{L} = -\frac{\mu_B}{\hbar}\vec{L}$

$$\vec{L} = \vec{r} \times (m_0\vec{v})$$

Bohr magneton $\mu_B = \frac{\hbar e}{2m_0}$

μ_B = 9,274009994(57)×10^{-24} J/T



$$H' = -\vec{m}\vec{B} = \frac{\mu_B}{\hbar}\hat{L}\vec{B}$$

$$\hat{L} = (\hat{L}_x, \hat{L}_y, \hat{L}_z)$$

Pole magnetyczne i spin

Magnetic field:

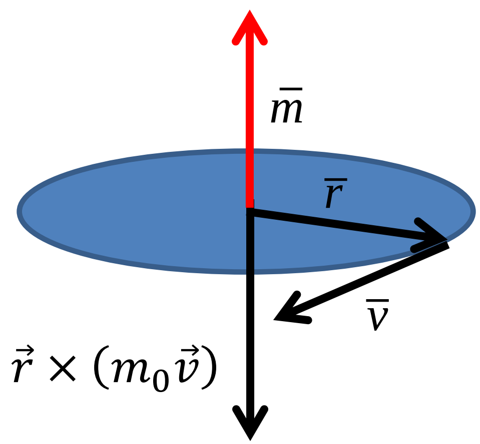
$$H' = -\vec{m}\vec{B} = \frac{\mu_B}{\hbar}\hat{L}\vec{B}$$

for $\vec{B} = (0,0,B_z)$

Here $\vec{m}$ is the magnetic moment

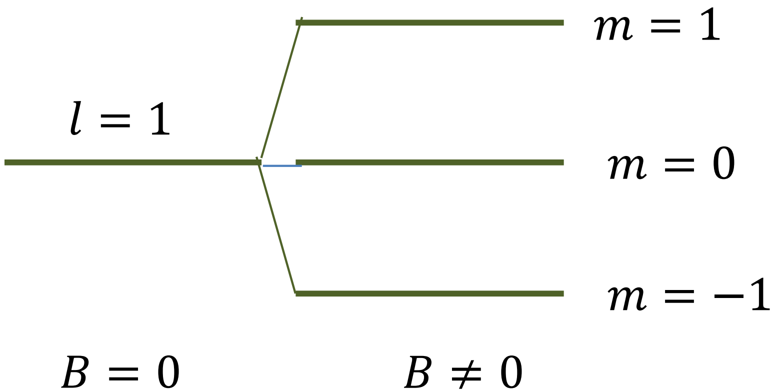
we have: $H' = \frac{\mu_B}{\hbar}\hat{L}_z B_z = \mu_B B_z m$ where $m = -l, -l+1, \dots l-1, l$

Here m is quantum number $|n, l, m\rangle$



$\vec{L} = \vec{r} \times (m_0\vec{v})$

the base: $|l, m\rangle$



Pole magnetyczne i spin

Magnetic field:

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Here $\vec{m}$ is the magnetic moment

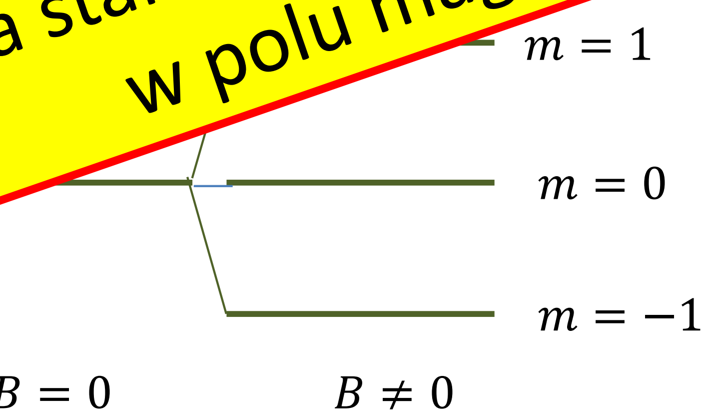
for $\vec{B} = (0,0,B_z)$

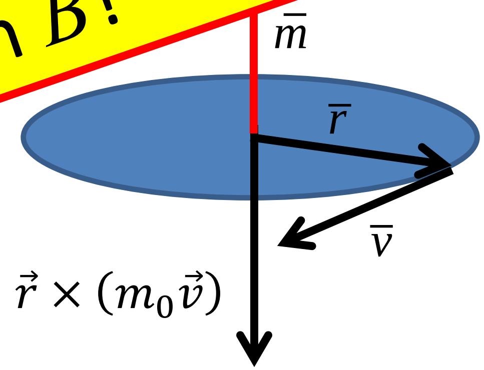
we have: $H' = \frac{\mu_B}{\hbar}\hat{L}_z B_z = \mu_B B_z m$ where $m = -l, -l+1$

Here m is quant

Czy dla stanów s (l=0) nie ma rozszczepienia w polu magnetycznym B?

