Physics of Condensed Matter I

1100-4INZ`PC

Faculty of Physics UW

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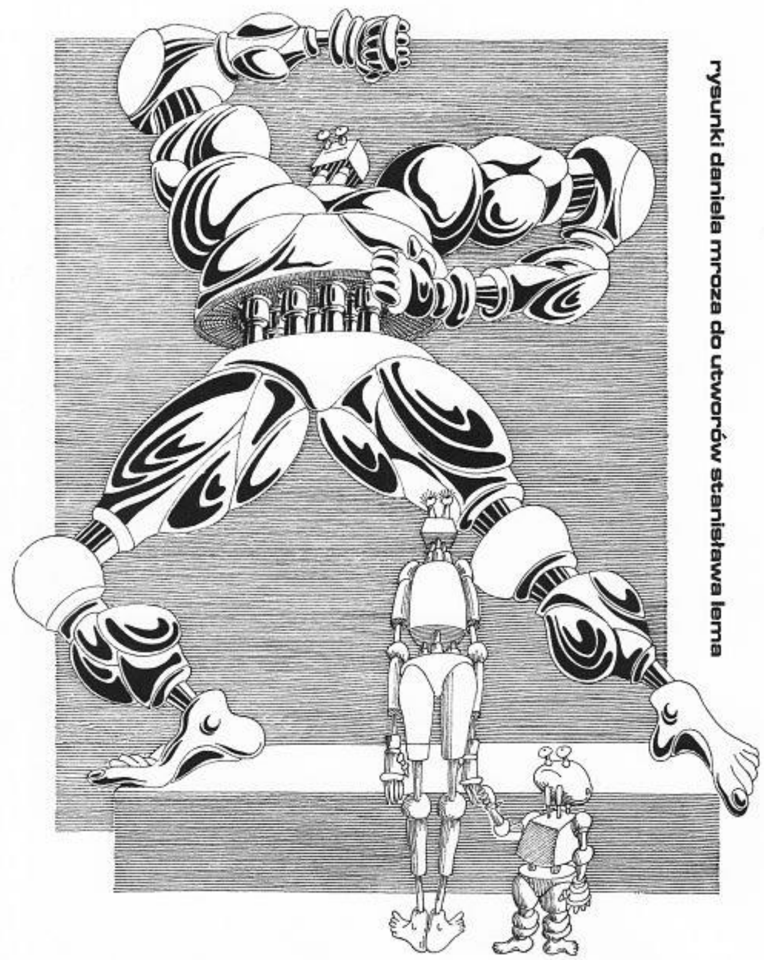
Summary of the lecture

1. Quantum mechanics
2. Optical transitions
3. Lasers
4. Optics
5. Molecules
6. Properties of molecules
7. Crystals
8. Crystalography
9. Solid state
10. Electronic band structure
11. Effective mass approximation
12. Electrons and holes
13. Carriers
14. Transport
15. Optical properties of solids



Classical and quantum universe

Hydrogen atom:

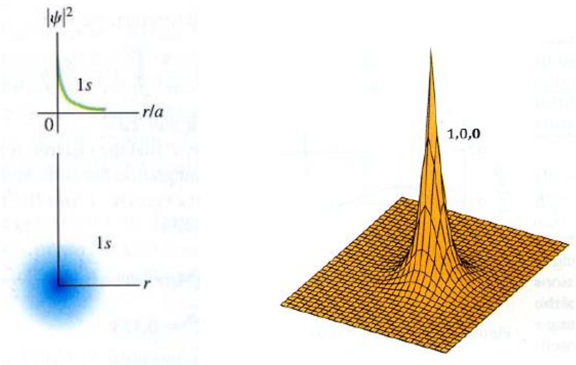
<u>Eigenstates of L:</u>

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

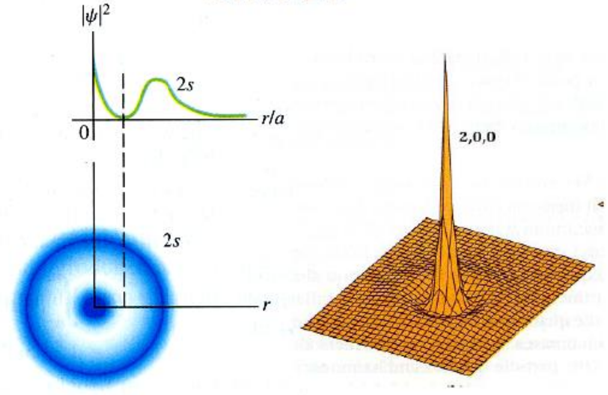
$$\psi_{2s} = \frac{1}{4\sqrt{2\pi a^3}} (2 - \frac{r}{a}) \exp(-\frac{r}{2a})$$

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

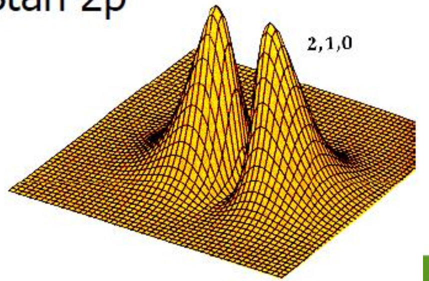
$$\psi_{2p\pm} = \frac{1}{8\sqrt{\pi a^3}} \frac{r}{a} \exp(-\frac{r}{2a}) \sin\theta \exp(\pm i\varphi)$$



Stan 2s



Stan 2p



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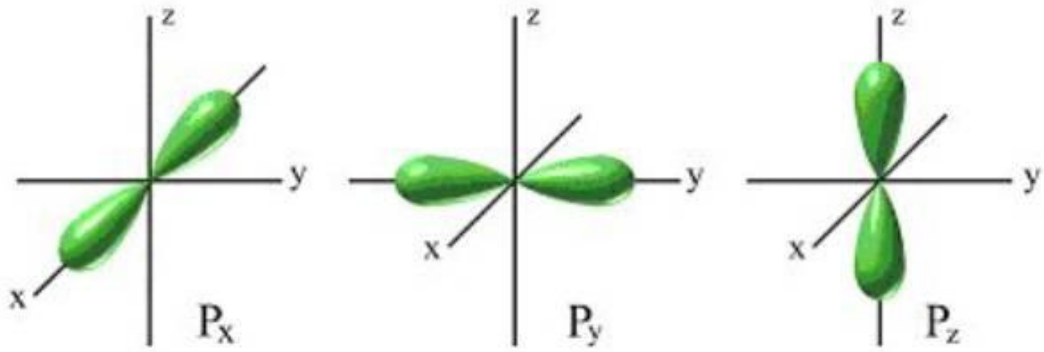
Real functions:

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

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

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

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



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Spherical harmonics Y_{lm}:

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

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

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

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

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

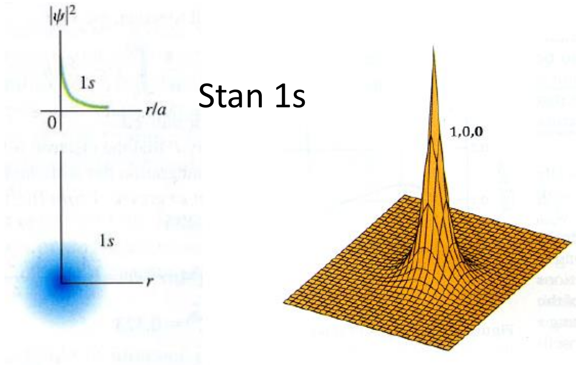
$$Y_{1\pm 1}(\theta,\varphi) = \sqrt{\frac{3}{8\pi}} \sin(\theta) \exp(\pm i\varphi)$$

Classical and quantum universe

Eigenstate:

E.g. hydrogen wavefunction

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



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

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

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

Quantum numbers!

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

Electric field

Stark effect of hydrogen atom

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

electric field E

dipole moment p

Eigenfunctions of hydrogen atom for 2p state:

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

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

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

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Exercises !

Eigenfunctions of hydrogen atom for 2p state:

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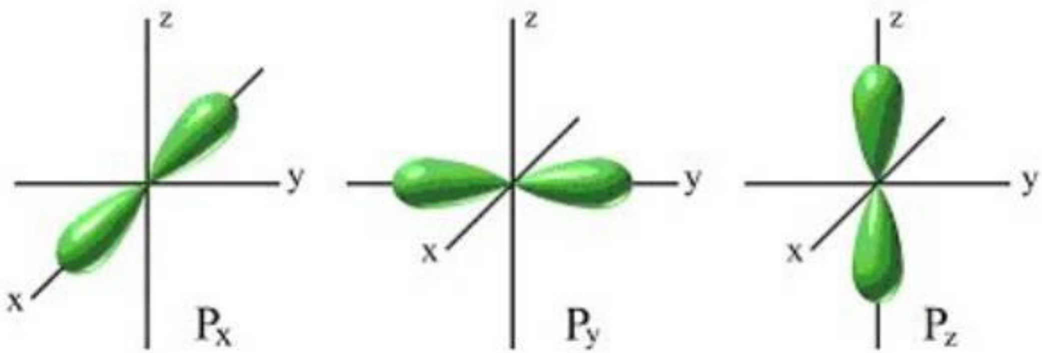
Atom in ligand field



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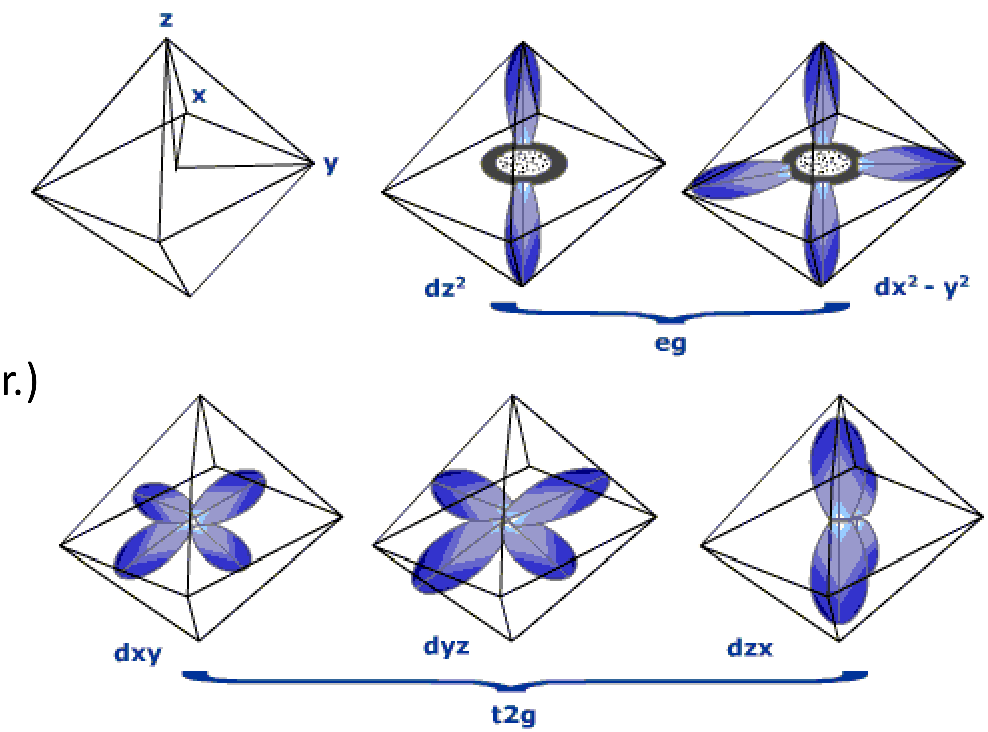
Atom in ligand field
Crystal Field Theory (CFT)
(magnetic properties as well as color.)



http://www.tutorvista.com/content/chemistry/chemistry-iv/coordination-compounds/crystal-field-splitting.php

Magnetic field and spin

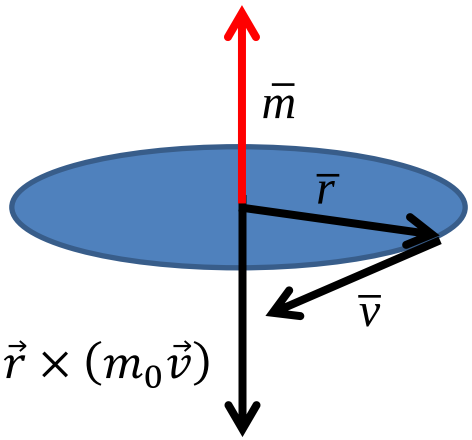
Magnetic field:

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

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

clasically:

$$|\vec{m}| = |I\vec{S}|$$



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

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

Magnetic field and spin

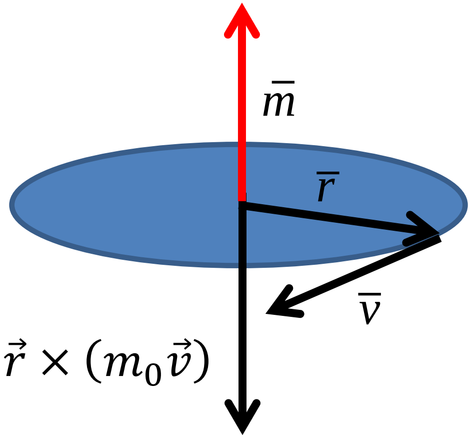
Magnetic field:

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

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

clasically:

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

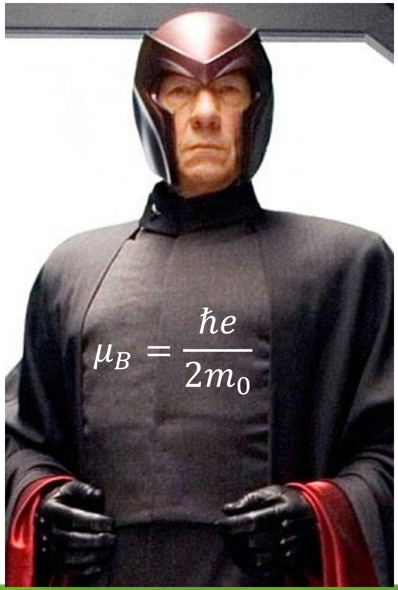


thus: $\vec{m} = -\frac{e}{2m_0}\vec{L} = -\frac{\mu_B}{\hbar}\vec{L}$

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

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

$\mu_B = 9{,}274009994(57)\times 10^{-24}$ J/T



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

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

Magnetic field and spin

Magnetic field:

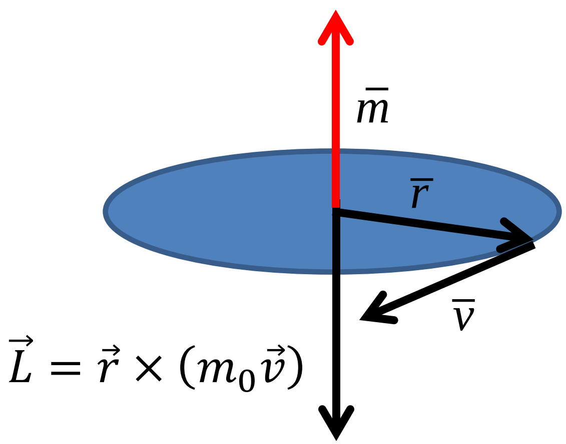
$$H' = -\vec{m}\vec{B} = \frac{\mu_B}{\hbar}\hat{L}\vec{B}$$

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

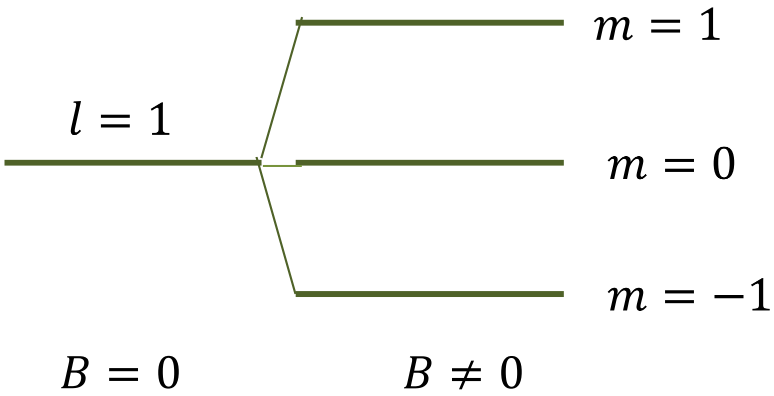
Here $\vec{m}$ is the magnetic moment

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

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



the base: $|l,m\rangle$



Magnetic field and spin

Magnetic field:

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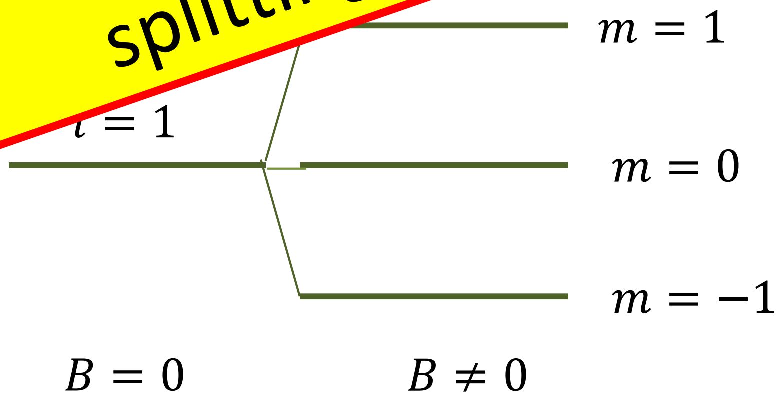
for $\vec{B} = (0,0,B_z)$

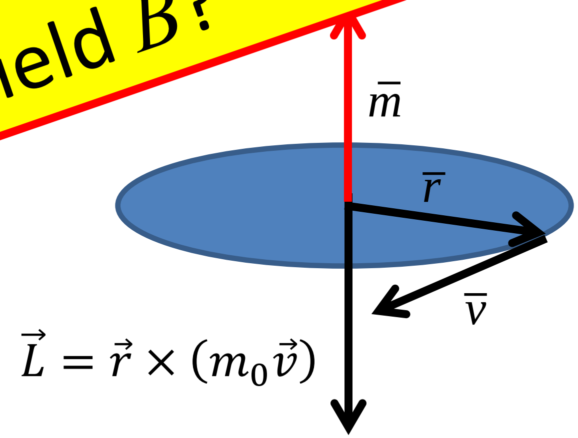
we have: $H' = \frac{\mu_B}{\hbar}\hat{L}_z B_z = \mu_B B_z m$ where $m = -l$ ...

Here ...

the b... $m)$

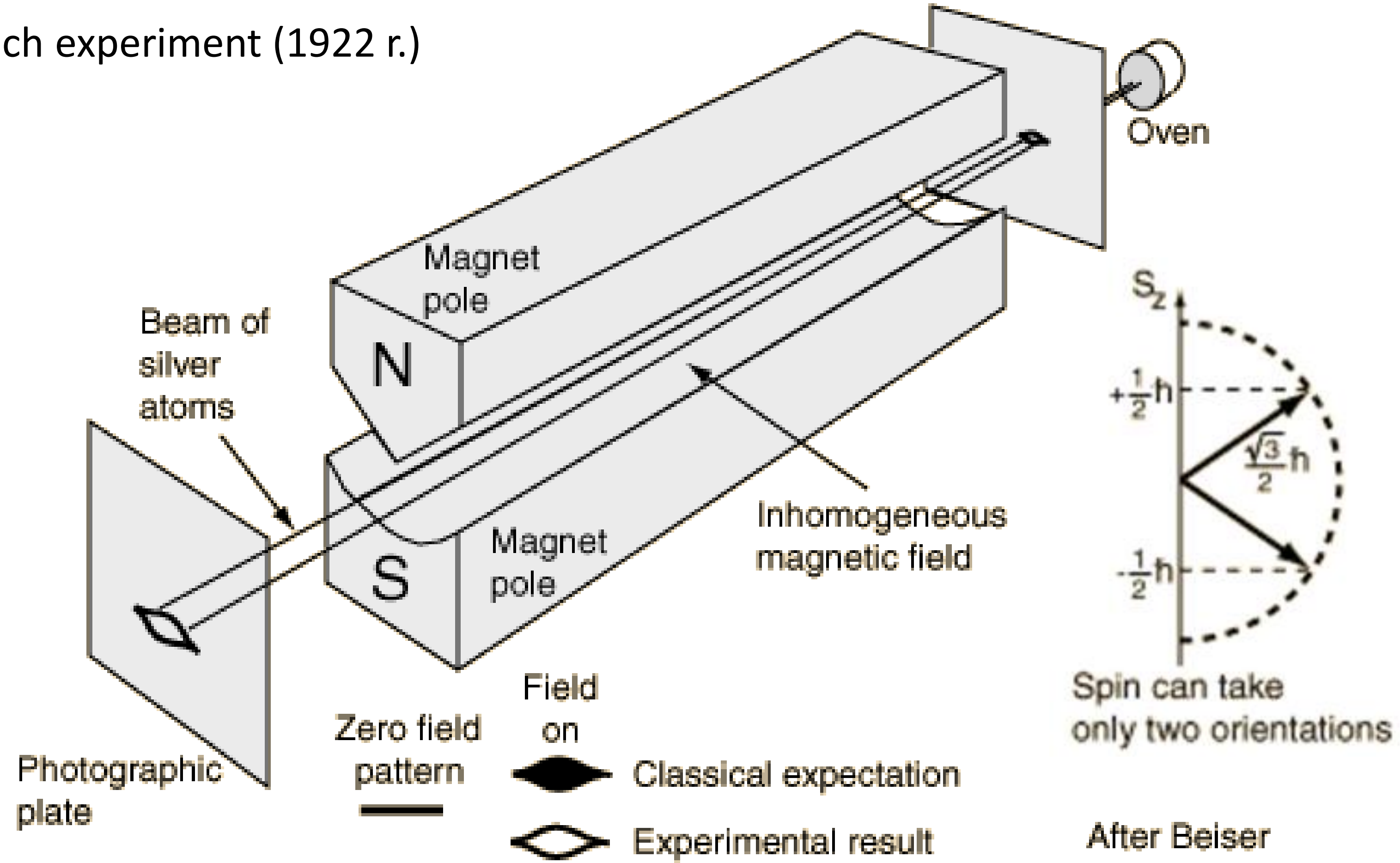
Does it mean that for s-state($l=0$) there is no splitting in magnetic field B?





Magnetic field and spin

Stern-Gerlach experiment (1922 r.)



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

What is the „spin”?

- What is „mass”?

$$\overrightarrow{F} = m\,\overrightarrow{a}$$

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

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

What is the „spin”?

- What is „momentum”?

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

What is the „spin”?

- What is „charge”?

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

What is the „spin”?

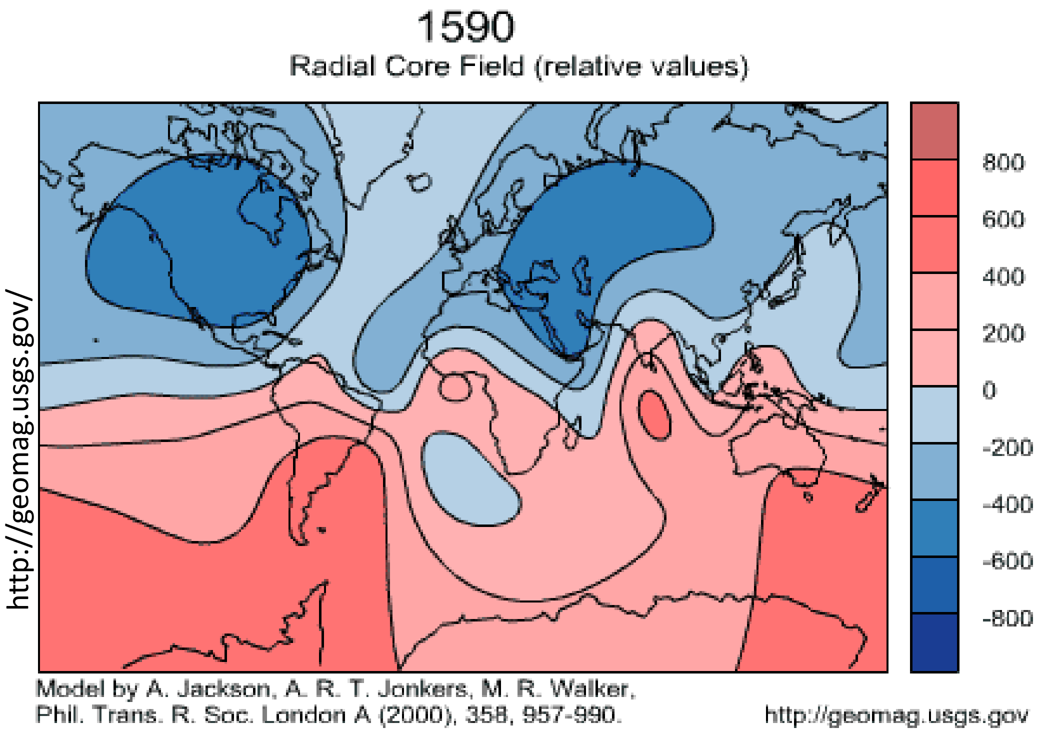
- Spin? 

