Plan of lectures

- 1 15.04.2015 Preliminary Discussion / Introduction

- 2 22.04.2015 Experiments (discovery of the positron, formation of antihydrogen, ...)
- 3 29.04.2015 Experiments (Lamb shift, hyperfine structure, quasimolecules and MO spectra)
- 4 06.05.2015 Theory (from Schrödinger to Dirac equation, solutions with negative energy)
- 5 13.05.2015 Theory (bound-state solutions of Dirac equation, quantum numbers)

- 6 20.05.2015 Theory (matrix elements and their evaluation, radiative decay and absorption)
- 7 27.05.2015 Experiment (photoionization, radiative recombination, ATI, HHG...)

- 8 03.06.2015 Theory (single and multiple scattering, energy loss mechanisms, channeling regime)
- 9 10.06.2015 Experiment (Kamiokande, cancer therapy, ….)

- 10 17.06.2015 Experiment (Auger decay, dielectronic recombination, double ionization)
- 11 24.06.2015 Theory (interelectronic interactions, extension of Dirac (and Schrödinger) theory for the description of many-electron systems, approximate methods)

- 12 01.07.2015 Theory (atomic-physics tests of the Standard Model, search for a new physics)
- 13 08.07.2015 Experiment (Atomic physics PNC experiments (Cs,...), heavy ion PV research)

From Schrödinger to Dirac equation

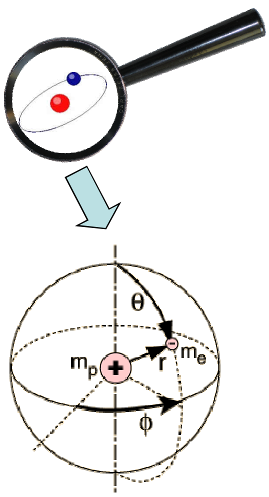
(Spin, relativity, general structure of Dirac equation)

06 May 2015

Plan of lecture

- Solutions of Schrödinger equation: Wavefunctions, energies, quantum numbers
- Particle's spin and relativity: Ideas which brought us to Dirac equation
- Dirac equation and free-particle solutions
- Negative-energy solutions of Dirac equation: Concept of antiparticles

Schrödinger equation for hydrogen atom



From www.hyperphysics.phy-astr.gsu.edu

- 3D Schrödinger equation (time-independent):

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r})+V(\mathbf{r})\psi(\mathbf{r})=E\psi(\mathbf{r})$$

- Where Coulomb potential is:

$$V(\mathbf{r})=-\frac{Ze^2}{|\mathbf{r}|}$$

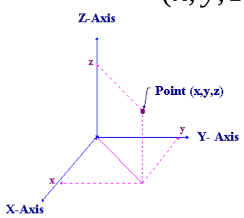
- Electron is bound to nucleus by the central force. It depends only on the radial distance between an electron and nucleus!

✓ It is natural to solve Schrödinger equation for central force in spherical coordinates!

Cartesian vs. spherical coordinates
(just a reminder)

Cartesian coordinates

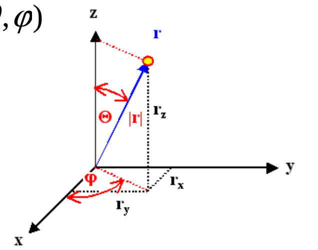
(x, y, z)



$$x = r\sin\theta\cos\varphi$$
$$y = r\sin\theta\sin\varphi$$
$$z = r\cos\theta$$

Spherical coordinates

(r, θ, φ)



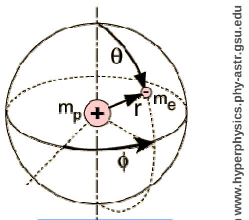
$$r = \sqrt{x^2 + y^2 + z^2}$$
$$\theta = \arccos\left(\frac{z}{\sqrt{x^2 + y^2 + z^2}}\right)$$
$$\varphi = \arctan\left(\frac{y}{x}\right)$$

06 May 2015

Schrödinger equation for hydrogen atom

- **It is natural to solve Schrödinger equation for central force in spherical coordinates!**

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r}) + V(\mathbf{r})\psi(\mathbf{r}) = E\psi(\mathbf{r})$$



$\mathbf{r} = (r, \theta, \varphi)$

- **Potential term:** $V(\mathbf{r}) = -\frac{Ze^2}{|\mathbf{r}|} = -\frac{Ze^2}{r}$

- **Laplace operator:** $\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}$

We can re-write Laplace operator as:

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{1}{r^2\hbar^2}\left[-\hbar^2\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right)\right]$$

Operator $\hat{\boldsymbol{L}}^2$ (depends only on θ and ϕ)

06 May 2015

Problem 4.1 (Angular momentum operator)

Prove that Cartesian components of the angular momentum operator:

$$\hat{\boldsymbol{L}} = \hat{\boldsymbol{r}} \times \hat{\boldsymbol{p}} = -i\hbar(\boldsymbol{r} \times \nabla)$$

read as:

$$\hat{L}_x = i\hbar\left(\sin\varphi\frac{\partial}{\partial\theta} + \cot\theta\cos\varphi\frac{\partial}{\partial\varphi}\right), \quad \hat{L}_y = i\hbar\left(-\cos\varphi\frac{\partial}{\partial\theta} + \cot\theta\sin\varphi\frac{\partial}{\partial\varphi}\right)$$

$$\hat{L}_z = -i\hbar\frac{\partial}{\partial\varphi}$$

and find $\hat{\boldsymbol{L}}^2 = L_x^2 + L_y^2 + L_z^2$

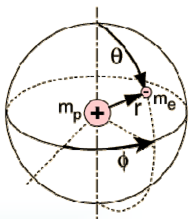
Schrödinger equation for hydrogen atom

- **In spherical coordinates Schrödinger equation reads:**

$$\left(-\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{\hat{\boldsymbol{L}}^2}{2mr^2} - \frac{Ze^2}{r}\right)\psi(\boldsymbol{r}) = E\psi(\boldsymbol{r})$$

r-dependence   *r*-dependence

(θ,ϕ) – dependence



$\boldsymbol{r} = (r,\theta,\varphi)$

From www.hyperphysics.phy-astr.gsu.edu

Such a decomposition of Hamiltonian operator gives us a hint to search for similar angle-radial decompositions of a wavefunction!

