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)

Bound-state solutions of Dirac equation

(Spectroscopic notations and wavefunctions)

Plan of lecture

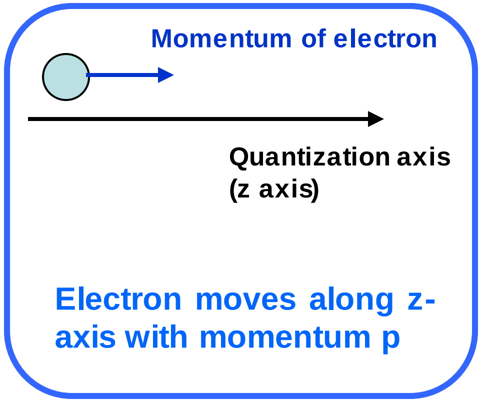
- Reminder from the last lecture: Free-particle solution
- Dirac’s spectroscopic notations
    - Integrals of motion
    - Parity of states
- Energy levels of the bound-state Dirac’s particle
- Structure of Dirac’s wavefunction
- Radial components of the Dirac’s wavefunction

Dirac equation: Free-particle solution

(reminder from the last lecture)

- **Dirac equation for the free particle in time-independent form:**

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



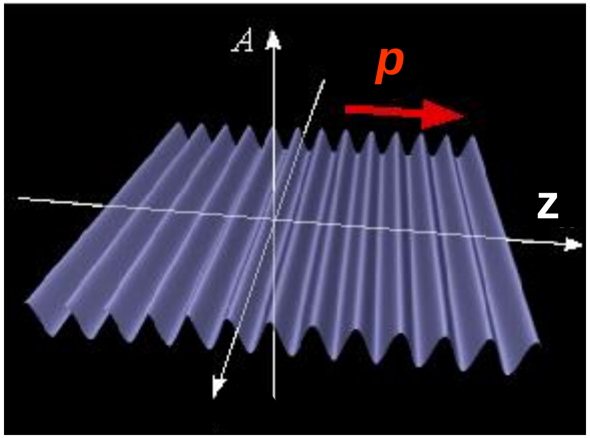
Momentum of electron

Quantization axis (z axis)

Electron moves along z-axis with momentum p

- **We have found the plane-wave solutions of this equation:**

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



Picture from: www.rpi.edu

- **Where *w(p)* were found as a solution of:**

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

Dirac equation: Free-particle solution

(reminder from the last lecture)

- **Dirac equation for the free particle in time-independent form:**

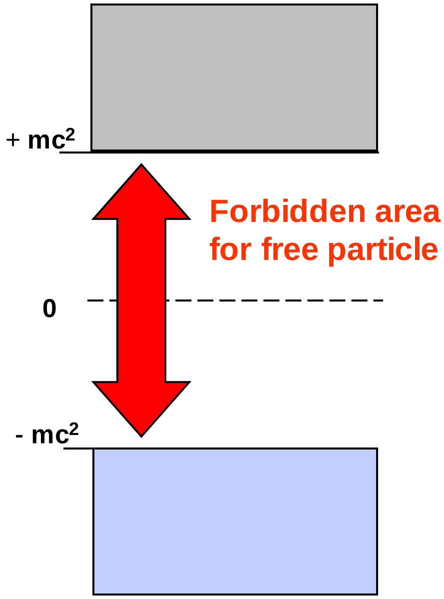
$$\left(-i\hbar c\boldsymbol{\alpha}\cdot\nabla + m_e c^2\alpha_0\right)\psi(\mathbf{r}) = E\psi(\mathbf{r})$$

- **Positive- and negative-energy solutions have been found:**

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

and

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



- **With the wavefunctions:**

$$w^+_{m_s} = N\begin{pmatrix} \chi_{sm_s} \\ \dfrac{cp\sigma_z}{E_+ + m_e c^2}\chi_{sm_s} \end{pmatrix} \quad \textbf{and} \quad w^-_{m_s} = N\begin{pmatrix} -\dfrac{cp\sigma_z}{\left|E_-\right| + m_e c^2}\chi_{sm_s} \\ \chi_{sm_s} \end{pmatrix}$$

Dirac equation: Free-particle solution

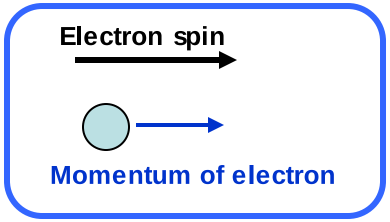
(reminder from the last lecture)

- **For each eigenvalue *E* there are two eigenfunctions which correspond to two different spin states of the particle:**