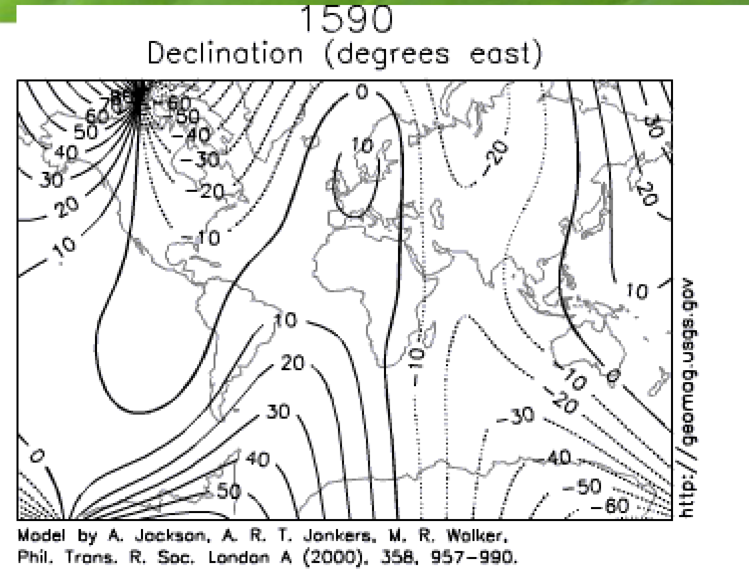
http://www.floridahistory.com/us@1570.html

Sebastian Münster, Cosmographia in 1544

Disney

The history


1590
Radial Core Field (relative values)
800
600
400
200
0
-200
-400
-600
-800
Model by A. Jackson, A. R. T. Jonkers, M. R. Walker,
Phil. Trans. R. Soc. London A (2000), 358, 957-990.
http://geomag.usgs.gov
http://geomag.usgs.gov/


1590
Declination (degrees east)
Model by A. Jackson, A. R. T. Jonkers, M. R. Walker,
Phil. Trans. R. Soc. London A (2000), 358, 957–990.
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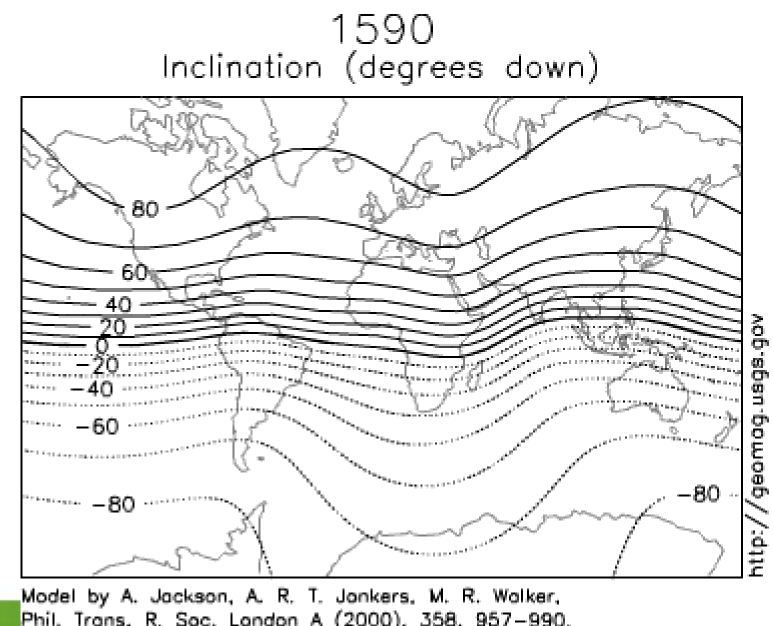
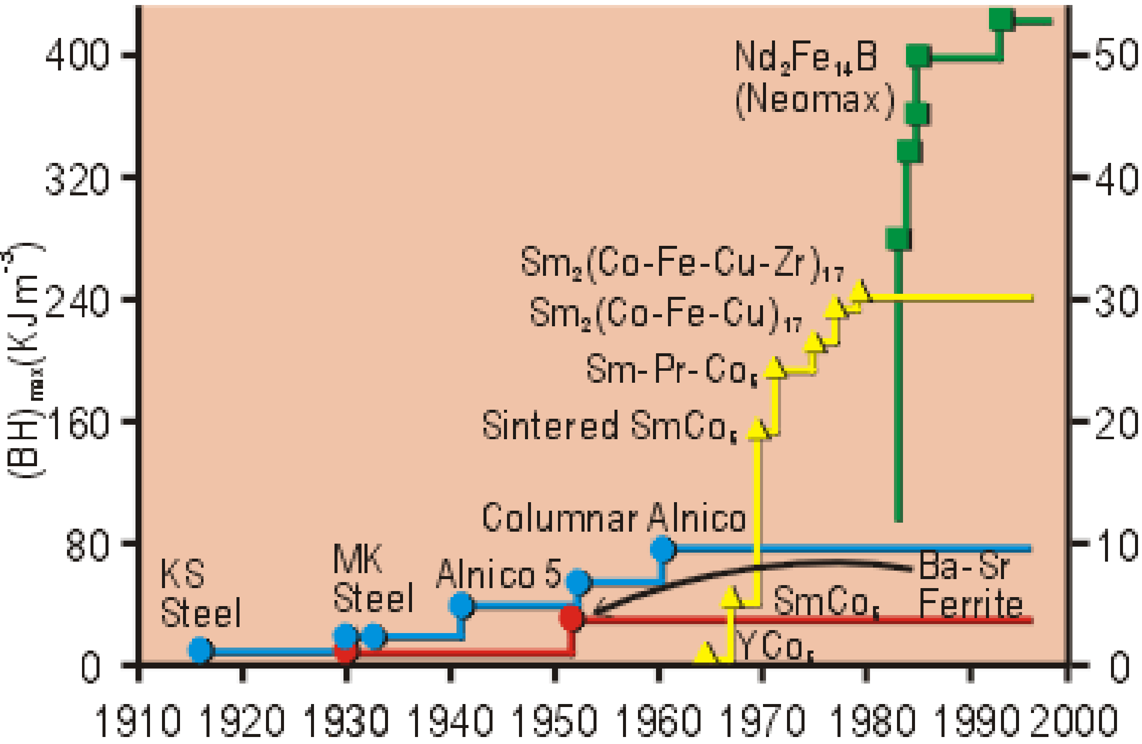

1590
Inclination (degrees down)
80
60
40
20
0
−20
−40
−60
−80
Model by A. Jackson, A. R. T. Jonkers, M. R. Walker,
Phil. Trans. R. Soc. London A (2000), 358, 957–990.
http://geomag.usgs.gov

The history



http://www.azom.com/details.asp?ArticleID=637

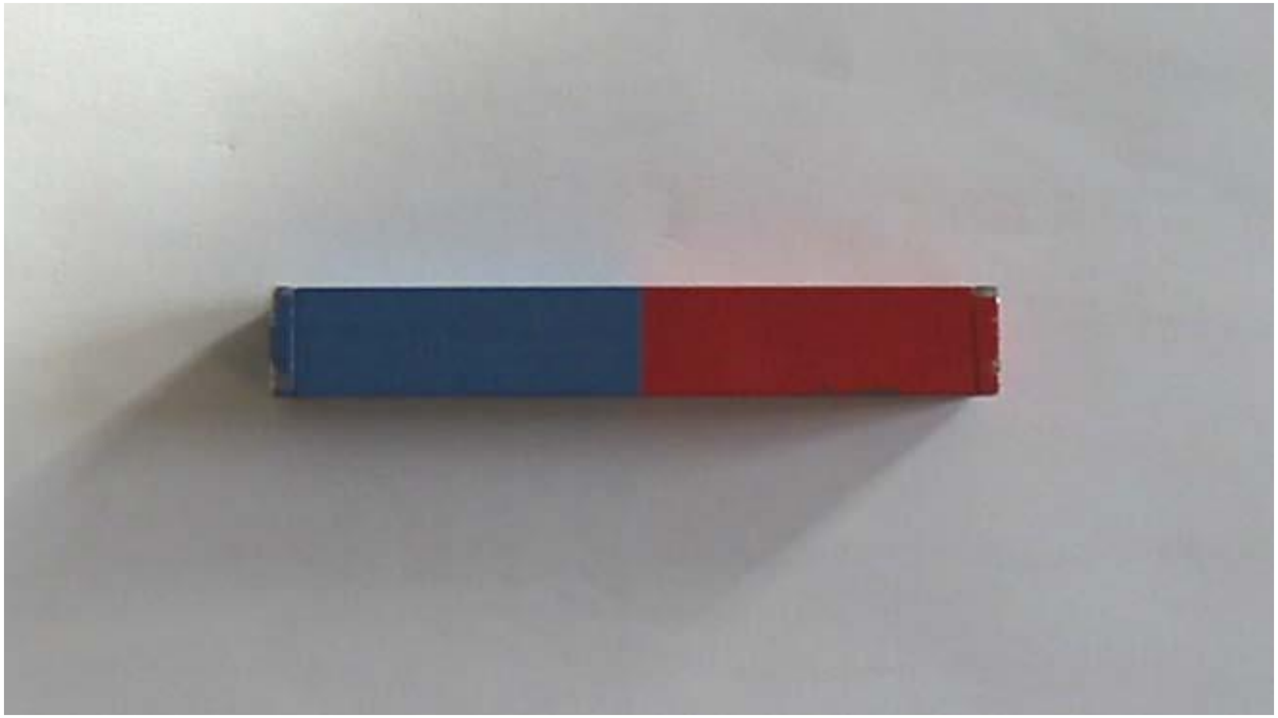
Magnetyt (z 1750 r.) typowy ferryt i magnes z ziem rzadkich. Każdy z nich o gęstości energii 1J.

http://www.tcd.ie/Physics/Schools/what/materials/magnetism/seven.html

A lodestone magnet from the 1750's and typical ferrite and rare earth used in modern appliances. Each of these produce about 1J of energy.

What is the „spin”?

How magnets work?



http://lucy.troja.mff.cuni.cz/~tichy/elektross/magn_pole/stac_mp.html

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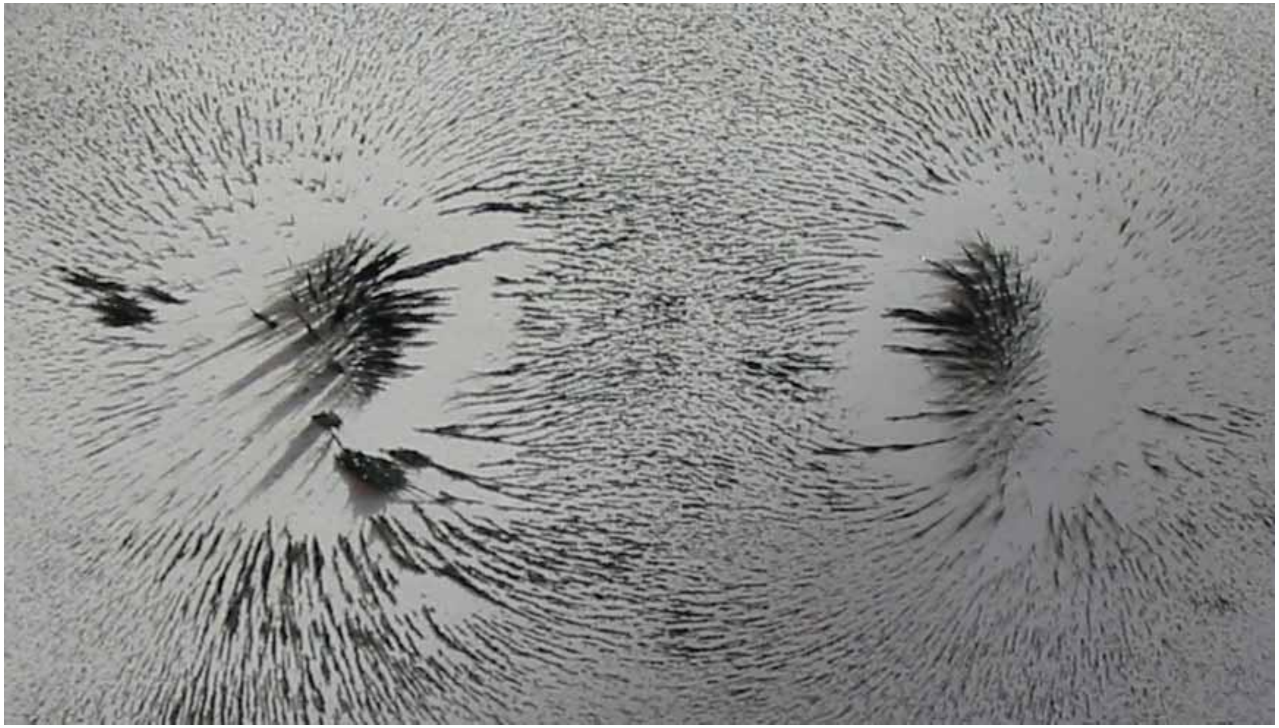