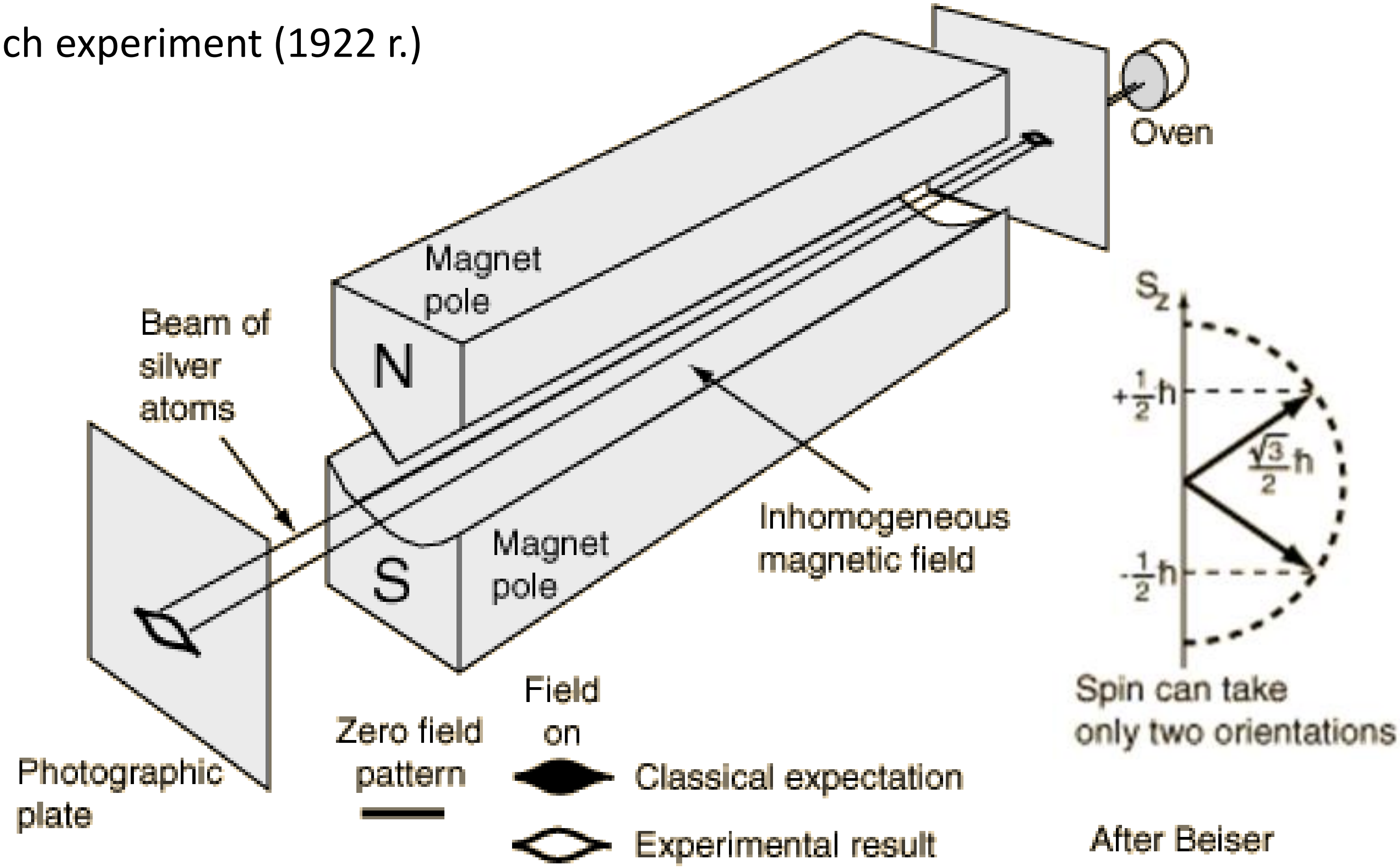
the base:





Pole magnetyczne i spin

Stern-Gerlach experiment (1922 r.)



http://hyperphysics.phy-astr.gsu.edu

Pole magnetyczne i spin

Spin, spin-orbit interaction

Spin operators $\hat{S}_x, \hat{S}_y, \hat{S}_z, \hat{S}^2$

$$\psi(\vec{r}, S_z) = \psi(\vec{r})\chi(S_z)$$

Spinor

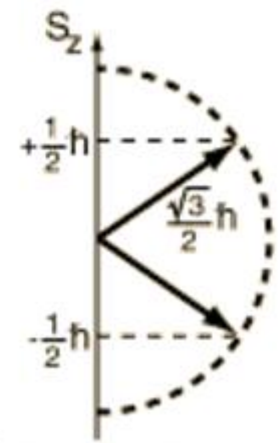
$$[\hat{S}_x, \hat{S}_y] = i\hbar\hat{S}_z, \text{ etc.}$$

Pauli matrices: $\sigma_x, \sigma_y, \sigma_z$

$$\hat{S}_x = \frac{1}{2}\hbar\sigma_x = \frac{1}{2}\hbar\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

$$\hat{S}_y = \frac{1}{2}\hbar\sigma_y = \frac{1}{2}\hbar\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$$

$$\hat{S}_x = \frac{1}{2}\hbar\sigma_z = \frac{1}{2}\hbar\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$



Spin can take only two orientations

projections of the spin on the axis z

$$\chi_\uparrow = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \chi_\downarrow = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

Pole magnetyczne i spin

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$$H' = \frac{\mu_B}{\hbar}\left(\hat{L} + g\hat{S}\right)\vec{B}$$

g-factor (g-czynnik) for the agreement with experiments

$\left[\hat{S}_x, \hat{S}_y\right] = i\hbar\hat{S}_z$, etc.

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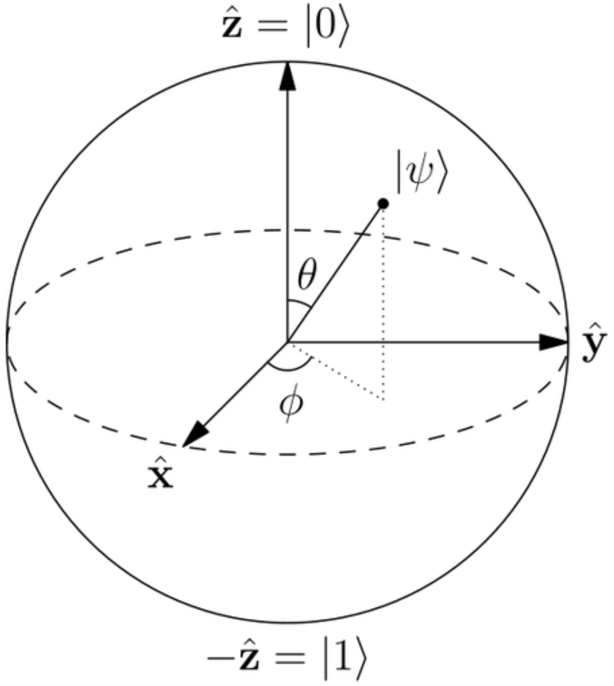
projections of the spin on the axis z

$$\chi_\uparrow = \begin{pmatrix}1\\0\end{pmatrix}, \chi_\downarrow = \begin{pmatrix}0\\1\end{pmatrix}$$