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

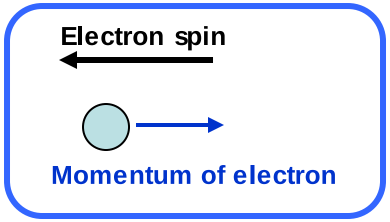
$$\chi_{1/2\ +1/2} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$\chi_{1/2\ -1/2} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$


Electron spin

Momentum of electron

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


Electron spin

Momentum of electron

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

Plan of lecture

- **Reminder from the last lecture: Free-particle solution**
- **Dirac's spectroscopic notations**
  - **Integrals of motion**
  - **Parity of states**
- **Energy levels of the bound-state Dirac's particle**
- **Structure of Dirac's wavefunction**
- **Radial components of the Dirac's wavefunction**

Dirac equation for particle in the potential

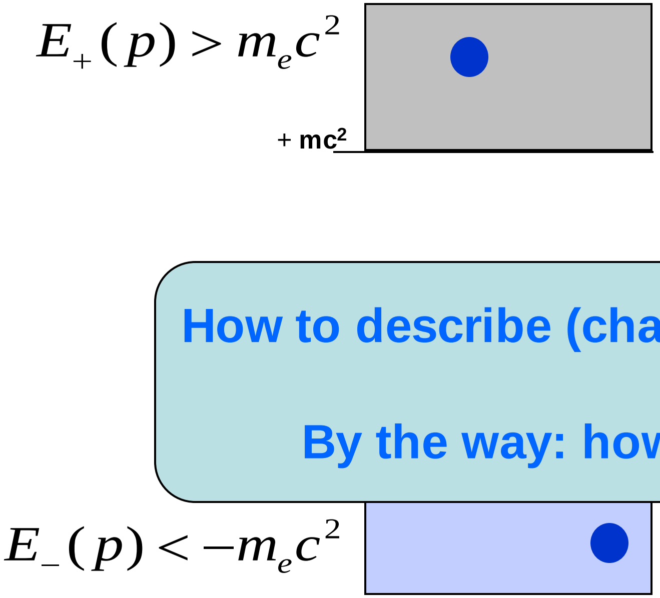
- **Stationary Dirac equation reads (let us add potential):**

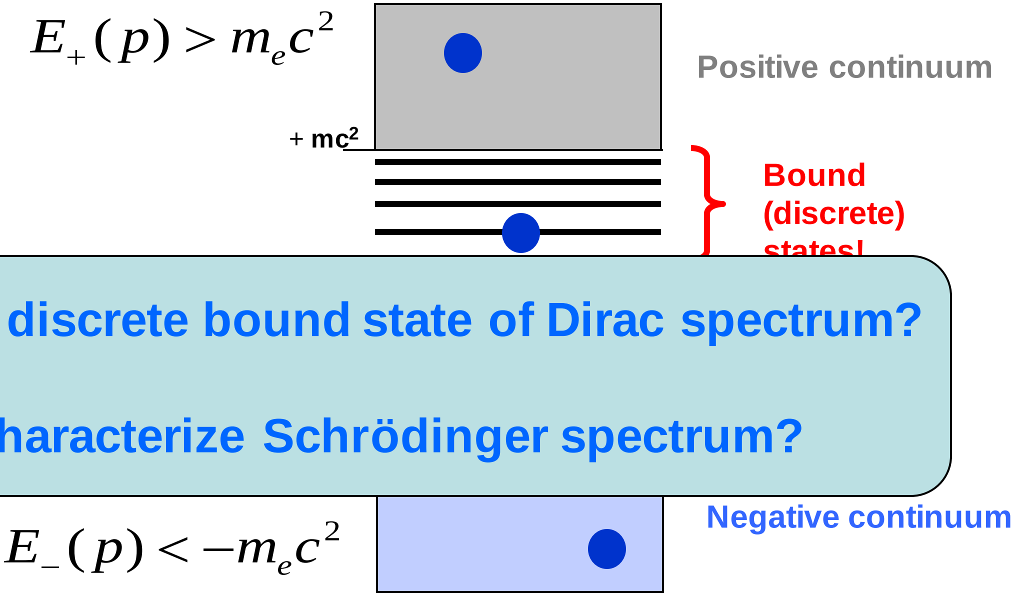
$$\left(-i\hbar c\boldsymbol{\alpha}\cdot\nabla+V(\boldsymbol{r})+m_e c^2\alpha_0\right)\psi(\boldsymbol{r})=E\psi(\boldsymbol{r})$$

- **Its solutions depend, of course, on the particular form of** $V(\boldsymbol{r})$

Free particle (discussed before): $V(\boldsymbol{r})=0$

Particle in Coulomb potential: $V(\boldsymbol{r})=-\frac{Ze^2}{r}$





How to describe (characterize) discrete bound state of Dirac spectrum?