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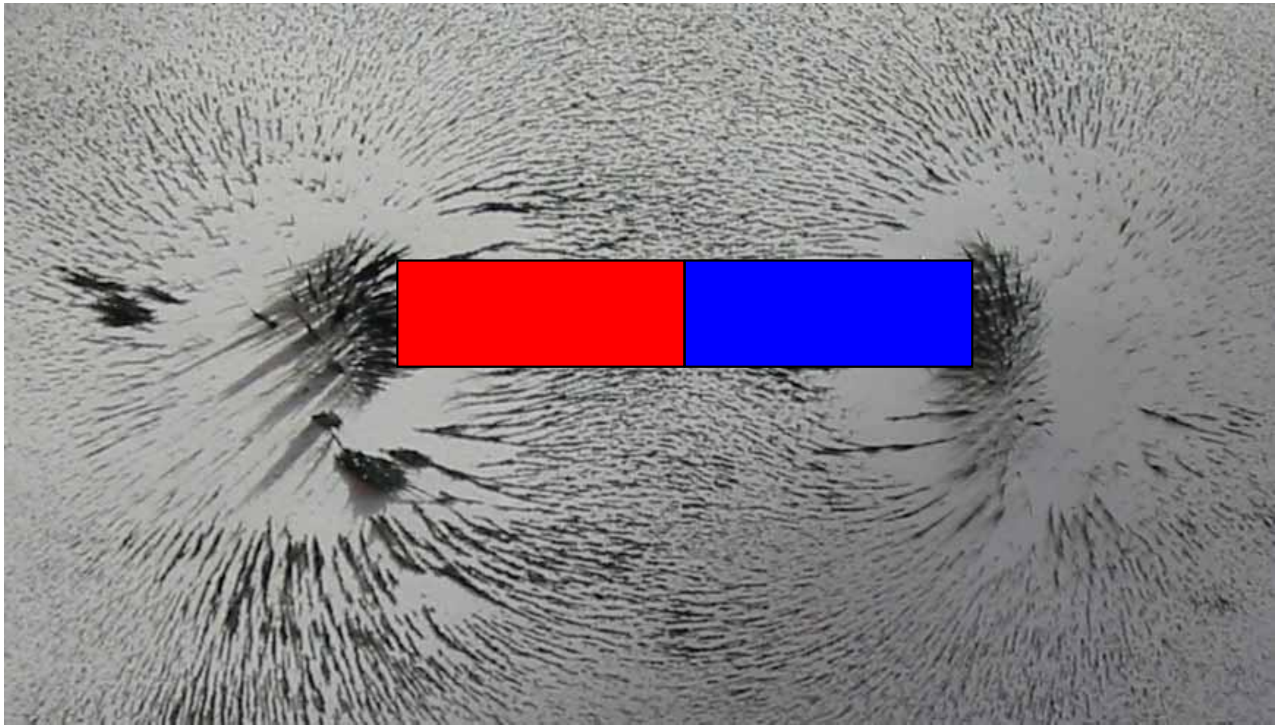

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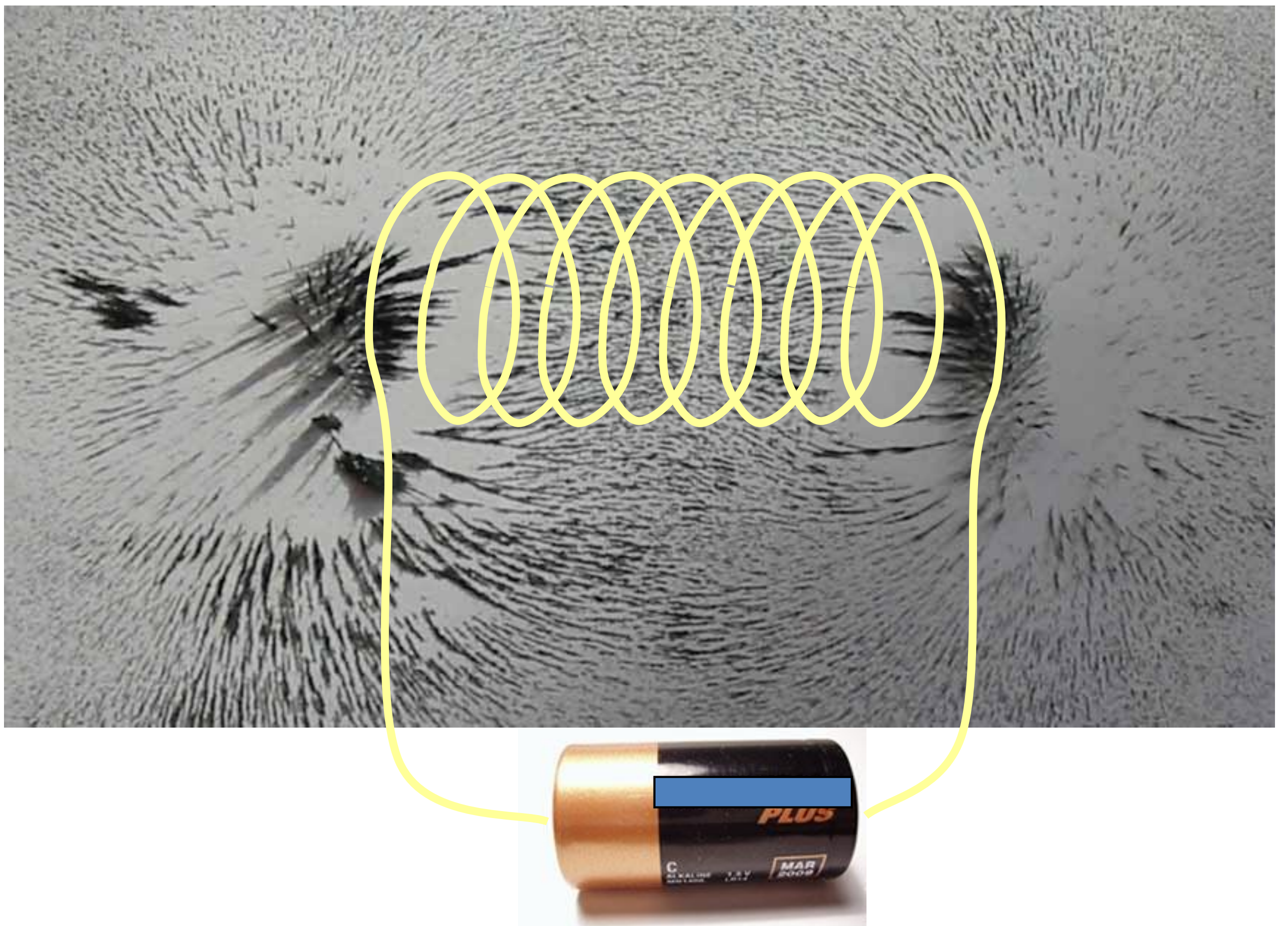

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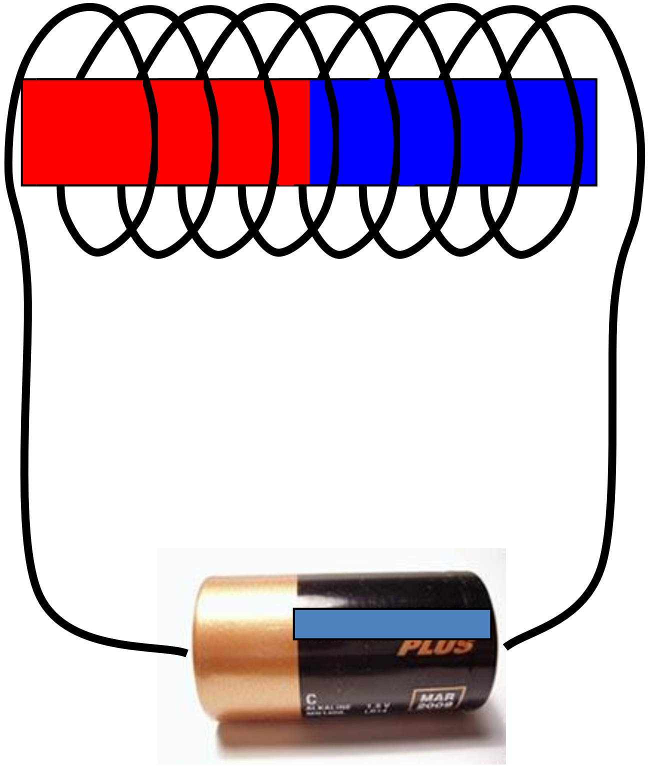
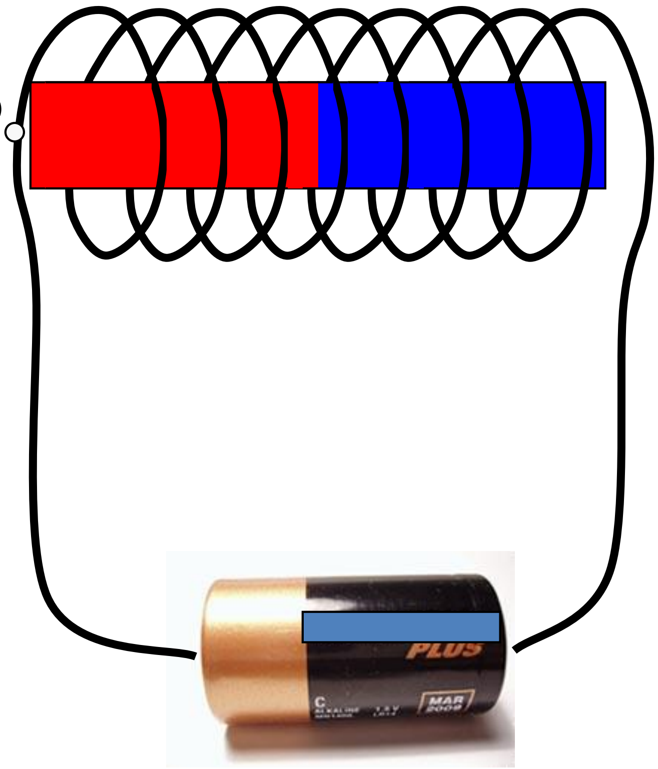


What is the „spin”?

How magnets work?

Moving charges produce a magnetic field…



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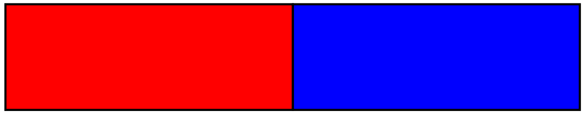

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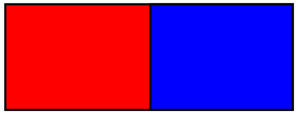

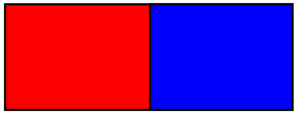

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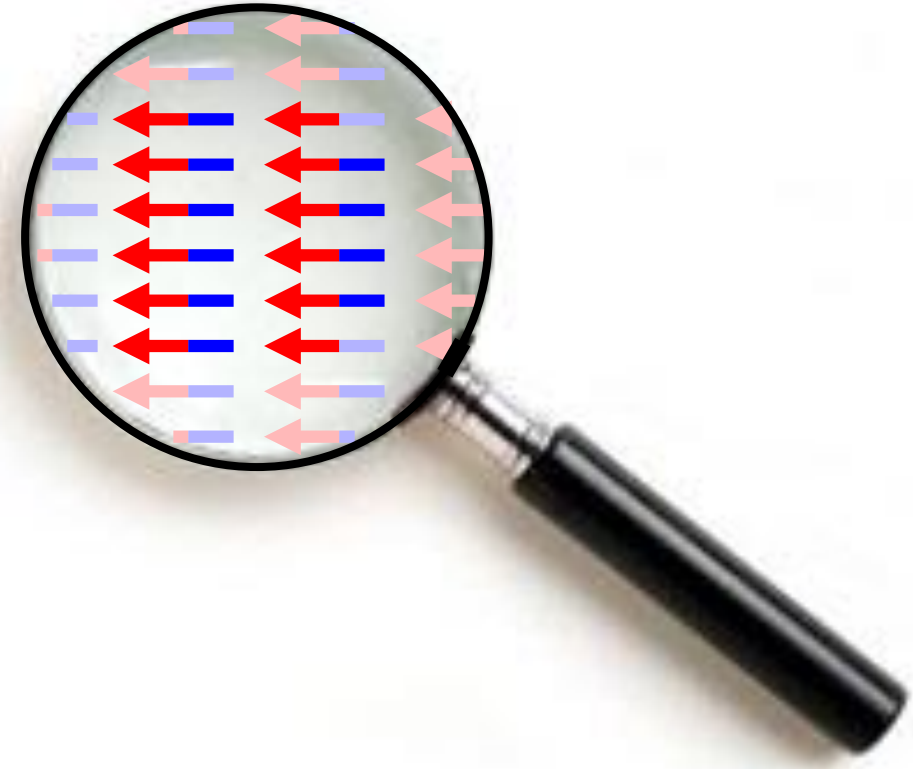