- **Moreover, L^2 and L_z commute with Hamiltonian (and with each other):**

$$[\hat{\boldsymbol{L}}^2, \hat{H}] = 0, \; [\hat{L}_z, \hat{H}] = 0$$

Eigenfunctions of Hamiltonian operators are at the same time eigenfunctions of operators L^2 and L_z.

Problem 4.2 (Commutation relations)

Prove that:

$$[\hat{\boldsymbol{L}}^2, \hat{H}] = 0, \ [\hat{L}_z, \hat{H}] = 0$$

and

$$[\hat{L}_x, \hat{L}_y] = i\hbar L_z, [\hat{L}_y, \hat{L}_z] = i\hbar L_x, [\hat{L}_z, \hat{L}_x] = i\hbar L_y$$

Just a reminder: $[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$

Schrödinger equation for hydrogen atom

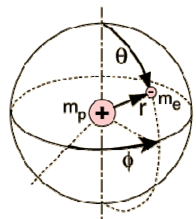
- **In spherical coordinates Schrödinger equation reads:**

$$\left(-\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{\hat{\boldsymbol{L}}^2}{2mr^2} - \frac{Ze^2}{r}\right)\psi(\boldsymbol{r}) = E\psi(\boldsymbol{r})$$

r-dependence

r-dependence

(θ,ϕ) – dependence



$\boldsymbol{r} = (r, \theta, \varphi)$

From www.hyperphysics.phy-astr.gsu.edu

- **We may thus look for solutions of the Schrödinger equation which are simultaneously eigenfunctions of the operators H, L^2 (and L_z):**

$$\psi(\boldsymbol{r}) = \psi(r, \theta, \varphi) = R_{nl}(r) Y_{lm_l}(\theta, \varphi)$$

Radial wavefunction

Angular part (spherical harmonics)

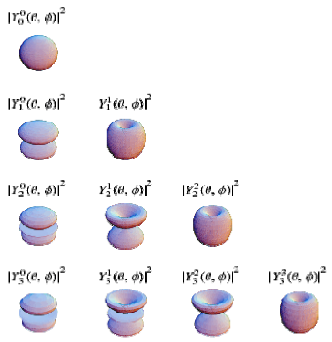
Spherical harmonics are the eigenfunctions of the operators L^2 and L_z .

Spherical harmonics
(just a reminder)

- Spherical harmonics are the eigenfunctions of the operators L^2 and L_z :

$$\hat{L}^2 Y_{lm}(\theta,\varphi) = l(l+1)\hbar^2 Y_{lm}(\theta,\varphi)$$

$$\hat{L}_z Y_{lm}(\theta,\varphi) = m\hbar\, Y_{lm}(\theta,\varphi)$$



From http://mathworld.wolfram.com/

- Analytic expressions for the spherical harmonics are well known:

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

$$Y_{10}(\theta,\varphi) = \sqrt{\frac{3}{4\pi}}\cos\theta\,, \quad Y_{1\pm1}(\theta,\varphi) = \mp\sqrt{\frac{3}{8\pi}}\sin\theta\, e^{\pm i\varphi}$$

...

See, for example, in Mathematica:

SphericalHarmonicY

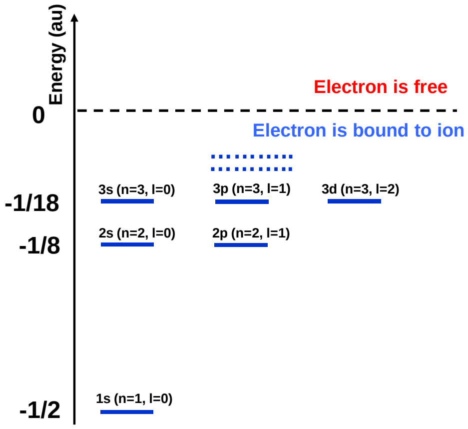
Schrödinger equation: Quantum numbers

- One needs three quantum numbers to define the state of hydrogen (hudrogen-like) atom:
  - n = 1, 2, 3... (principal)
  - l = 0, ... n-1 (orbital)
  - m_l = -l, ... +l (magnetic)
- The energy depends only on the principal quantum number:

$$E_n = -\frac{\varepsilon_0 Z^2}{2n^2}$$

- i.e. in nonrelativistic theory the states are degenerate (l, m)!

$$\psi(\mathbf{r}) = \psi(r,\theta,\varphi) = R_{nl}(r) Y_{lm_l}(\theta,\varphi)$$



Schrödinger equation: Quantum numbers

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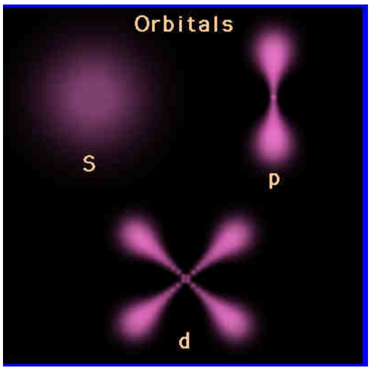
$$\psi(\mathbf{r}) = \psi(r,\theta,\varphi) = R_{nl}(r)Y_{lm_l}(\theta,\varphi)$$



- **Let us consider electron density distribution:**

$$\rho(\mathbf{r}) = |\psi(\mathbf{r})|^2 = |R_{nl}(r)|^2 |Y_{lm_l}(\theta,\varphi)|^2$$

- **By fixing *r* :**

$$\rho(r = const, \theta, \varphi) \sim |Y_{lm_l}(\theta,\varphi)|^2$$

By choosing *l* and *m* we define the shape of electron cloud!