By the way: how did we characterize Schrödinger spectrum?

Schrödinger equation: Quantum numbers

(just a reminder)

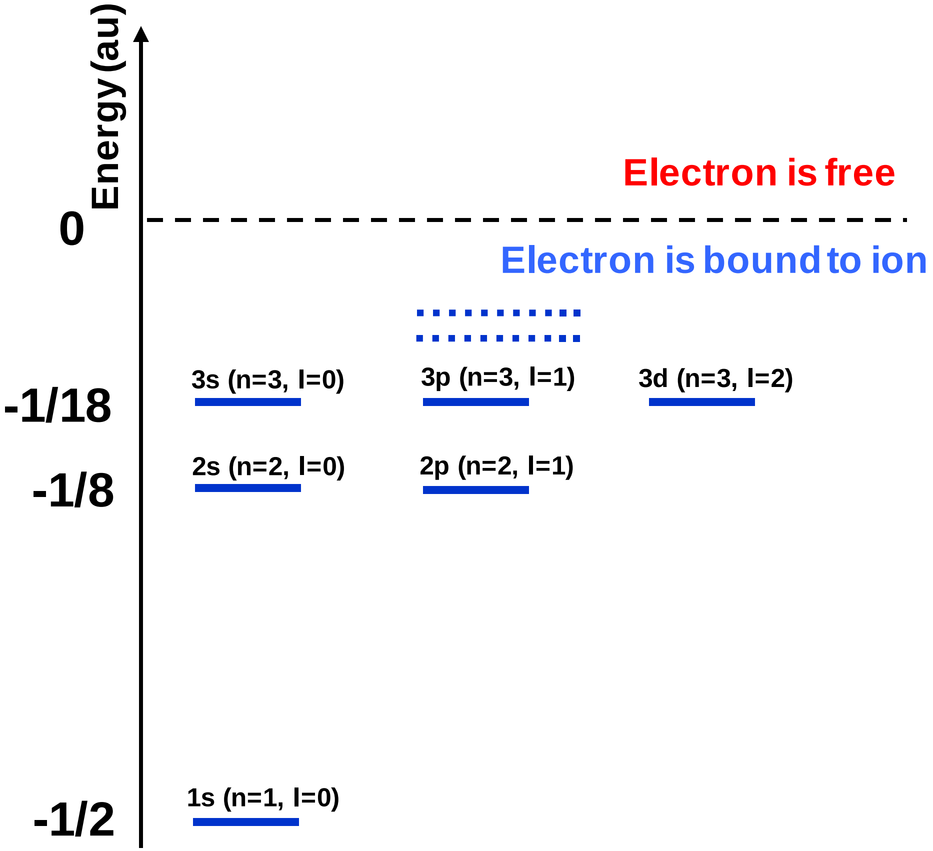
- **One needs three quantum numbers to define the state of hydrogen (hudrogen-like) atom:**
  - ***n*** **= 1, 2, 3… (principal)**
  - ***l*** **= 0, … *n*-1 (orbital)**
  - m_l **= -*l*, …. +*l* (magnetic)**

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

- **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)!**



Can we use the same set of quantum numbers (n,l,m) for Dirac spectrum?

Plan of lecture

- Reminder from the last lecture: Free-particle solution
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Constants of motion (1)

- **For the description of the (stable) atom we need to have a set of quantum numbers which do not change as time evolves.**

- **Let us take some observable (operator which represents some physical quantity) *Q* and its expectation value in some quantum state:**

$$\langle Q \rangle = \left\langle \Psi \middle| \hat{Q} \middle| \Psi \right\rangle$$

- **To find the general requirement for $\langle Q \rangle$ being not dependent on time, let us first derive the (matrix form of) Heisenberg equation of motion:**

$$\frac{d}{dt}\langle Q \rangle = \frac{d}{dt}\left\langle \Psi \middle| \hat{Q} \middle| \Psi \right\rangle = \frac{i}{\hbar}\left\langle \Psi \middle| \left[\hat{H}, \hat{Q}\right] \middle| \Psi \right\rangle + \left\langle \Psi \middle| \frac{\partial \hat{Q}}{\partial t} \middle| \Psi \right\rangle$$

Constants of motion (2)