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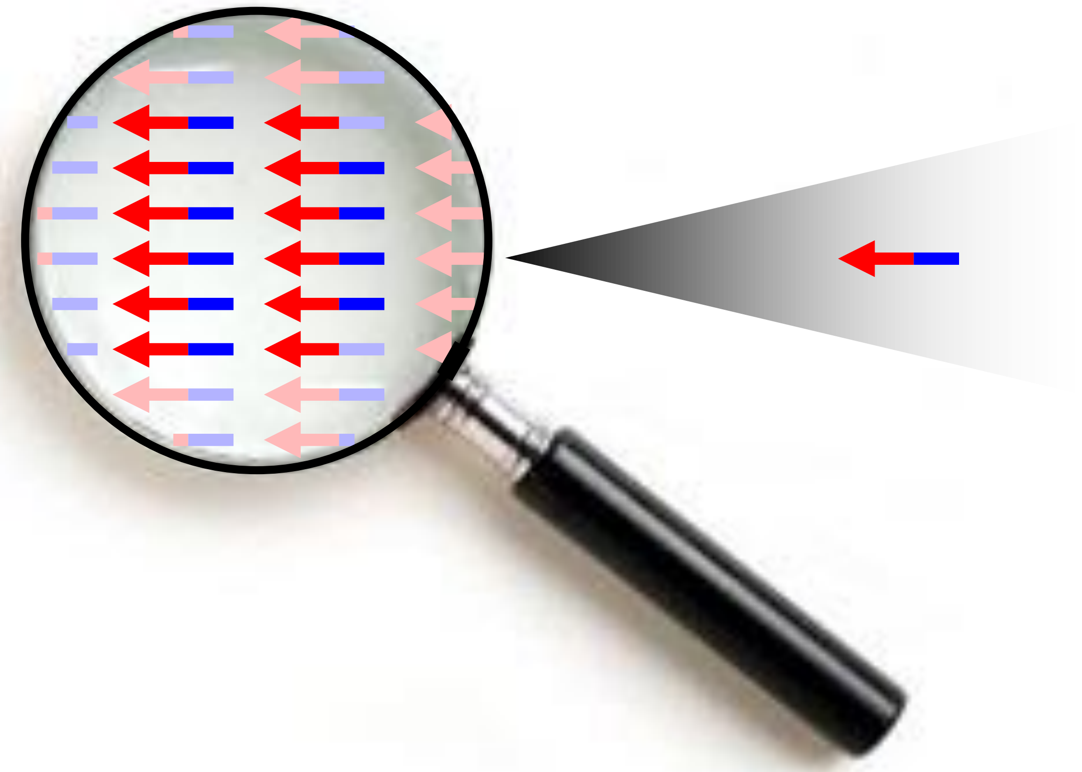


These smal magnets
are electrons

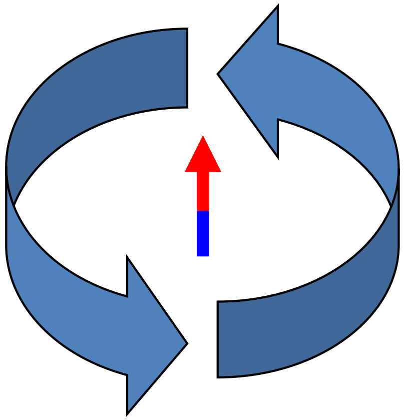
What is the „spin”?

How magnets work?

These smal magnets
are electrons

What is the „spin”?

Skąd się biorą magnesy?



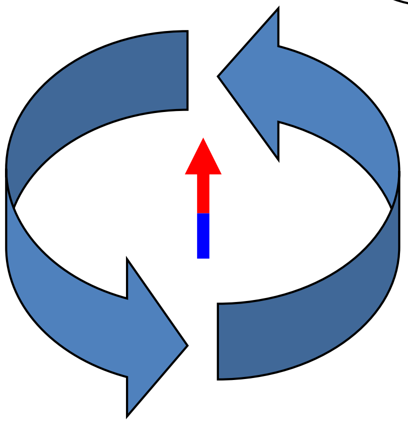
A więc płynie jakiś prąd?

What is the „spin”?

How magnets work?

The movement of electrons around the nucleus?

The spin of electrons around it’s own axis?



So, there is a current?

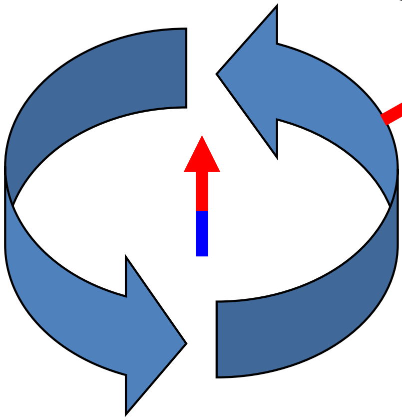
Internal property of electrons?

What is the „spin”?

How magnets work?

The movement of electrons around the nucleus?

The spin of electrons around it’s own axis?



So, there is a current?

Internal property of electrons?

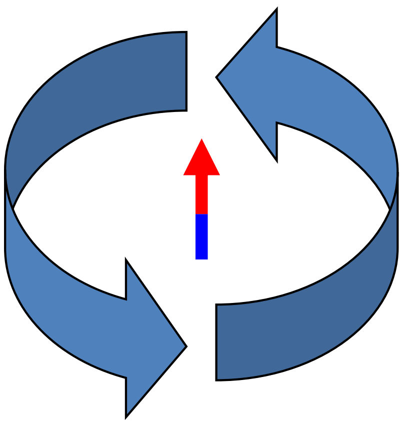
!

internal angular momentum
SPIN

What is the „spin”?

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

internal angular momentum

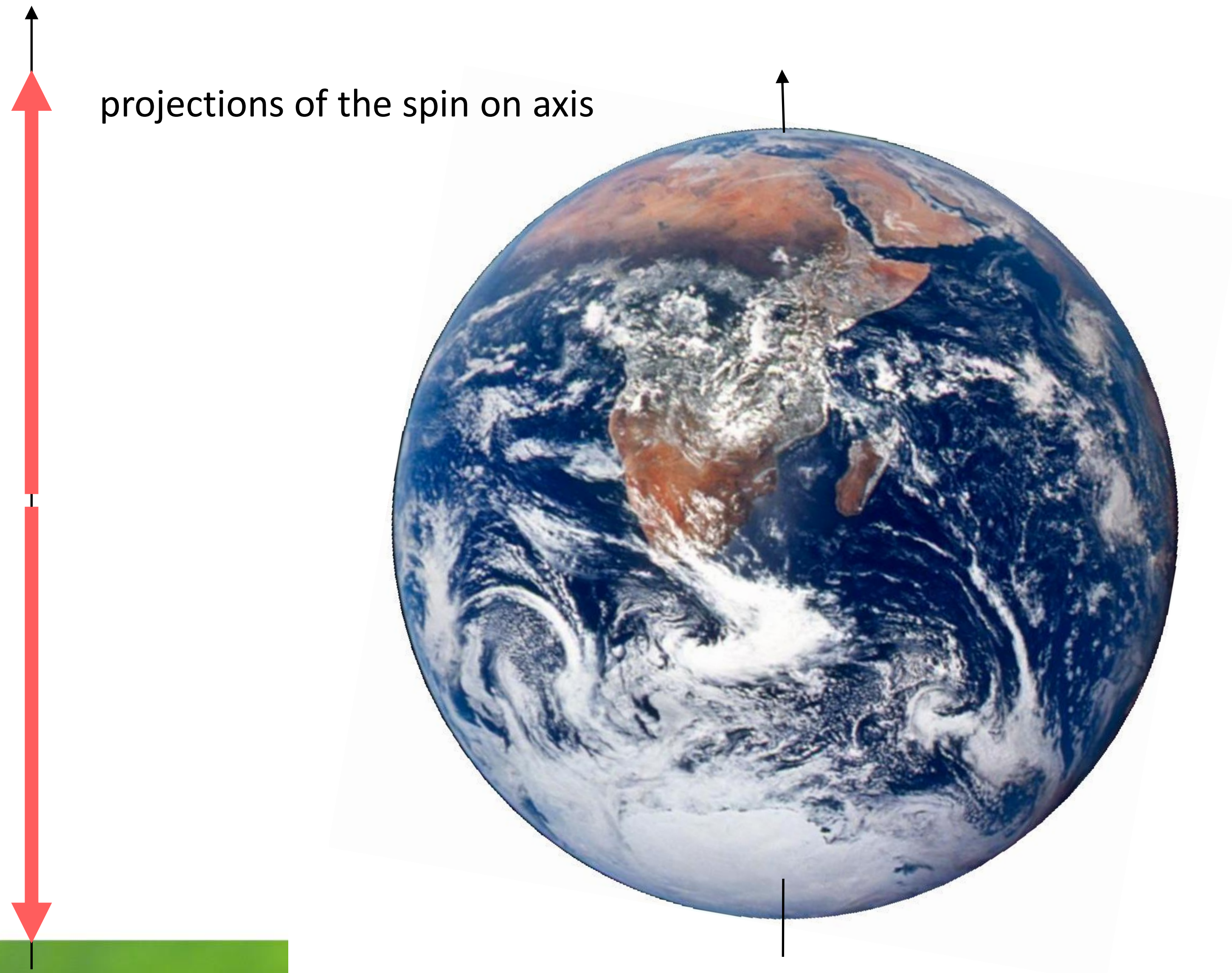


Internal property of electrons

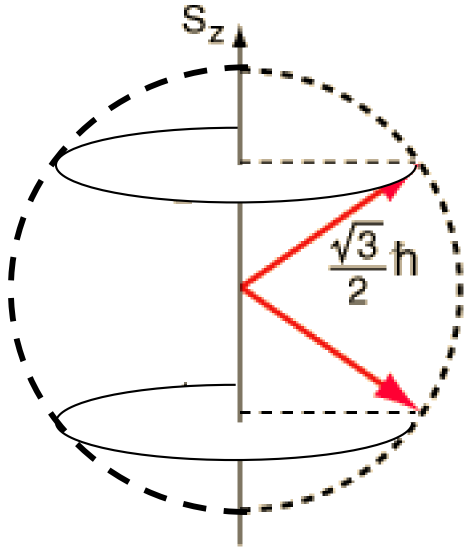
!

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

What is the „spin”?



What is the „spin”?



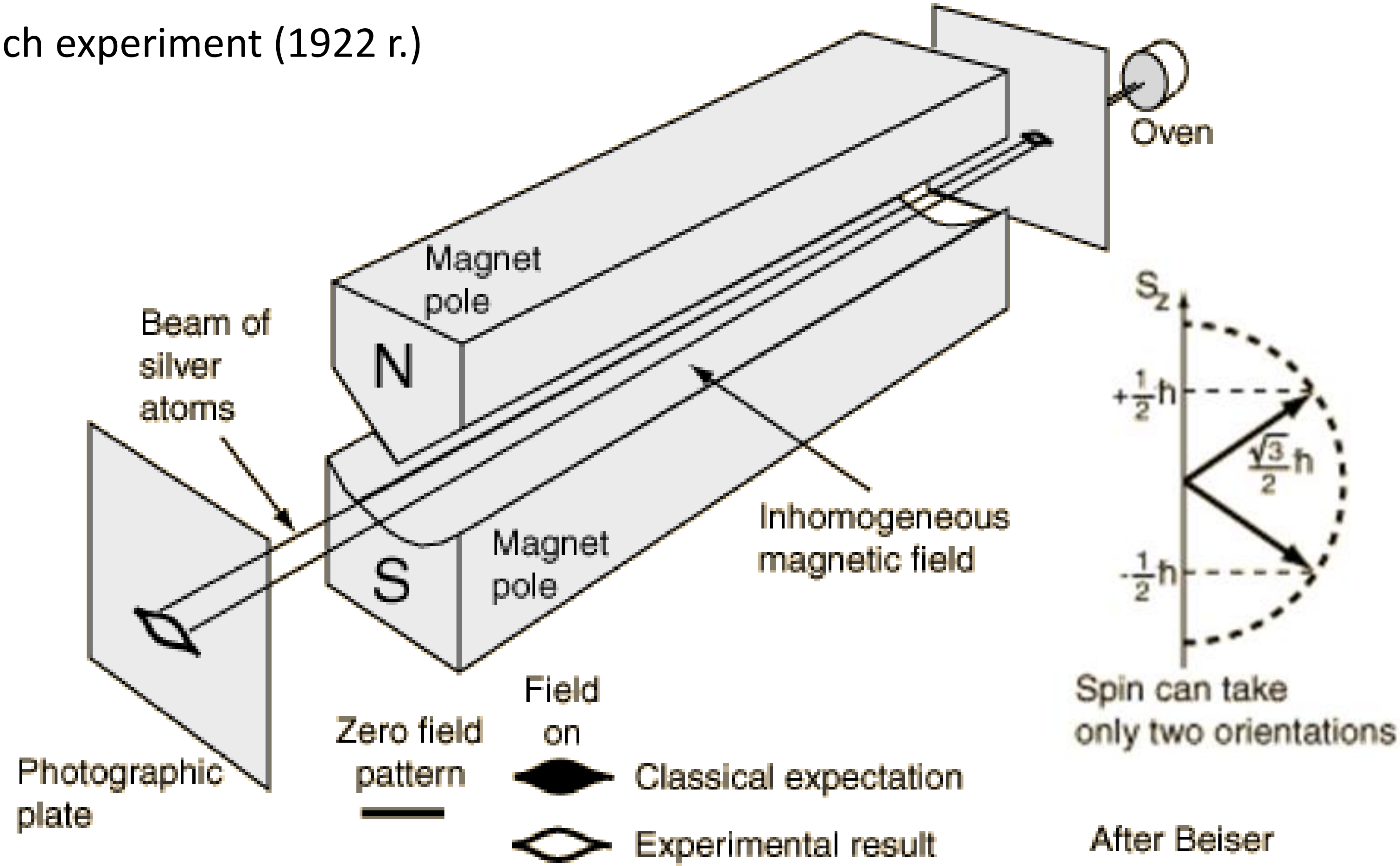
projections of the spin on ANY of axes has only TWO values:

$$+\frac{1}{2}\hbar \quad -\frac{1}{2}\hbar$$

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

Magnetic field and spin

Stern-Gerlach experiment (1922 r.)