Polaryzacja światła

Wykład 2

Bloch sphere



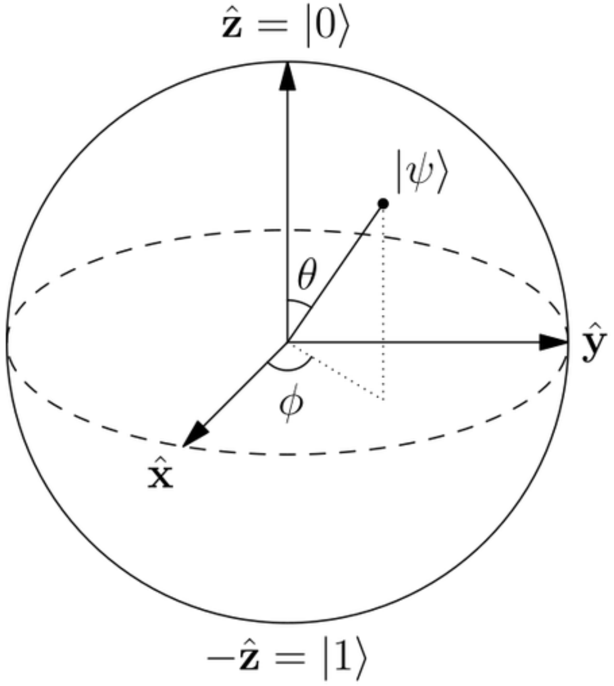
$$\sigma_1 = \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$
$$\sigma_2 = \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$
$$\sigma_3 = \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\psi_{x+} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}, \qquad \psi_{x-} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix},$$
$$\psi_{y+} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix}, \qquad \psi_{y-} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \end{pmatrix},$$
$$\psi_{z+} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \uparrow \qquad \psi_{z-} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \downarrow$$

Polaryzacja światła

Wykład 2

Poincaré ~~Bloch~~ sphere



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$$\psi_{x+} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}, \qquad \psi_{x-} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix},$$

$$\psi_{y+} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix}, \sigma^+ \quad \psi_{y-} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \end{pmatrix}, \sigma^-$$

$$\psi_{z+} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad \psi_{z-} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

Pole magnetyczne i spin

Spin, spin-orbit interaction

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$$H' = \frac{\mu_B}{\hbar}(\hat{L} + g\hat{S})\vec{B}$$

g-factor (g-czynnik) for the agreement with experiments

$$[\hat{S}_x, \hat{S}_y] = i\hbar\hat{S}_z, \text{ etc.}$$

Pauli matrices (macierze Pauliego): $\sigma_x, \sigma_y, \sigma_z$

$$\hat{S}_x = \frac{1}{2}\hbar\sigma_x = \frac{1}{2}\hbar\begin{bmatrix}0 & 1\\1 & 0\end{bmatrix}$$

$$g = -2.00231930436182 \pm 0.00000000000052$$

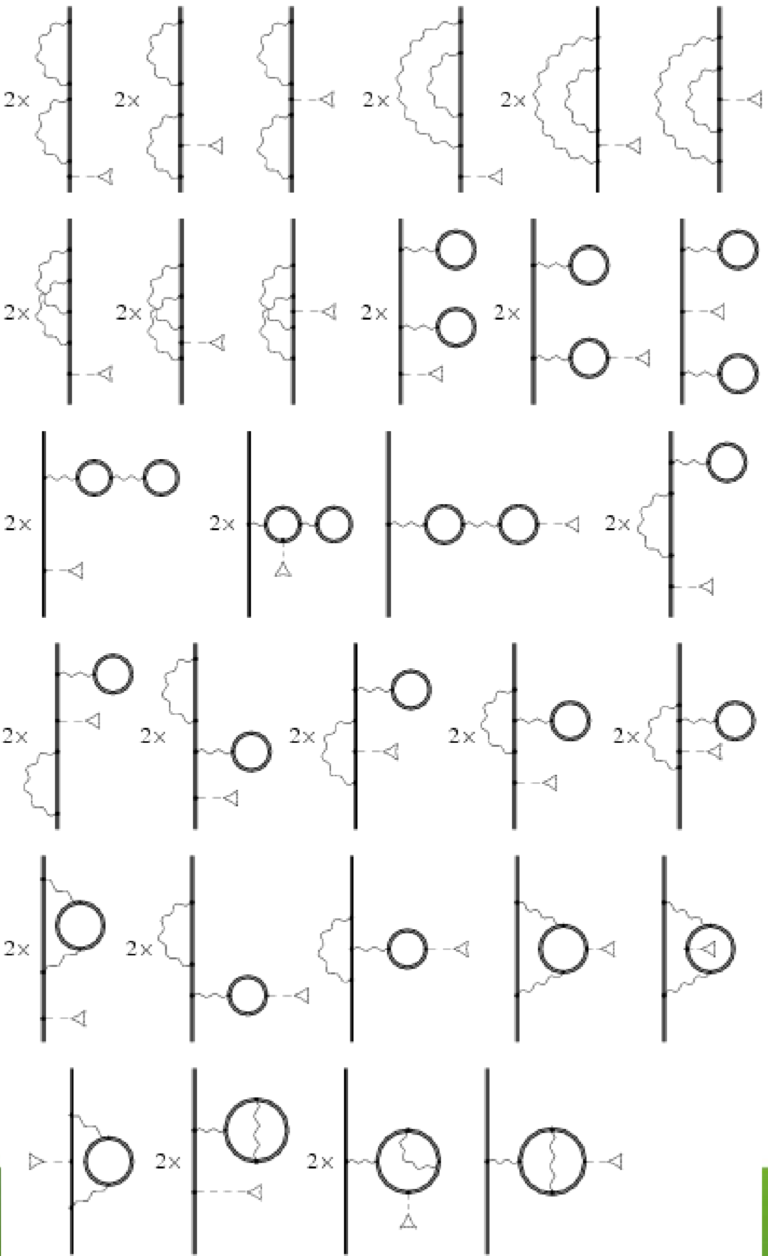
$$\hat{S}_y = \frac{1}{2}\hbar\sigma_y = \frac{1}{2}\hbar\begin{bmatrix}0 & -i\\i & 0\end{bmatrix}$$