✓ Please, remember: states with different *l* and *m* (but the same *n*) have the same energies!

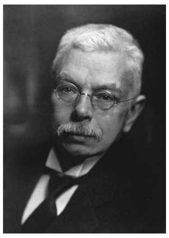
06 May 2015

Plan of lecture

- **Solutions of Schrödinger equation: Wavefunctions, energies, quantum numbers**
- **Particle's spin and relativity: Ideas which brought us to Dirac equation**
- **Dirac equation and free-particle solutions**
- **Negative-energy solutions of Dirac equation: Concept of antiparticles**

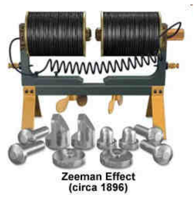
06 May 2015

Breaking of symmetry: „Normal“ Zeeman effect

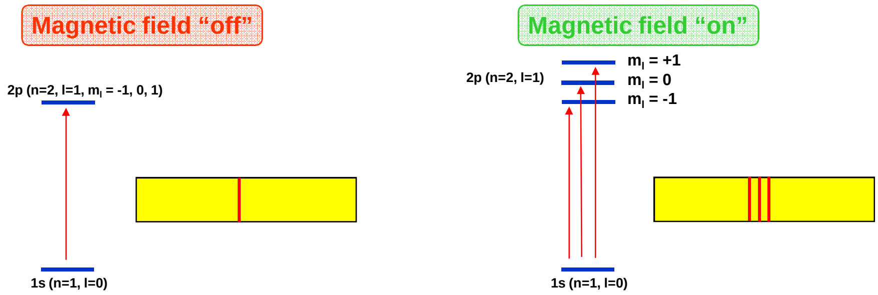


Pieter Zeeman
1902 Nobel prize

- **Zeeman effect: splitting of a spectral line into several components in the presence of a static magnetic field.**

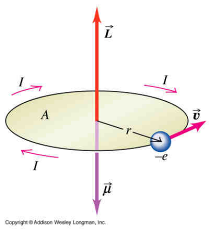


Picture from: www.magnet.fsu.edu



This effect was understood within the Quantum Mechanics.

Electron magnetic dipole moment



In classical electrodynamics:

$$|\mu| = \boldsymbol{I}\cdot\boldsymbol{A}$$

current — vector area of the current loop

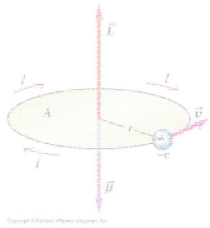
$$|\mu| = \boldsymbol{I}\cdot\boldsymbol{A} = \frac{q}{T}\pi r^2 = \frac{qv}{2\pi r}\pi r^2 = \frac{q}{2m}mrv = \frac{q}{2m}L$$

In quantum mechanics, for electron: q=-e

$$\hat{\boldsymbol{\mu}}_l = -\mu_0 \hat{\boldsymbol{L}}/\hbar, \qquad \mu_0 = \frac{e\hbar}{2m_e}$$

Bohr magneton

Electron magnetic dipole moment



In classical electrodynamics:

$|\mu| = I \cdot A$

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$$|\mu| = I \cdot A = \frac{q}{T}\pi r^2 = \frac{qv}{2\pi r}\pi r^2 = \frac{q}{2m} mrv = \frac{q}{2m} L$$

In quantum mechanics, for electron: q=-e

$$\hat{\mu}_l = -\mu_0 \hat{L}/\hbar, \qquad \mu_0 = \frac{e\hbar}{2m_e}$$

Bohr magneton

Interaction with external magnetic field

$$\hat{H}_{\text{int}} = -\hat{\boldsymbol{\mu}}_l \cdot \boldsymbol{B}$$

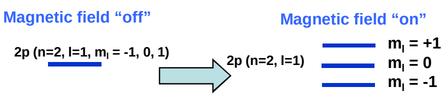
By choosing *z*-axis along *B*:

$$\hat{H}_{\text{int}} = -\hat{\mu}_{l,z} B = \mu_0 B L_z / \hbar$$

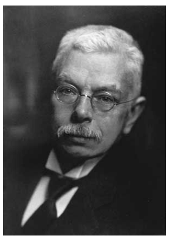
⇩

Energy shift (1st order perturbation):

$$\Delta E_{m_l} = \left\langle \psi_{nlm_l} \middle| \hat{H}_{\text{int}} \middle| \psi_{nlm_l} \right\rangle = \mu_0 B m_l$$

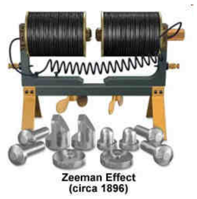


„Normal“ Zeeman effect

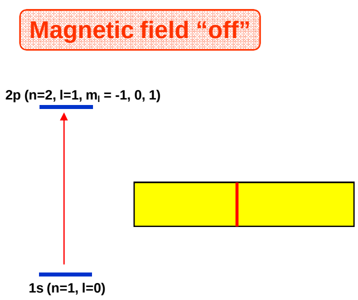


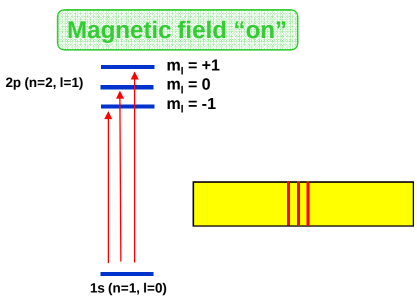
Pieter Zeeman
1902 Nobel prize

- **Zeeman effect: splitting of a spectral line into several components in the presence of a static magnetic field.**



Picture from: www.magnet.fsu.edu





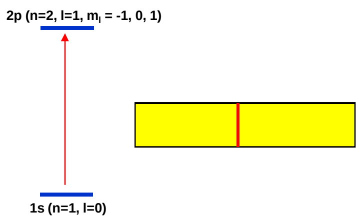
So far everything looks clear...