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

Magnetic field and spin

Spin, spin-orbit interaction

Spin operators $\hat{S}_x, \hat{S}_y, \hat{S}_z, \hat{S}^2$ $\quad$ $\psi(\vec{r}, S_z) = \psi(\vec{r})\chi(S_z)$

Spinor

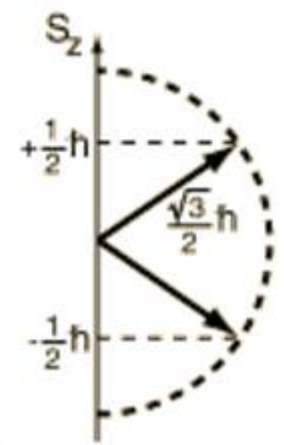
$$[\hat{S}_x, \hat{S}_y] = i\hbar\hat{S}_z, \text{ etc.}$$

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

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

Magnetic field and 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 for the agreement with experiments

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

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$$g = -2.00231930436182 \pm 0.00000000000052$$

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projections of the spin on the axis z

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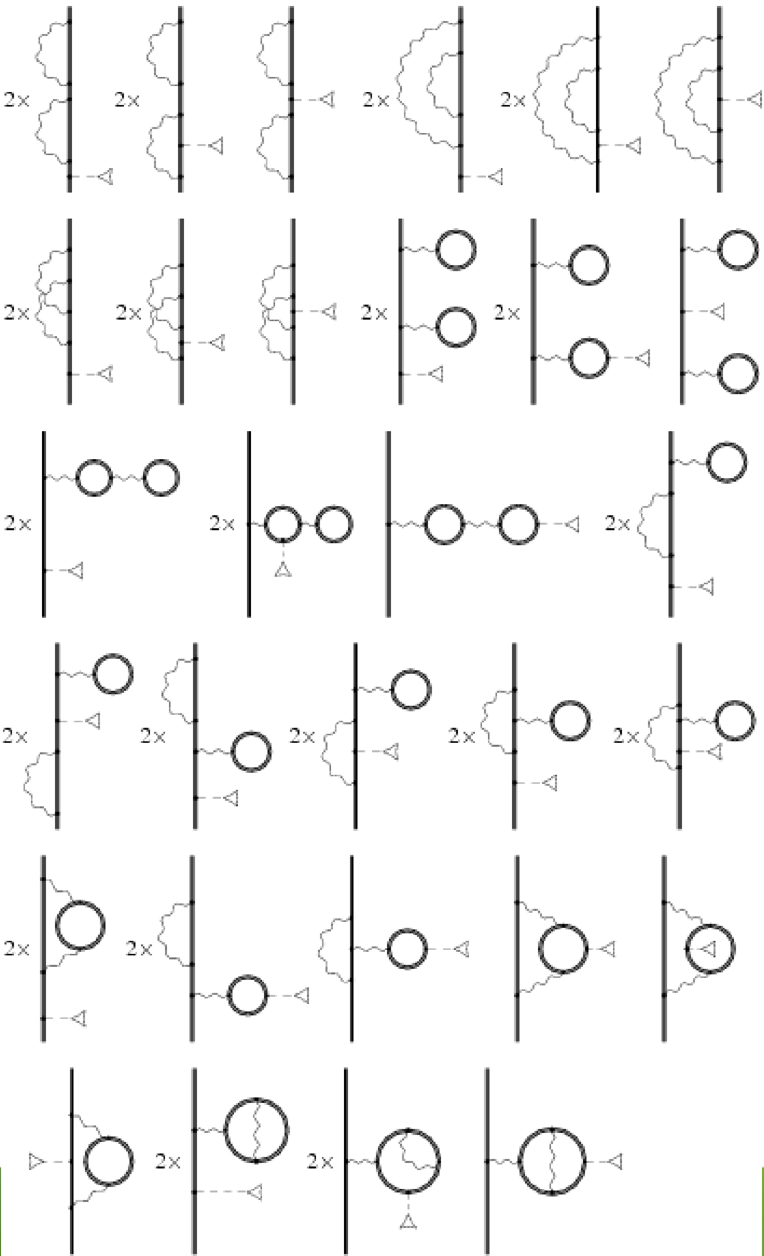
QED – Quantum ElectroDynamics



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Magnetic field and spin

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

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

g-factor 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

Magnetic field and 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 $\hat{L} = 0 \Rightarrow \hat{L}\hat{S} = 0$

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

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

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

fine-structure constant

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

$$Ry = hcR_\infty$$

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

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

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

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

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

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

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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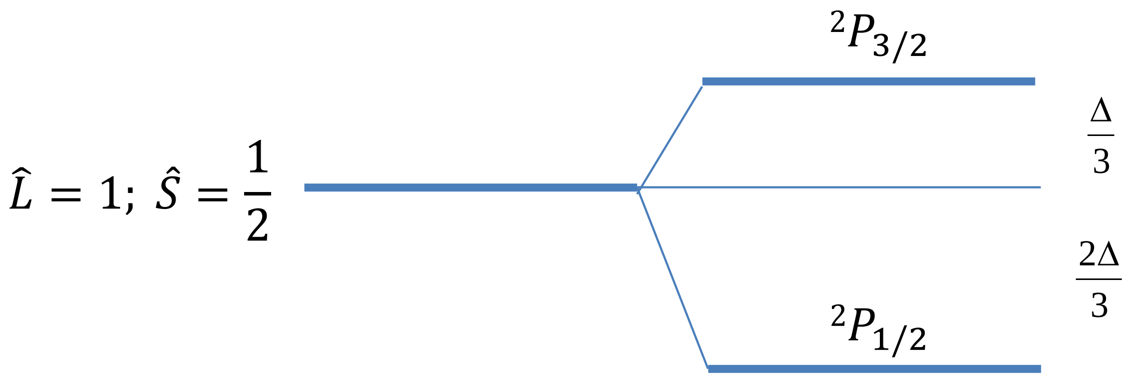

the base: $|n, l, s, j, m_j\rangle$

shortly: $|j, m_j\rangle$

Fine structure

The fine structure means the splitting of the spectral lines of atoms due to electron spin and relativistic corrections to the Schrödinger equation. We got corrections to the value of energy levels.

- Kinetic energy relativistic correction
- Spin-orbit coupling
- Darwin term

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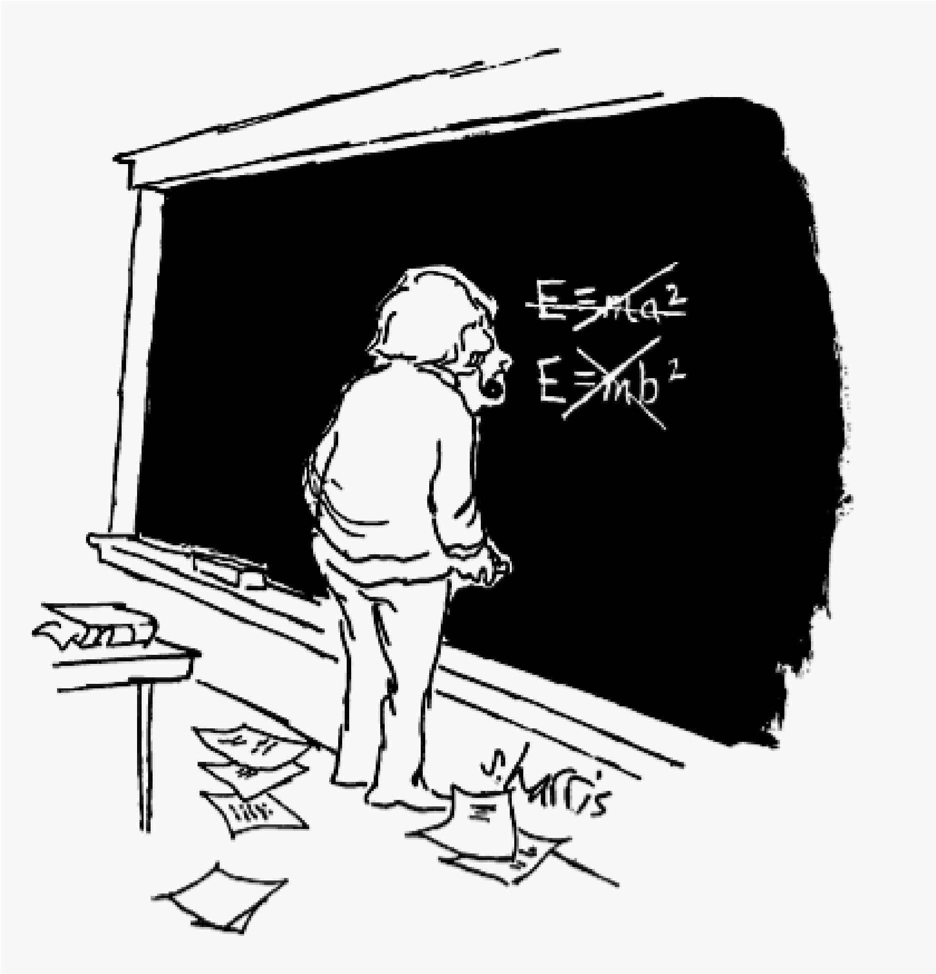

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- Kinetic energy relativistic correction

$$E = \sqrt{\vec{p}^2 c^2 + m_0^2 c^4}$$

The correct description of the atom requires taking into account the relativistic effects which lead to the Dirac Hamiltonian.

The square root can be expanded into a series:

$$E = m_0 c^2 \left(1 + \frac{p^2}{2m_0^2 c^2} - \frac{p^4}{2m_0^4 c^4} + \cdots \right) = m_0 c^2 + \frac{p^2}{2m_0} - \frac{p^4}{8m_0^3 c^2} + \cdots$$

thus kinetic energy can be expressed as

$$E_K = E - m_0 c^2 = \frac{p^2}{2m_0} - \frac{p^4}{8m_0^3 c^2} + \cdots$$

and the Hamiltonian is:

$$i\hbar \frac{\partial}{\partial t} \Psi(\vec{r}, t) = \left[-\frac{\hbar^2}{2m} \nabla^2 + \mathrm{V}(\vec{r}) - \frac{\hbar^4}{8m_0^3 c^2} \nabla^4 \right] \Psi(\vec{r}, t)$$

Fine structure

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Using perturbation theory one can find correction due to the **relativistic mass change** for each principal quantum number and corresponding energy E_n.
For instance the electron speed of $1s$ in gold ^{79}Au $v = 53\%\ c$!

$$m = \frac{m_0}{\sqrt{1-\frac{v^2}{c^2}}}$$

$$\Delta E_n' = -\frac{E_n^2}{2mc^2}\left[\frac{4n}{l+\frac{1}{2}} - 3\right] = -\frac{\alpha^2 Z^2}{2n^4}E_n\left[\frac{n}{l+\frac{1}{2}} - \frac{3}{4}\right]$$

$$\alpha = \frac{e^2}{4\pi\epsilon_0\,\hbar c} \approx \frac{1}{137}$$

$$E_n = -\frac{mc^2\alpha^2}{2}\frac{Z^2}{n^2}$$

Correction from this perturbation:

- Small for light atoms
- Rapidly decreases with the principal quantum number n
- Significant for large Z

Tadeusz Stacewicz

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

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)