$$\hat{S}_x = \frac{1}{2}\hbar\sigma_z = \frac{1}{2}\hbar\begin{bmatrix}1 & 0\\0 & -1\end{bmatrix}$$

projections of the spin on the axis z

$$\chi_\uparrow = \begin{pmatrix}1\\0\end{pmatrix}, \chi_\downarrow = \begin{pmatrix}0\\1\end{pmatrix}$$

QED – Quantum ElectroDynamics



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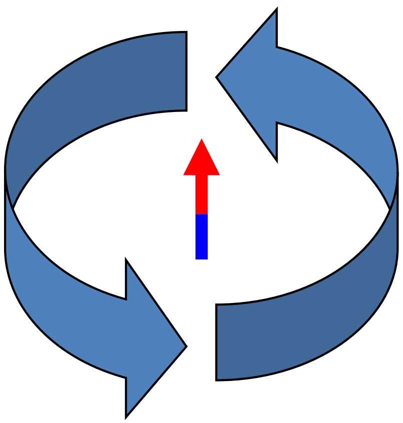
Co to jest spin?

Albert **Einstein** - Johannes Wander **de Haas**, Berlin 1914,

Kwantowy moment pędu



Wewnętrzna własność elektronów?

!

http://www.ptb.de/en/publikationen/jahresberichte/jb2005/nachrdjahres/s23e.html

Spintronika

No dobra, ale…

- **Co to jest spin?**

Co to jest spin?

- Co to jest masa?

$$\vec{F} = m\vec{a}$$

$$F = G\frac{m_1 m_2}{r^2}$$

Mariusz Pudzianowski http://www.pudzian.pl/

Co to jest spin?

- Co to jest ładunek?

$$F = k\frac{q_1 q_2}{r^2}$$

Co to jest spin?

- Co to jest pęd?

$$\overrightarrow{p} = m\overrightarrow{v}$$

Co to jest spin?

- Co to jest moment pędu?

$$\overrightarrow{L} = \overrightarrow{r} \times \overrightarrow{p}$$

Co to jest spin?

- Spin?

http://www.floridahistory.com/us@1570.html

Sebastian Münster, Cosmographia in 1544

Disney

Pole magnetyczne i spin

Spin, spin-orbit interaction

Spin operators $\hat{S}_x, \hat{S}_y, \hat{S}_z, \hat{S}^2$

$$H' = \frac{\mu_B}{\hbar}\left(\hat{L} + g\hat{S}\right)\vec{B}$$

g-factor (g-czynnik) for the agreement with experiments

Total angular momentum operator $\hat{J} = \hat{L} + \hat{S}$, the base $|j, m_j\rangle$

Total magnetic moment $\widehat{M} = \widehat{M}_L + \widehat{M}_S = -g_L \frac{\mu_B}{\hbar}\hat{L} - g_S \frac{\mu_B}{\hbar}\hat{S}$

g_L =1, g_S =2

$\widehat{M} \neq \hat{J}$ - magnetic anomaly of spin

Pole magnetyczne i spin

Spin-orbit interaction $\hat{H}_{SO} = \lambda \hat{L}\hat{S}$ with the base $|n, l, s, m_l, m_s\rangle$