„Anamalous“ Zeeman effect

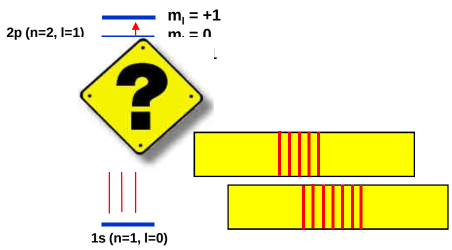
Alfred Lande

- Zeeman effect: splitting of a spectral line into several components in the presence of a static magnetic field.
- But… a lot of experimental data have been obtained which can not be explained within the “Schrödinger picture”.

Magnetic field “off”



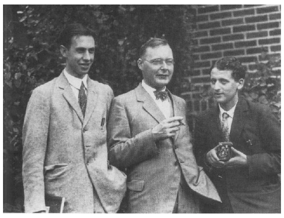
Magnetic field “on”



From Zeeman effect to concept of spin

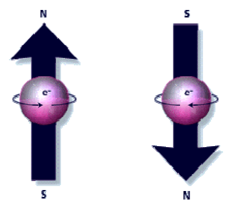
Wolfgang Pauli

“How can one avoid despondency if one thinks of the anomalous Zeeman effect?” (1925)



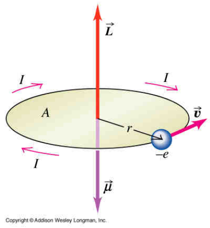
Uhlenbeck Goudsmit

- Pauli introduced the idea of a new quantum degree of freedom (or quantum number) for electron with two possible values.
- Ralph Kronig, George Uhlenbeck and Samuel Goudsmit: every electron carries intrinsic angular momentum called spin.
- Magnetic moment can be associated with spin and is “responsible” for the interaction with magnetic field.



Electron spin

Orbital magnetic moment



In classical electrodynamics:

$$|\mu| = \boldsymbol{I} \cdot \boldsymbol{A}$$

current — vector area of the current loop

$$|\mu| = \boldsymbol{I} \cdot \boldsymbol{A} = \frac{q}{T}\pi r^2 = \frac{qv}{2\pi r}\pi r^2 = \frac{q}{2m} mrv = \frac{q}{2m} L$$

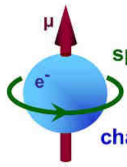
In quantum mechanics, for electron: q=-e

$$\hat{\boldsymbol{\mu}}_l = -\mu_0 \hat{\mathbf{L}} / \hbar, \qquad \mu_0 = \frac{e\hbar}{2m_e}$$

Bohr magneton

Spin magnetic moment

classical picture



$$\hat{\boldsymbol{\mu}}_s = -g_s \mu_0 \hat{\mathbf{S}} / \hbar$$

Gyromagnetic rato

06 May 2015

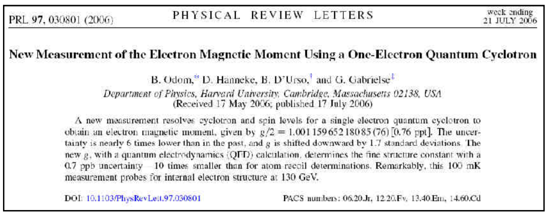
Total magnetic moment

- **Total magnetic moment is given finally by:**

$$\hat{\boldsymbol{\mu}} = -\mu_0 (\hat{\boldsymbol{L}} + g\hat{\mathbf{S}}) / \hbar$$

- **And it interacts with external magnetic field as:** $H = -\hat{\boldsymbol{\mu}} \cdot \boldsymbol{B}$

  - **Measurements of the total magnetic momentum is of fundamental importance for analysis of gyromagnetic ratio:**



PRL 97, 030801 (2006) PHYSICAL REVIEW LETTERS week ending 21 JULY 2006

New Measurement of the Electron Magnetic Moment Using a One-Electron Quantum Cyclotron

B. Odom,* D. Hanneke, B. D'Urso,† and G. Gabrielse‡

Department of Physics, Harvard University, Cambridge, Massachusetts 02138, USA

(Received 17 May 2006; published 17 July 2006)

A new measurement resolves cyclotron and spin levels for a single electron quantum cyclotron to obtain an electron magnetic moment, given by $g/2 = 1.001\,159\,652\,180\,85\,(76)$ [0.76 ppt]. The uncertainty is nearly 6 times lower than in the past, and g is shifted downward by 1.7 standard deviations. The new g, with a quantum electrodynamics (QED) calculation, determines the fine structure constant with a 0.7 ppb uncertainty—10 times smaller than for atom recoil determinations. Remarkably, this 100 mK measurement probes for internal electron structure at 130 GeV.

DOI: 10.1103/PhysRevLett.97.030801 PACS numbers: 06.20.Jr, 12.20.Fv, 13.40.Em, 14.60.Cd

g/2=1 (Dirac theory)

g/2=1.001 159 180 ...