- To find the general requirement for $\langle Q \rangle$ being not dependent on time, let us first derive the (matrix form of) Heisenberg equation of motion:

$$\frac{d}{dt}\langle Q \rangle = \frac{d}{dt}\left\langle \Psi \middle| \hat{Q} \middle| \Psi \right\rangle = \frac{i}{\hbar}\left\langle \Psi \middle| \left[\hat{H},\hat{Q}\right] \middle| \Psi \right\rangle + \left\langle \Psi \middle| \frac{\partial \hat{Q}}{\partial t} \middle| \Psi \right\rangle$$

$$\Downarrow$$

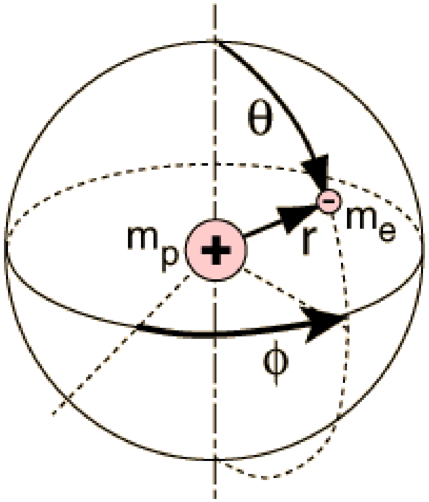
- Therefore, if $\left[\hat{H},\hat{Q}\right] = 0$ and $\hat{Q}$ do not depend (directly) on time, we find:

$$\frac{d}{dt}\langle Q \rangle = 0$$

- Expectation value $q = \langle Q \rangle$ does not change with time and provides us a “good quantum number” for the description of quantum system!

Non-relativistic hydrogen

Good quantum numbers



- **Schrödinger Hamiltonian in spherical coordinates:**

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

- **Its eigenfunctions:** $\psi(\mathbf{r}) = \psi(r,\theta,\varphi) = R_{nl}(r)Y_{lm_l}(\theta,\varphi)$

- **Operators** $\hat{H}, \hat{L}_Z, \hat{\boldsymbol{L}}^2$ **commute with each other:** $[\hat{\boldsymbol{L}}^2, \hat{H}] = 0,\ [\hat{L}_z, \hat{H}] = 0, [\hat{\boldsymbol{L}}^2, \hat{L}_z] = 0$

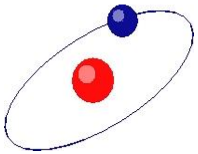
- **And:** $\hat{\boldsymbol{L}}^2\psi(\mathbf{r}) = l(l+1)\hbar^2\psi(\mathbf{r}),\quad \hat{L}_z\psi(\mathbf{r}) = m_l\hbar\psi(\mathbf{r}),\quad \hat{H}\psi(\mathbf{r}) = E\psi(\mathbf{r})$

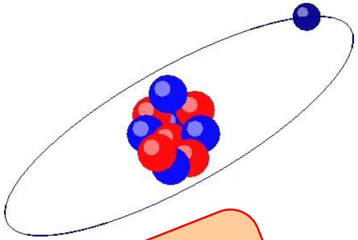
⬇

(n, l, m) are good quantum numbers.
… but only in the nonrelativistic case!

Relativistic hydrogen

„Bad“ quantum numbers





$$\hat{H}_S = -\frac{\hbar^2}{2m}\nabla^2 - \frac{Ze^2}{r}$$

$$\hat{H}_D = -i\hbar c\boldsymbol{\alpha}\cdot\nabla \quad \ldots \quad c^2\alpha_0$$

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

$$\psi \quad \ldots \quad (\theta,\varphi)\,\chi_{sm_s}(\sigma)$$

- **In Dirac’s theory, however, nei… …r *L* nor *L*^{2} commute with Hamiltonian. Instead, o…**

$$] = i\hbar c\boldsymbol{\alpha}\times\mathbf{p}$$

- **T… …ue for the spin operator:** $\hat{\mathbf{S}} = \frac{\hbar}{2}\begin{pmatrix}\hat{\boldsymbol{\sigma}} & 0\\ 0 & \hat{\boldsymbol{\sigma}}\end{pmatrix}$

$$[\hat{\mathbf{S}},\hat{H}] = -i\hbar c\boldsymbol{\alpha}\times\mathbf{p}$$

Quantum numbers *l*, *m*$_l$, *s*, *m*$_s$ are not “good” for relativistic Hamiltonian!
But what is good quantum number then?