For s-states $\hat{L} = 0 \Rightarrow \hat{L}\hat{S} = 0$

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$$\hat{H}_{SO} = \lambda \hat{L}\hat{S} = \lambda \frac{1}{2}(J^2 - L^2 - S^2) = \lambda\left(L_z S_z + \frac{1}{2}(L_+ S_- + L_- S_+)\right)$$

$$\lambda = hc\, A = \frac{Z\alpha^2}{2}\left\langle \frac{1}{r^3} \right\rangle$$

$Ry = hcR_\infty$

$R_\infty = \frac{m_e e^4}{8\varepsilon_0^2 h^3 c}$

$R_\infty = 1{,}097 \times 10^7 \mathrm{m}^{-1}$

Stała struktury subtelnej
fine-structure constant

$$\alpha = \frac{e^2}{4\pi\varepsilon_0 \hbar c} \approx \frac{1}{137.037}$$

$$E_{SO} = \int \psi^* H_{SO} \psi \, dV = \frac{Z}{2(137)^2} \int \psi^* \frac{\hat{L}\hat{S}}{r^3} \psi \, dV$$

e.g. for ψ_{210} we get $\left\langle \frac{1}{r^3} \right\rangle = \frac{1}{24}\left(\frac{Z}{a_0}\right)^3$ and for general n (principal quantum number)

$$E_{SO} = \frac{Z^4}{2(137)^2 a_0^3 n^3}\left(\frac{j(j+1) - l(l+1) - s(s+1)}{2l(l+1/2)(l+1)}\right)$$

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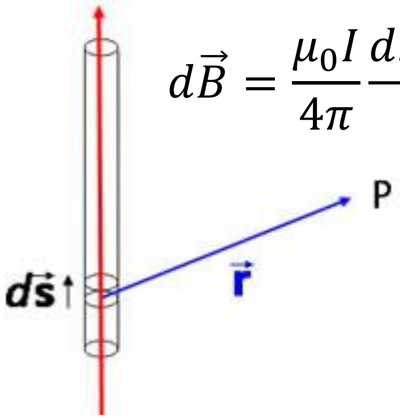
Biot-Savart law – magnetic field of en electron of angular momentum L



$$d\vec{B} = \frac{\mu_0 I}{4\pi}\frac{d\vec{s} \times \vec{r}}{|r|^3}$$

Orbiting charge: $v\, d\vec{s} = \vec{v}\, ds$ $\qquad I = \frac{Zqv}{2\pi a_B}$

Classically

$$\vec{B}_L = \frac{Ze\mu_0}{4\pi m_e}\frac{1}{r^3}\vec{L}$$

Electron in the external field $\vec{B}_L$

http://www.chem.ox.ac.uk/teaching/Physics%20for%20CHemists/Magnetism/Field.html

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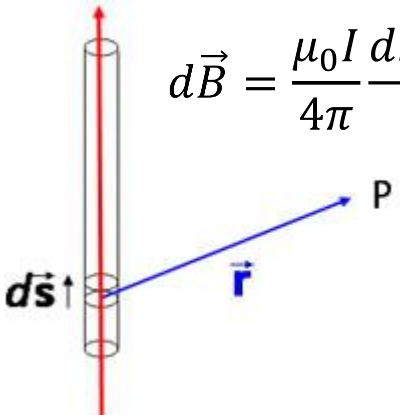

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Quantum

$$\vec{B}_L = \frac{1}{2}\frac{Ze\mu_0}{4\pi m_e}\frac{1}{r^3}\vec{L}$$

$$\vec{\mu}_S = g_S \frac{\mu_B}{\hbar}\hat{S}$$

Thomas factor from relativistic calculations

http://www.st-andrews.ac.uk/~dc43/PH4021/Lectures%2011-13%20SPIN-ORBIT%20INTERACTION.pdf

Pole magnetyczne i spin

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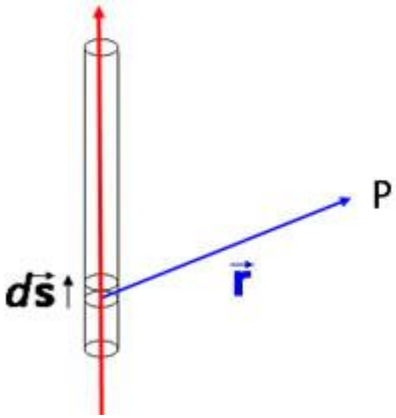

$$H' = \frac{e}{m_e}\hat{S}\cdot\vec{B}_L = \frac{Ze^2\mu_0}{8\pi m_e^2}\frac{1}{r^3}\hat{S}\cdot\hat{L} = \frac{\lambda}{\hbar^2}\hat{L}\hat{S}$$