06 May 2015

Total magnetic moment

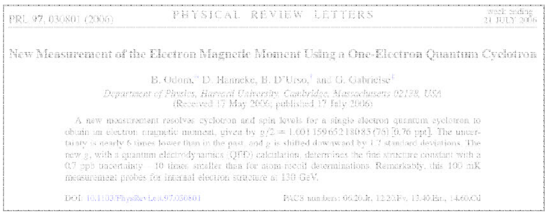
- **Total magnetic moment is given finally by:**

$$\hat{\boldsymbol{\mu}} = -\mu_0(\hat{\boldsymbol{L}} + g\hat{\boldsymbol{S}})/\hbar$$

- **And it interacts with external magnetic field as:** $H = -\hat{\boldsymbol{\mu}} \cdot \boldsymbol{B}$

But what is actually spin operator ***S***?

...agnetic momentum is of fundamental importance for analysis of gyromagnetic ratio: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DOI: 10.1103/PhysRevLett.97.030801 PACS numbers: 06.20.Jr, 12.20.Fv, 13.40.Em, 14.60.Cd

g/2=1 (Dirac theory)

⇩

g/2=1.001 159 180 ...

Orbital and spin angular momentum operators

Orbital magnetic moment

- **We have discussed already the properties of angular momentum operator *L*:**

$$\hat{\boldsymbol{L}}^2 Y_{lm}(\theta,\varphi) = l(l+1)\hbar^2 Y_{lm}(\theta,\varphi)$$

$$\hat{L}_z Y_{lm}(\theta,\varphi) = m\hbar\, Y_{lm}(\theta,\varphi)$$

$$m = -l,....+l$$

- **And its commutation relations:**

$$[\hat{L}_x,\hat{L}_y] = i\hbar L_z, [\hat{L}_y,\hat{L}_z] = i\hbar L_x,$$

$$[\hat{L}_z,\hat{L}_x] = i\hbar L_y$$

We shall assume that all angular momentum operators satisfy these commutation relations!

Orbital and spin angular momentum operators

Orbital magnetic moment

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$$m = -l,....+l$$

- **And its commutation relations:**

$$[\hat{L}_x,\hat{L}_y] = i\hbar\hat{L}_z, [\hat{L}_y,\hat{L}_z] = i\hbar\hat{L}_x,$$
$$[\hat{L}_z,\hat{L}_x] = i\hbar\hat{L}_y$$

Spin magnetic moment

- **We shall expect the following properties of spin angular momentum operator *S*:**

$$\hat{S}^2 \chi_{sm_s} = s(s+1)\hbar^2 \chi_{sm_s}$$

$$\hat{S}_z \chi_{sm_s} = m_s\hbar\, \chi_{sm_s}$$

$$m_s = -s,....+s$$

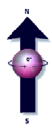
- **And its commutation relations:**

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

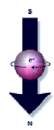
Spin operator and wavefunctions

- **Let us restrict ourselves to the case of electron (two possible spin states).**
- **Spin-1/2 basis wavefunctions:** $| s\, m_s >= \chi_{sm_s}$

$$| s\, m_s >=| 1/2\ +1/2 >= \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$



$$| s\, m_s >=| 1/2\ -1/2 >= \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$



- **Spin-1/2 operators are the 2x2 matrices:**

$$\hat{S}_x = \frac{\hbar}{2}\hat{\sigma}_x\ ,\ \hat{S}_y = \frac{\hbar}{2}\hat{\sigma}_y\ ,\ \hat{S}_z = \frac{\hbar}{2}\hat{\sigma}_z$$

- **Where Pauli matrices are:**

$$\hat{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \hat{\sigma}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \hat{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

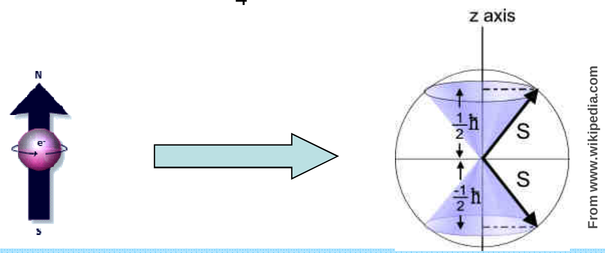
Spin operator and wavefunctions

- **What does it mean that electron is in the state with spin projection +1/2?**
- **Let us calculate matrix elements (mean values of spin projections):**

$$< s_x > = < \chi_{1/2} | \hat{s}_x | \chi_{1/2} > = 0 \,, < s_y > = < \chi_{1/2} | \hat{s}_y | \chi_{1/2} > = 0 \,, < s_z > = < \chi_{1/2} | \hat{s}_z | \chi_{1/2} > = \frac{\hbar}{2}$$

- **Can we now say that "electron spin is along *z* axis"?**
- **Let us calculate the variance:**

$$< \chi_{1/2} | (\hat{s}_x - < s_x >)^2 | \chi_{1/2} > = \frac{\hbar^2}{4} \,, \quad < \chi_{1/2} | (\hat{s}_y - < s_y >)^2 | \chi_{1/2} > = \frac{\hbar^2}{4}$$

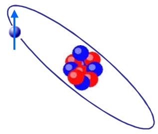


Problem 4.3

Find the state vector for the electron with spin projection $\pm 1/2$ on the x-axis.

Nonrelativistic theory with spin included

(... the simplest approach)



- **We may include electron spin into consideration:**

$$\psi_{nlm_l}(\mathbf{r}) = \psi_{nlm_l}(r,\theta,\varphi) = R_{nl}(r)Y_{lm_l}(\theta,\varphi)$$

$$\Downarrow$$

$$\psi_{nlm_l sm_s}(\mathbf{r}) = \psi_{nlm_l sm_s}(r,\theta,\varphi,\sigma) = R_{nl}(r)Y_{lm_l}(\theta,\varphi)\,\chi_{sm_s}(\sigma)$$

- **These wavefunctions are spinors:** $\psi_{nlm_l sm_s}(\mathbf{r}) \Rightarrow \begin{pmatrix} f(\mathbf{r}) \\ g(\mathbf{r}) \end{pmatrix}$

- This (rather simple) approach can be used for the case studies where particles are slow enough so that the relativistic effects are negligible.
- We are still missing something.