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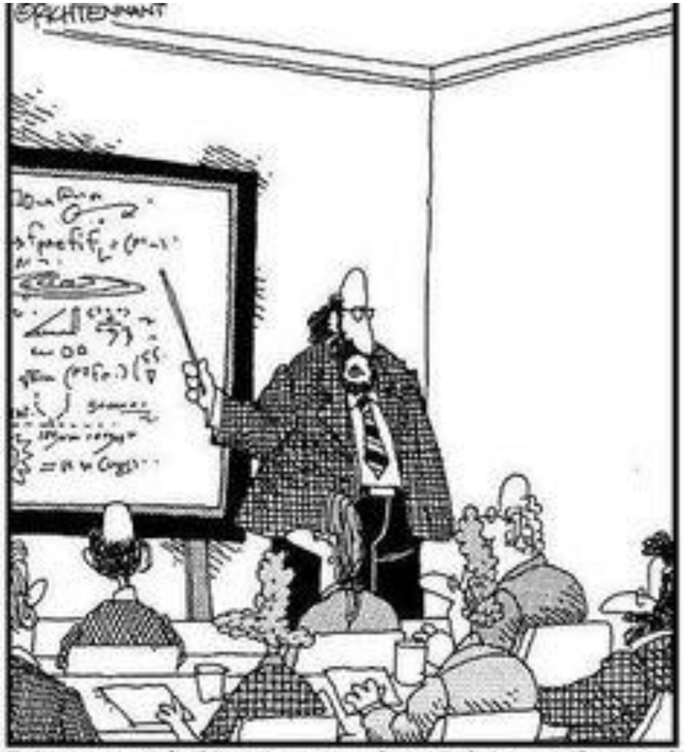
Darwin term is the non-relativistic expansion of the Dirac equation:

$$\left[\beta mc^2 + c\left(\sum_{n}^{3} \alpha_n p_n\right)\right]\psi(\vec{r},t) = i\hbar \frac{\partial \psi(\vec{r},t)}{\partial t}$$

Negative E solutiuons to the equation → antimatter



"Along with 'Antimatter,' and 'Dark Matter,' we've recently discovered the existence of 'Doesn't Matter,' which appears to have no effect on the universe whatsoever."

https://pl.wikibooks.org/wiki/Mechanika_kwantowa/Relatywistyczna_teoria_kwant%C3%B3w_Diraca

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$$\alpha_x = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$$

$$\beta = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \qquad \alpha_y = \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix} \qquad \alpha_z = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}$$

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$$H_{Darwin} = \frac{\hbar^2}{8m^2c^2} 4\pi \left(\frac{Ze^2}{4\pi\epsilon_0} \right) \delta(\vec{r}\,)$$

$$\langle H_{Darwin} \rangle = \frac{\hbar^2}{8m^2c^2} 4\pi \left(\frac{Ze^2}{4\pi\epsilon_0} \right) |\psi(\vec{r} = 0)|^2$$

Only for s-orbit, because: $\psi(\vec{r} = 0) = 0$ for $l > 0$

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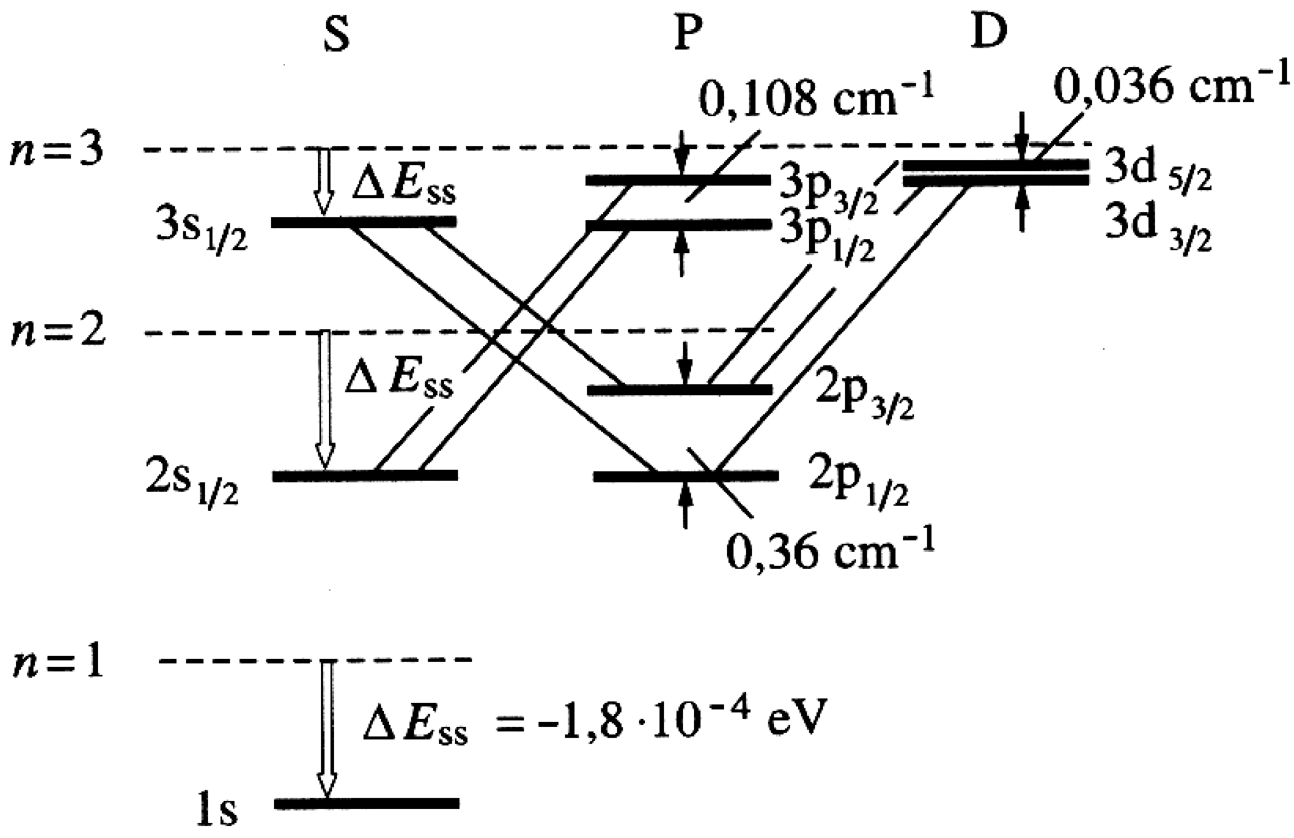
- Darwin term → $$E_{Darwin} = \frac{\hbar^2}{8m^2c^2} 4\pi \left(\frac{Ze^2}{4\pi\epsilon_0}\right) |\psi(\vec{r}=0)|^2$$

Total effect:

$$\Delta E_n' = -\frac{\alpha^2 Z^2}{n^2} E_n \left[\frac{n}{j+\frac{1}{2}} - \frac{3}{4}\right]$$

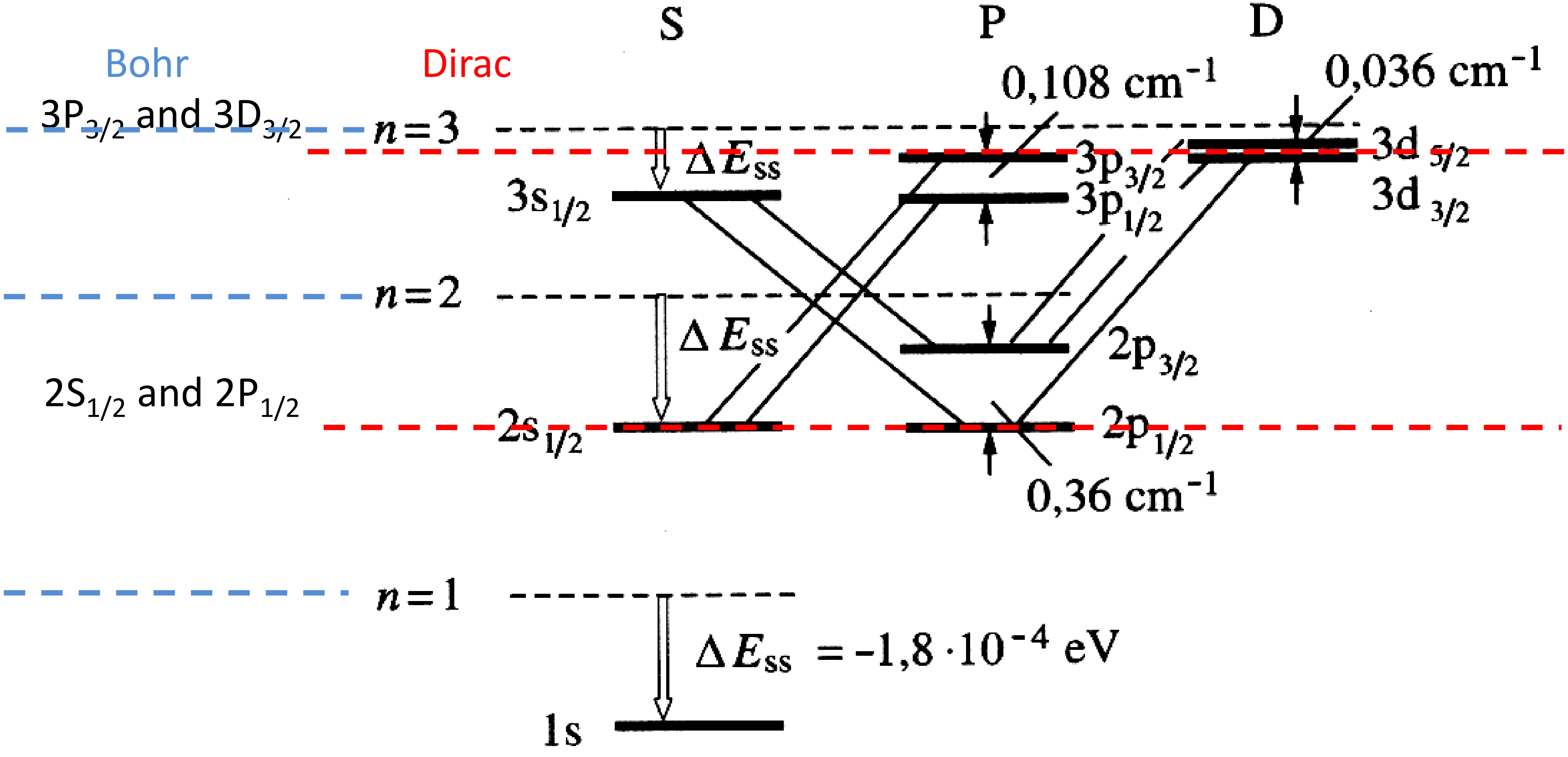
Fine structure

Paul Dirac calculations:



Fine structure

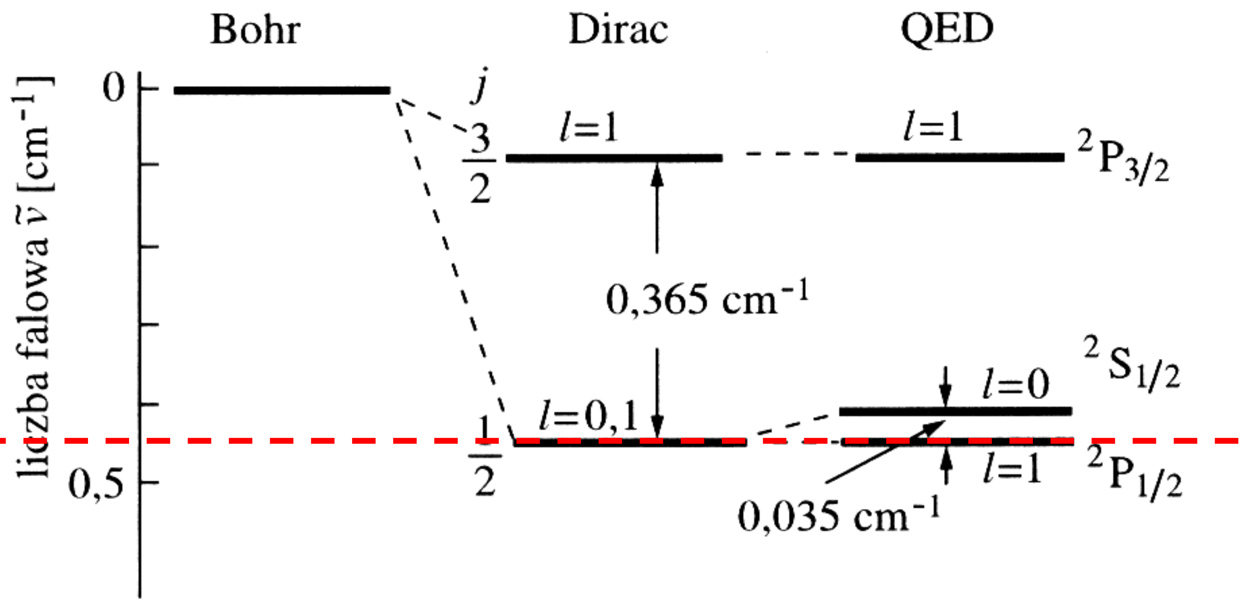
Paul Dirac (Nobel 1933) calculations:



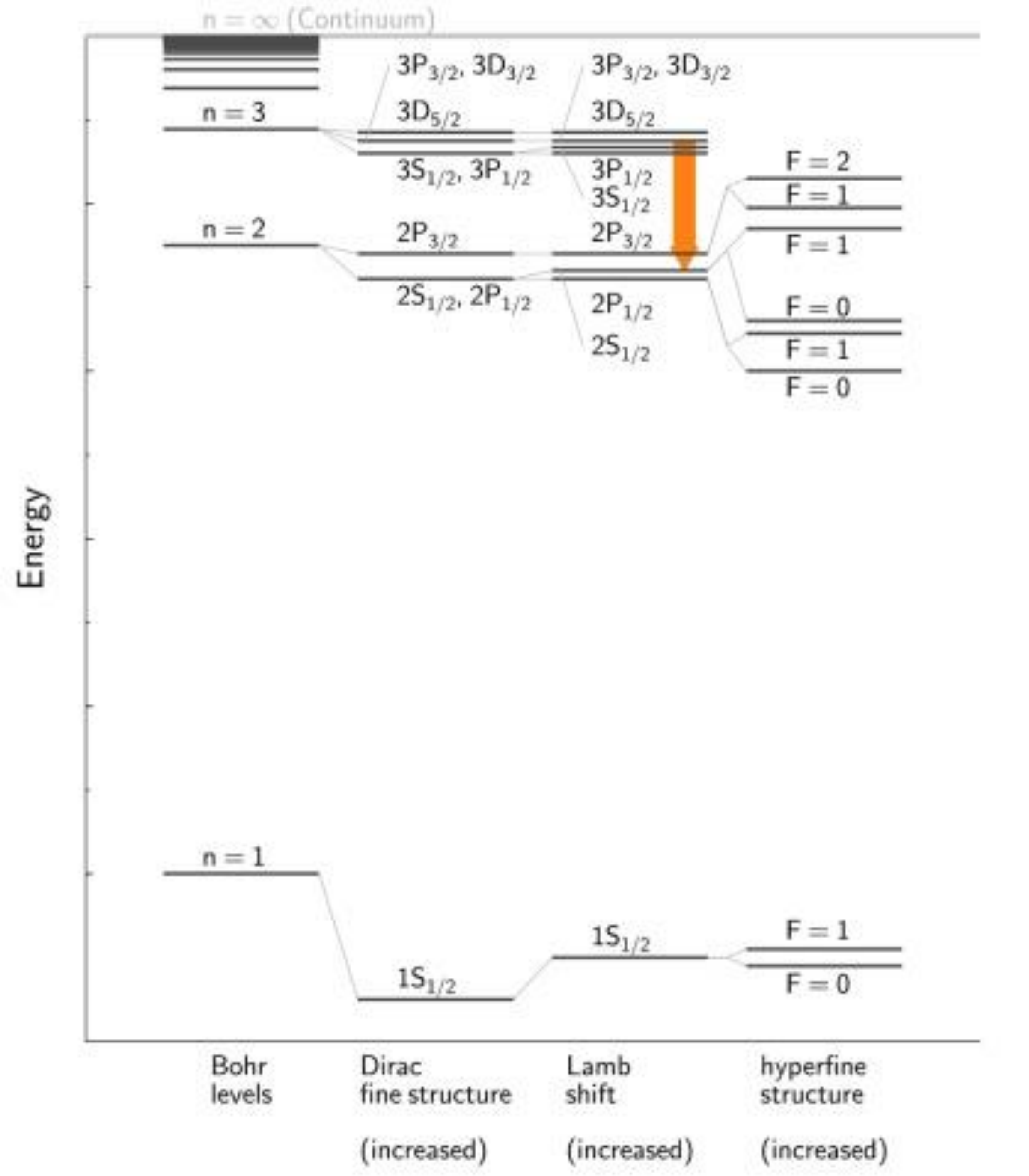
Fine structure

Willis Lamb (Nobel 1955) calculations:

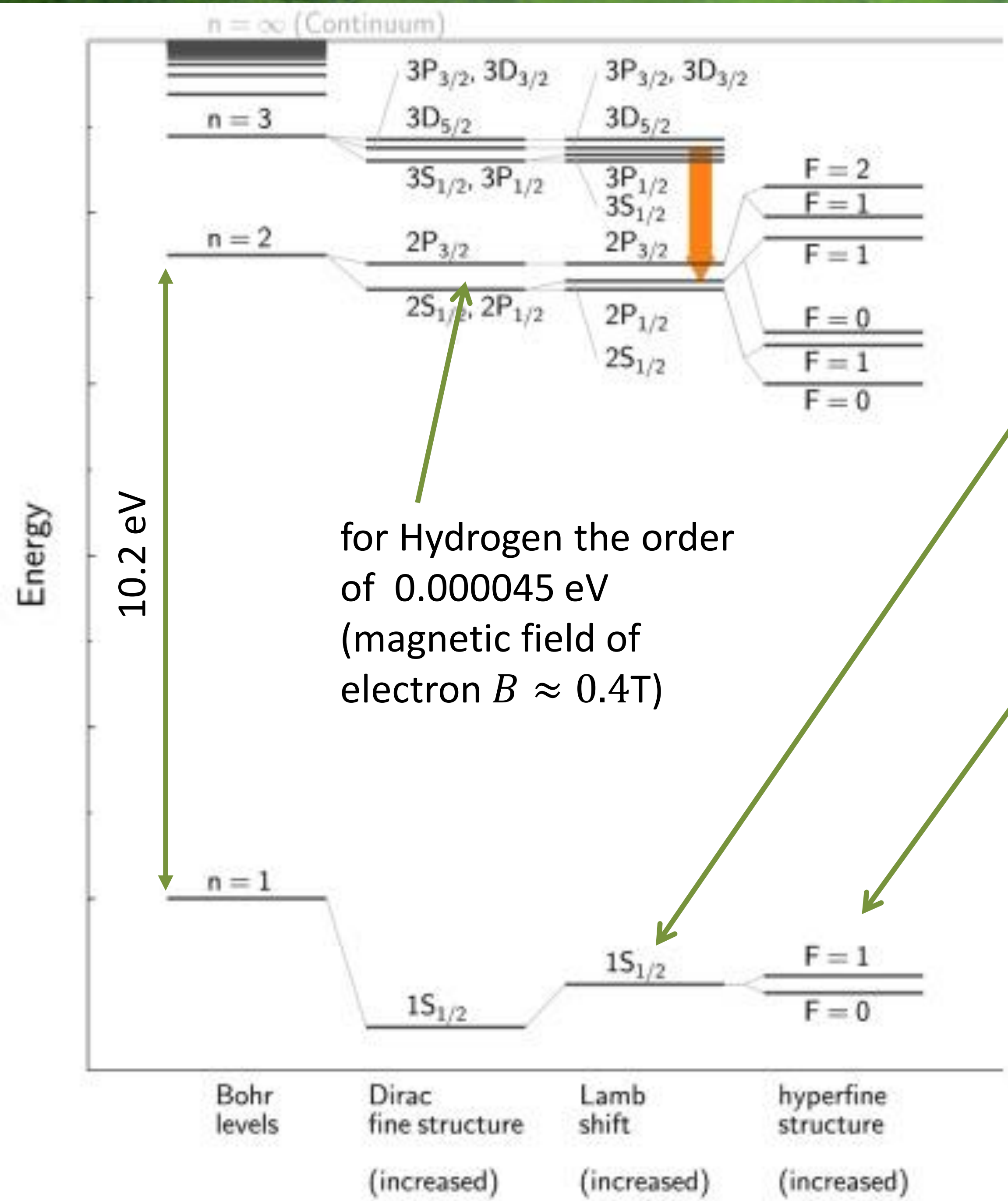
$2S_{1/2}$ and $2P_{1/2}$



QED – Quantum ElectroDynamics – Lamb shift due to the interaction of the atom with virtual photons emitted and absorbed by it. In quantum electrodynamics the electromagnetic field is quantized and therefore its lowest state cannot be zero ($E_{min} = \frac{\hbar\omega}{2}$), which perturbs Coulomb potential.



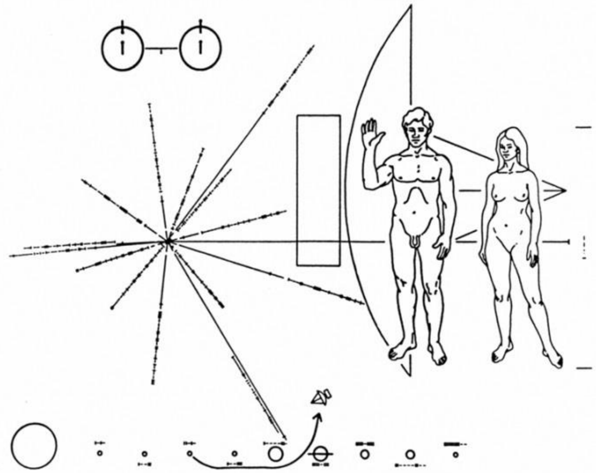
http://backreaction.blogspot.com/2007/12/hydrogen-spectrum-and-its-fine.html



for Hydrogen the order of 0.000045 eV (magnetic field of electron $B \approx 0.4\mathrm{T}$)

Lamb shift – (Willis Lamb) QED
size of the proton!
(hydrogen vs muonic hydrogen)
[about 1 GHz]

Hyperfine interaction: interaction with nuclear moment
[21 cm (1420 MHz) for atomic H]



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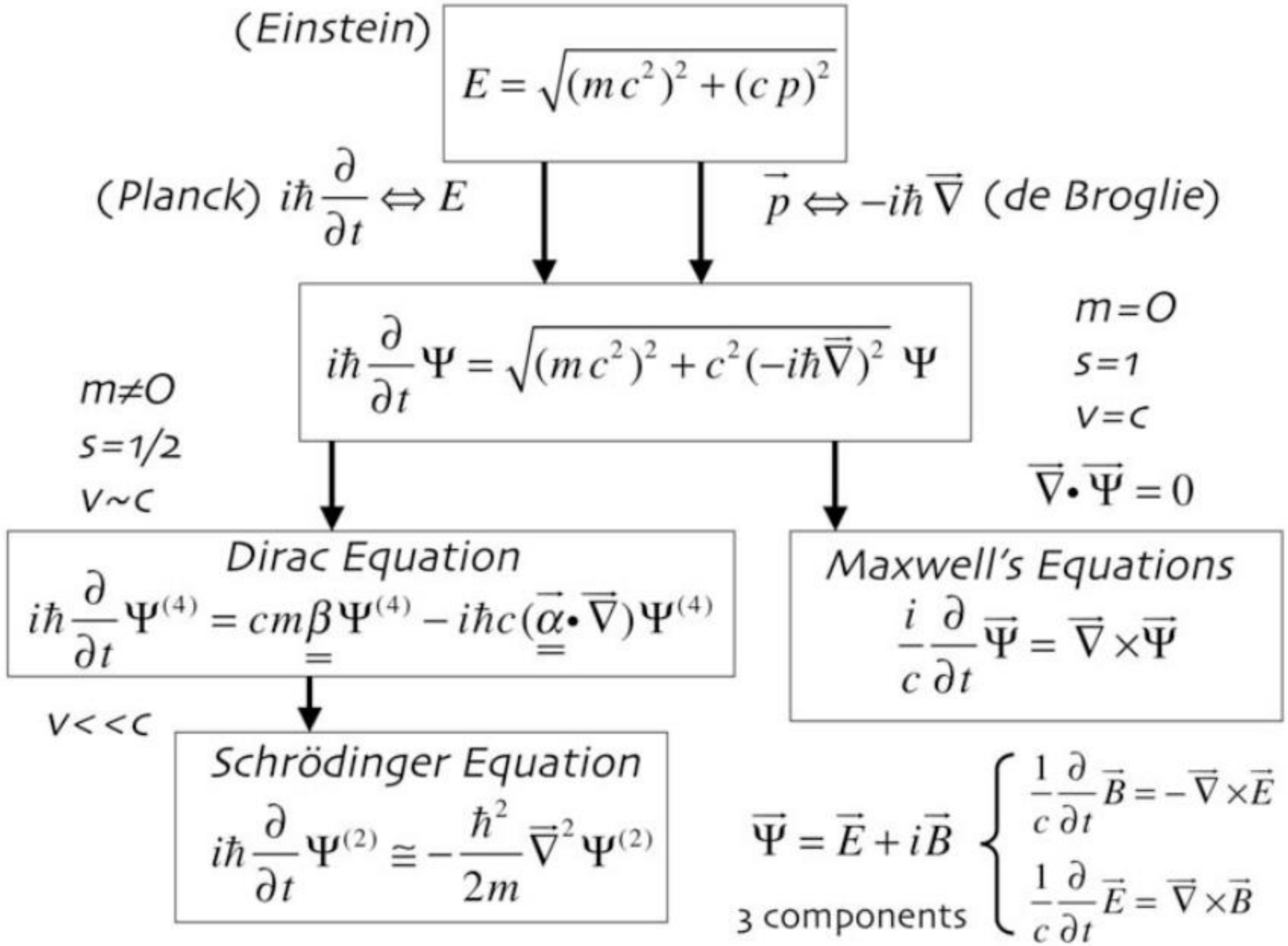

Fig.1 Flow chart for derivations of electron and photon wave equations, m = rest mass, s = spin, v = velocity.

The Maxwell wave function of the photon M. G. Raymer and Brian J. Smith, SPIE conf. Optics and Photonics 2005