(Note: sometimes convection is $H' = \lambda\hat{l}\hat{s}$)

$$H_{SO} = \frac{1}{2}\left(\frac{Ze^2}{4\pi\epsilon_0}\right)\left(\frac{g_s}{2m^2c^2}\right)\frac{\hat{L}\hat{S}}{r^3}$$

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fine-structure constant α

$$\lambda = \frac{Ze^2\mu_0\hbar^2}{8\pi m_e^2}\left\langle\frac{1}{r^3}\right\rangle = \frac{Z\hbar^3\alpha}{2m_e^2\, c}\left\langle\frac{1}{r^3}\right\rangle$$

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$$\left\langle\frac{1}{r^3}\right\rangle = uff \dots ufff \dots ufffff \dots = \frac{Z^3}{n^3 a_B^3}\frac{1}{l\left(l+\frac{1}{2}\right)(l+1)}$$

$$\langle\hat{L}\hat{S}\rangle = \frac{\hbar^2}{2}[j(j+1) - l(l+1) - s(s+1)]$$

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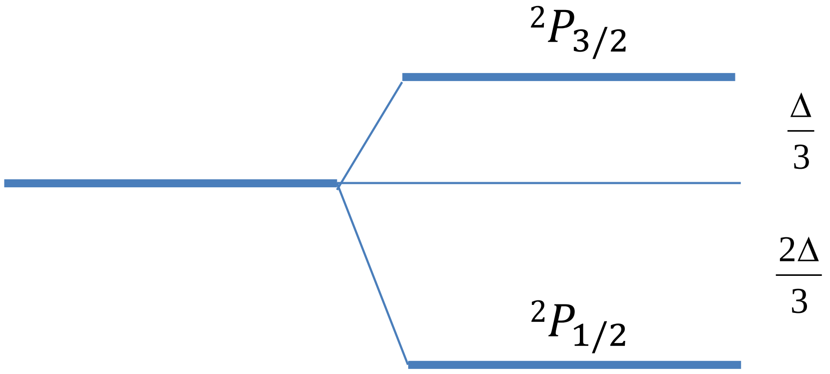
$\hat{L} = 1;\ \hat{S} = \frac{1}{2}$



the base: $|n, l, s, j, m_j\rangle$

shortly: $|j, m_j\rangle$

Multi-electron atom

Term symbol $\quad {}^{2S+1}L_J$

an abbreviated description of the angular momentum quantum numbers in a multi-electron atom

Total wavefunction must be antisymmetric (under interchange of any pair of particle)

$$\psi(\vec{r}, S_z) = \psi(\vec{r})\chi(S_z)$$

Orbital part $\quad$ **Spin part**

Multi-electron wavefunction:

$$\psi\left(\vec{r}_1, \dots, \vec{r}_N, \vec{S}_1, \dots, \vec{S}_N\right) = \psi(\vec{r}_1, \dots, \vec{r}_N)\chi\left(\vec{S}_1, \dots, \vec{S}_N\right)$$

Antisymmetric wavefunction + Pauli exclusion principle + Coulomb interaction =

Exchange interaction

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Hund's rules (soon!)

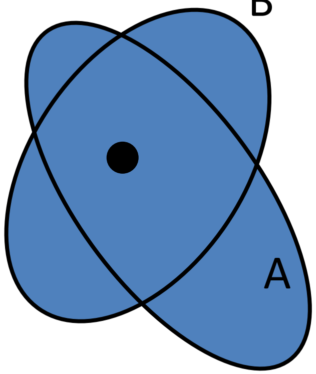
Antisymmetric wavefunction + Pauli exclusion principle + Coulomb interaction =
Exchange interaction

Rodzaje oddziaływań wymiennych

Oddziaływanie wymienne = Odziaływanie kulombowskie + Zasada Pauliego

$\Psi = \Psi_{orbital} \times \Psi_{spin}$ Antysymetryczna!