Plan of lecture

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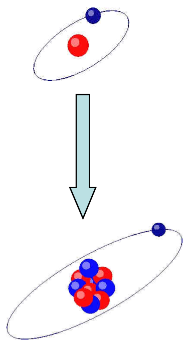
- **Particle's spin and relativity: Ideas which brought us to Dirac equation**
- **Dirac equation and free-particle solutions**
- **Negative-energy solutions of Dirac equation: Concept of antiparticles**

Hydrogen-like ions: Relativistic effects



- **We want to study very heavy (*Z* >> 1) ionic systems!!!**
- **From the simple model one can “estimate” the electron “velocity” in the ground state:**

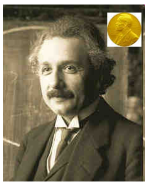
$$v = (\alpha Z)\, c$$

Speed of light

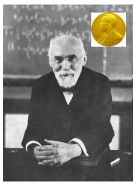
- **For hydrogen (Z=1):** $\alpha Z \approx 1/137 \approx 0.00729$
- **For hydrogen-like Uranium (Z=92):** $\alpha Z \approx 0.67$

Electron is moving at velocities very close to the speed of light!
The relativistic effects have to be taken into account!

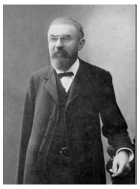
Special relativity



Albert Einstein

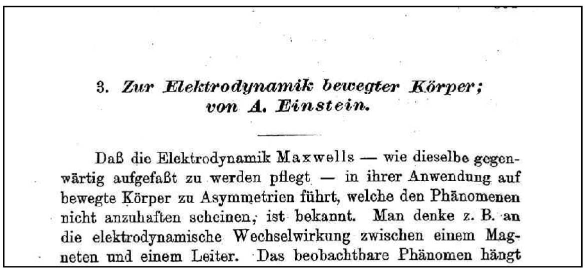


Hendrik Lorentz



Henri Poincaré

- Special theory of relativity is the theory of measurement in inertial frames of reference.
- It generalizes Galileo’s principle of relativity.

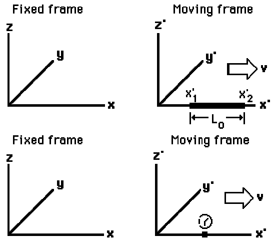


3. *Zur Elektrodynamik bewegter Körper;*
von A. Einstein.

Daß die Elektrodynamik Maxwells — wie dieselbe gegenwärtig aufgefaßt zu werden pflegt — in ihrer Anwendung auf bewegte Körper zu Asymmetrien führt, welche den Phänomenen nicht anzuhaften scheinen, ist bekannt. Man denke z. B. an die elektrodynamische Wechselwirkung zwischen einem Magneten und einem Leiter. Das beobachtbare Phänomen hängt

Relativistic kinematics

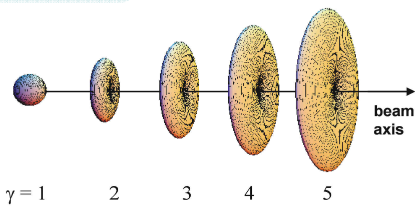
(just a reminder)



- **By approaching speed of light, we find:**
  - **Length contraction** $L = L_0 / \gamma$
  - **Time dilation** $T = T_0\, \gamma$
  - **The increase in effective mass** $m = m_0\, \gamma$
  - **The change in relativistic momentum** $p = m_0 v\, \gamma$

$$\gamma = \frac{1}{\sqrt{1-(v/c)^2}}$$

- **The electro-magnetic field is also transformed!**
  - **Example: Lienard-Wiechert potential (transformation of the Coulomb potential)**



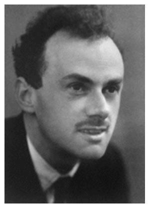
Plan of lecture

- **Solutions of Schrödinger equation: Wavefunctions, energies, quantum numbers**
- **Particle's spin and relativity: Ideas which brought us to Dirac equation**
- **Dirac equation and free-particle solutions**
- **Negative-energy solutions of Dirac equation: Concept of antiparticles**

Dirac equation

- A quantum treatment of the electron motion in heavy ions requires the use of the Dirac equation which is the relativistic wave equation for a ½-spin particles.
- Time-dependent Dirac equation reads:

Paul Dirac
1933 Nobel prize



$$i\hbar\frac{\partial\psi(\mathbf{r},t)}{\partial t}=\hat{H}\psi(\mathbf{r},t)$$

Which looks like Schrödinger equation but ....
... what is the Dirac Hamiltonian?

Let us consider Dirac Hamiltonian for the simplest case: free particle.

Dirac equation for free particle

- A quantum treatment of the electron motion in heavy ions requires the use of the Dirac equation which is the relativistic wave equation for a ½-spin particles.
- Time-dependent Dirac equation reads:

Paul Dirac
1933 Nobel prize

$$i\hbar\frac{\partial\psi(\mathbf{r},t)}{\partial t}=\left(-i\hbar c\boldsymbol{\alpha}\cdot\nabla+mc^2\alpha_0\right)\psi(\mathbf{r},t)$$

Kinetic term — Rest mass term

$$\boldsymbol{p}=-i\hbar\nabla$$

- Note: Dirac equation is the first-order differential equation (in contrast to Schrödinger one)!
- The important consequence: the Dirac equation is relativistically invariant!