Przykład:



Dwa elektrony zlokalizowane na jednym centrum

$$\mathcal{H}(1,2) = H_0(1) + H_0(2) + \frac{e^2}{r_{12}}$$

Rodzaje oddziaływań wymiennych

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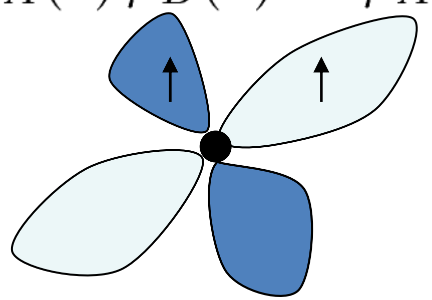
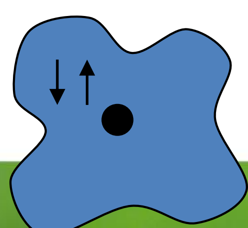
Reguły Hunda, $E_T < E_S$

$$\frac{1}{\sqrt{2}}\left[\varphi_A(1)\varphi_B(2) - \varphi_A(2)\varphi_B(1)\right] \times \begin{bmatrix} \chi_\uparrow(1)\chi_\uparrow(2) \\ \frac{1}{\sqrt{2}}\left[\chi_\uparrow(1)\chi_\downarrow(2) + \chi_\downarrow(1)\chi_\uparrow(2)\right] \\ \chi_\downarrow(1)\chi_\downarrow(2) \end{bmatrix}$$



$$\frac{1}{\sqrt{2}}\left[\varphi_A(1)\varphi_B(2) + \varphi_A(2)\varphi_B(1)\right] \quad \frac{1}{\sqrt{2}}\left[\chi_\uparrow(1)\chi_\downarrow(2) - \chi_\downarrow(1)\chi_\uparrow(2)\right]$$



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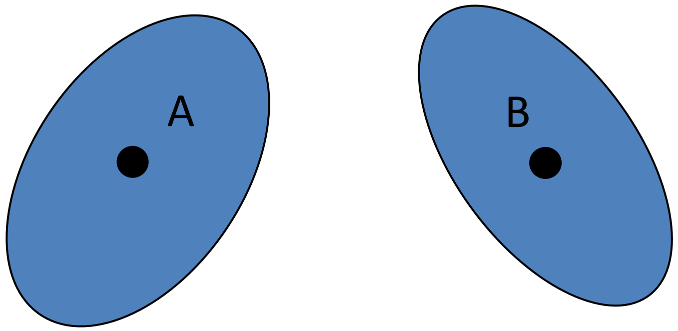


Dwa elektrony na dwóch różnych centrach

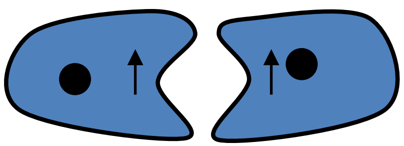
$$\mathcal{H}(1,2) = H_0^A(1) + H_0^B(2) + \frac{e^2}{r_{12}}$$

Rodzaje oddziaływań wymiennych

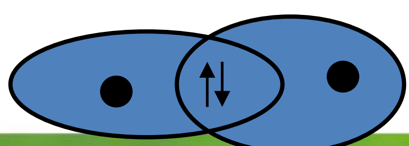
Oddziaływanie wymienne = Odziaływanie kulombowskie + Zasada Pauliego

$\Psi = \Psi_{orbital} \times \Psi_{spin}$ <u>Antysymetryczna!</u>

$$\frac{1}{\sqrt{2}}\left[\varphi_A(1)\varphi_B(2) - \varphi_A(2)\varphi_B(1)\right] \times \begin{bmatrix} \chi_\uparrow(1)\chi_\uparrow(2) \\ \frac{1}{\sqrt{2}}\left[\chi_\uparrow(1)\chi_\downarrow(2) + \chi_\downarrow(1)\chi_\uparrow(2)\right] \\ \chi_\downarrow(1)\chi_\downarrow(2) \end{bmatrix}$$



$$\frac{1}{\sqrt{2}}\left[\varphi_A(1)\varphi_B(2) + \varphi_A(2)\varphi_B(1)\right] \; \frac{1}{\sqrt{2}}\left[\chi_\uparrow(1)\chi_\downarrow(2) - \chi_\downarrow(1)\chi_\uparrow(2)\right]$$



Wiązania chemiczne, $E_S < E_T$