Dirac equation: What is what here?

$$i\hbar\frac{\partial\psi(\mathbf{r},t)}{\partial t}=\left(-i\hbar c\boldsymbol{\alpha}\cdot\nabla+mc^2\alpha_0\right)\psi(\mathbf{r},t)$$

Kinetic term — Rest mass term

- 4x4 matrices are built up from Pauli matrices:

$$\boldsymbol{\alpha}=\begin{pmatrix}0 & \boldsymbol{\sigma}\\ \boldsymbol{\sigma} & 0\end{pmatrix}\qquad \alpha_0=\begin{pmatrix}\boldsymbol{I} & 0\\ 0 & -\boldsymbol{I}\end{pmatrix}$$

- Wavefunctions in the Dirac equation are four-spinors:

$$\psi(\mathbf{r})=\begin{pmatrix}\varphi_1(\mathbf{r})\\ \varphi_2(\mathbf{r})\\ \varphi_3(\mathbf{r})\\ \varphi_4(\mathbf{r})\end{pmatrix}\qquad \psi^+(\mathbf{r})=\left(\varphi^*{}_1(\mathbf{r})\quad \varphi^*{}_2(\mathbf{r})\quad \varphi^*{}_3(\mathbf{r})\quad \varphi^*{}_4(\mathbf{r})\right)$$

Can we find explicit form of Dirac wavefunctions?

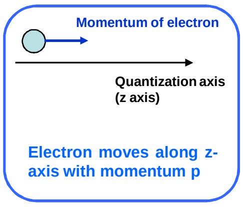
Dirac equation: Free-particle solution

- We may re-write Dirac equation in its time-independent form:

$$\left(-i\hbar c\boldsymbol{\alpha}\cdot\nabla+m_ec^2\alpha_0\right)\psi(\mathbf{r})=E\,\psi(\mathbf{r})$$

- We will look for plane wave solutions:

$$\psi_p(\mathbf{r})=w(p)\exp(ipz/\hbar)$$



- We obtain the system of equations (here written in matrix form):

$$\begin{bmatrix}m_ec^2 & 0 & pc & 0\\ 0 & m_ec^2 & 0 & -pc\\ pc & 0 & -m_ec^2 & 0\\ 0 & -pc & 0 & -m_ec^2\end{bmatrix}w=Ew$$

- … which is standard eigenvalue problem.

Task 4.3

Prove that plane wave solution for the Dirac equation of free particle:

$$\psi_p(\mathbf{r}) = w(p)\exp(ipz/\hbar)$$

leads to the system of equations:

$$\begin{bmatrix} m_ec^2 & 0 & pc & 0 \\ 0 & m_ec^2 & 0 & -pc \\ pc & 0 & -m_ec^2 & 0 \\ 0 & -pc & 0 & -m_ec^2 \end{bmatrix} w = Ew$$

Find solutions of this system of equations.

18 October 2010

Plane wave solution of Dirac equation

- **We obtain the system of equations (here written in matrix form):**

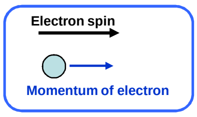
$$\begin{bmatrix} m_ec^2 & 0 & pc & 0 \\ 0 & m_ec^2 & 0 & -pc \\ pc & 0 & -m_ec^2 & 0 \\ 0 & -pc & 0 & -m_ec^2 \end{bmatrix} w = Ew$$

- **Two types of solutions can be obtained by solving this system (finding determinant of the matrix):**

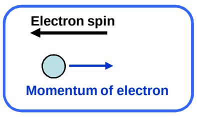
$$E_+(p) = \sqrt{(m_ec^2)^2 + (pc)^2} \qquad E_-(p) = -\sqrt{(m_ec^2)^2 + (pc)^2}$$

Solution with negative energy!

- **To each energy corresponds two wavefunctions. For example, positive-energy solutions are:**



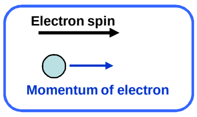
$$w_{+1/2} = N\begin{pmatrix} 1 \\ 0 \\ \dfrac{cp}{E_+ + m_ec^2} \\ 0 \end{pmatrix} \qquad w_{-1/2} = N\begin{pmatrix} 0 \\ 1 \\ 0 \\ \dfrac{-cp}{E_+ + m_ec^2} \end{pmatrix}$$



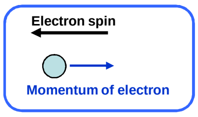
06 May 2015

Plane wave solution of Dirac equation

- **To each energy corresponds two wavefunctions. For example, positive-energy solutions are:**



$$w_{+1/2} = N\begin{pmatrix} 1 \\ 0 \\ \dfrac{cp}{E_+ + m_e c^2} \\ 0 \end{pmatrix} \qquad w_{-1/2} = N\begin{pmatrix} 0 \\ 1 \\ 0 \\ \dfrac{-cp}{E_+ + m_e c^2} \end{pmatrix}$$



- **By making use the properties of the Pauli matrices and the spin wavefunctions, we finally obtain:**

$$w_{m_s} = N\begin{pmatrix} \chi_{sm_s} \\ \dfrac{cp\sigma_z}{E_+ + m_e c^2}\chi_{sm_s} \end{pmatrix}$$

Free-electron wavefunction (plane wave solution) is written now as bispinor.

„Problem“ of negative energy solutions

- **We obtain the system of equations (here written in matrix form):**

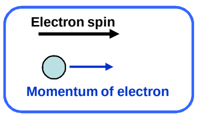
$$\begin{bmatrix} m_e c^2 & 0 & pc & 0 \\ 0 & m_e c^2 & 0 & -pc \\ pc & 0 & -m_e c^2 & 0 \\ 0 & -pc & 0 & -m_e c^2 \end{bmatrix} w = Ew$$

- **Two types of solutions can be obtained by solving this syste determinant of the matrix):**

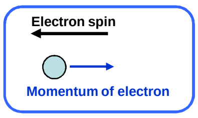
$$E_+(p) = \sqrt{(m_e c^2)^2 + (pc)^2} \qquad E_-(p) = -\sqrt{(m_e c^2)^2 + (pc)^2}$$

Solution with negative energy!

- **To each energy corresponds two wavefunctions. For example, positive-energy solutions are:**



$$w_{+1/2} = N\begin{pmatrix} 1 \\ 0 \\ \dfrac{cp}{E_+ + m_e c^2} \\ 0 \end{pmatrix} \qquad w_{-1/2} = N\begin{pmatrix} 0 \\ 1 \\ 0 \\ \dfrac{-cp}{E_+ + m_e c^2} \end{pmatrix}$$



Plan of lecture

- Solutions of Schrödinger equation: Wavefunctions, energies, quantum numbers
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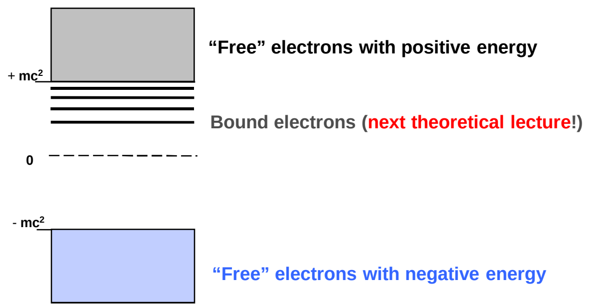
06 May 2015

Energy spectrum of the Dirac particle

- **For the free particles we found:** $E_{\pm}(p) = \pm\sqrt{(m_e c^2)^2 + (pc)^2}$
  - **Energy of positive energy particles:** $E_{+}(p) > m_e c^2$
  - **Energy of negative energy particles:** $E_{-}(p) < -m_e c^2$

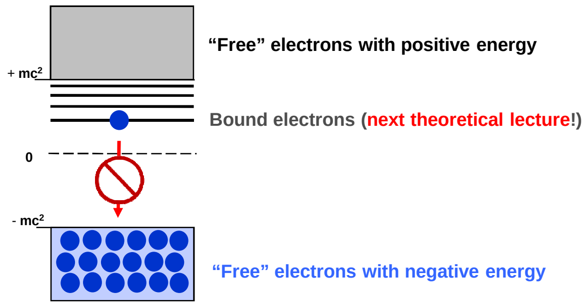


Where is the problem here?

06 May 2015

Concept of the Dirac sea

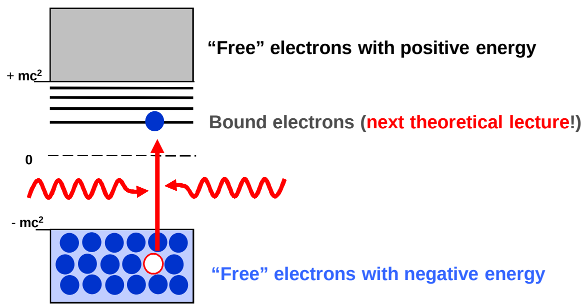
- In 1930 Paul Dirac have proposed a theoretical model of the vacuum as an infinite sea of particles possessing negative energy.



- Since all the states in Dirac sea are occupied “our” electron can not go down from the domain of positive energies. (Pauli principle.)

Particles and antiparticles

- Situation might exist in which all the negative-energy states are occupied except one. This "hole" in the sea of negative-energy electrons would respond to electric fields as though it were a positively-charged particle.



- How to understand the hole?

Antiparticles

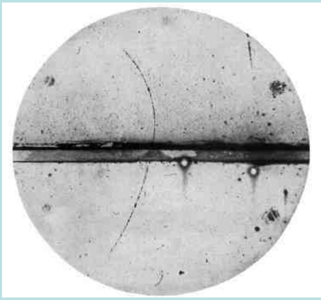
- How can one understand “holes” in the Dirac sea?

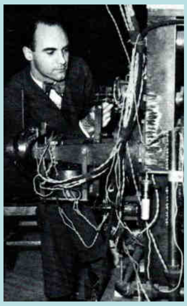
1931:2 QUANTISED SINGULARITIES IN THE ELECTROMAGNETIC FIELD 505

60

+ mc^2

- mc^2





“New kind of particle, unknown to experimental physics” was discovered just in 1932 by Carl David Anderson.

06 May 2015

Plan of lectures

- 1 15.04.2015 Preliminary Discussion / Introduction
- 2 22.04.2015 Experiments (discovery of the positron, formation of antihydrogen, ...)
- 3 29.04.2015 Experiments (Lamb shift, hyperfine structure, quasimolecules and MO spectra)
- 4 06.05.2015 Theory (from Schrödinger to Dirac equation, solutions with negative energy)
- 5 13.05.2015 Theory (bound-state solutions of Dirac equation, quantum numbers)
- 6 20.05.2015 Theory (matrix elements and their evaluation, radiative decay and absorption)
- 7 27.05.2015 Experiment (photoionization, radiative recombination, ATI, HHG...)
- 8 03.06.2015 Theory (single and multiple scattering, energy loss mechanisms, channeling regime)
- 9 10.06.2015 Experiment (Kamiokande, cancer therapy, ….)
- 10 17.06.2015 Experiment (Auger decay, dielectronic recombination, double ionization)
- 11 24.06.2015 Theory (interelectronic interactions, extension of Dirac (and Schrödinger) theory for the description of many-electron systems, approximate methods)
- 12 01.07.2015 Theory (atomic-physics tests of the Standard Model, search for a new physics)
- 13 08.07.2015 Experiment (Atomic physics PNC experiments (Cs,...), heavy ion PV research)