Task 5.1

Please, prove commutation relations for the Dirac Hamiltonian:

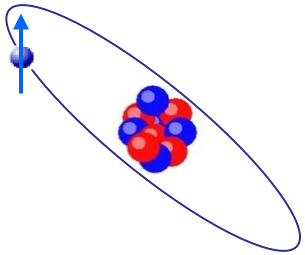
$$[\hat{\boldsymbol{L}}, \hat{H}] = i\hbar c\boldsymbol{\alpha} \times \boldsymbol{p}$$

and

$$[\hat{\boldsymbol{S}}, \hat{H}] = -i\hbar c\boldsymbol{\alpha} \times \boldsymbol{p}$$

Relativistic hydrogen

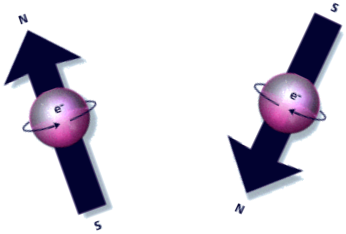
- **Dirac equation for the hydrogen-like ions:**



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

- **Why l, m_l, s, m_s are not good quantum numbers?**

- **The main difference from the non-relativistic picture is the spin of electron!**



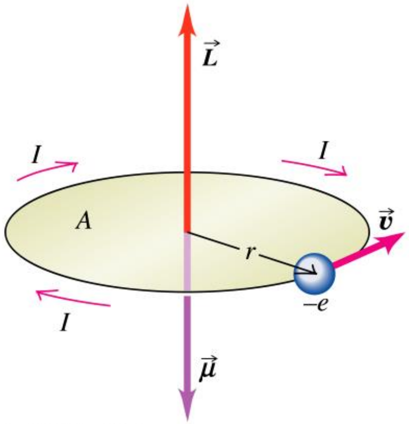
$$\Downarrow$$

Spin-orbit interaction!

Spin-orbit interaction (1)

(qualitative and rather rough derivation)

✓ **Please, remind yourself discussion from the last lecture concerning magnetic dipole moment**



In classical electrodynamics:

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

current

vector area of the current loop

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

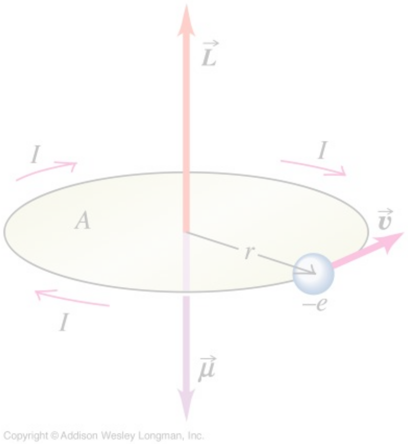
In quantum mechanics, for electron: q=-e

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

Bohr magneton

Spin-orbit interaction (1)

(qualitative and rather rough derivation)



In classical electrodynamics:

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

current

vector area of the current loop

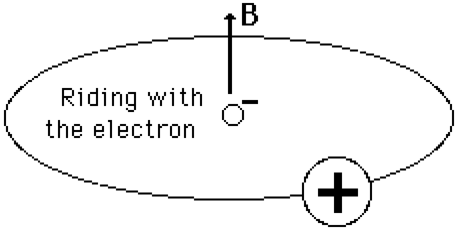
$$|\mu| = \boldsymbol{I} \cdot \boldsymbol{A} = \frac{q}{T} \pi r^2 = \frac{qv}{2\pi r} \pi r^2 = \frac{q}{2m} L$$

In quantum mechanics, for electron: q=-e

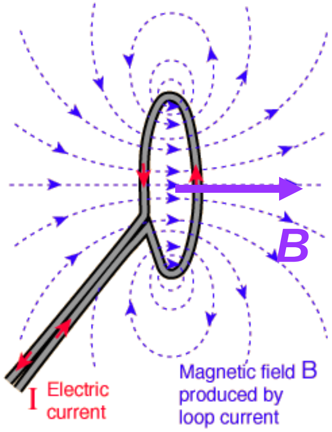
$$\hat{\boldsymbol{\mu}}_l = -\mu_0 \hat{\mathbf{L}} / \hbar, \qquad \mu_0 = \frac{e\hbar}{2m_e}$$

Bohr magneton

✓ Let us move to the rest frame of electron (we are riding with electron)



- In the rest frame of electron there is a magnetic filed caused by the relative motion of the nucleus (magnetic field of current loop)!



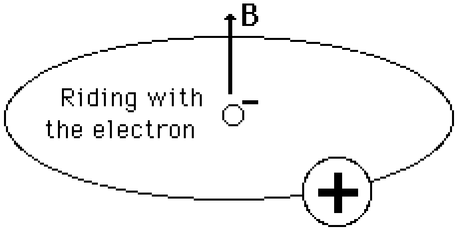
$$B = \frac{\mu_0 I}{2r}$$

where

$$I = \frac{Ze}{T} = \frac{Zev}{2\pi r} = \frac{Ze}{2\pi r^2 m} mvr$$

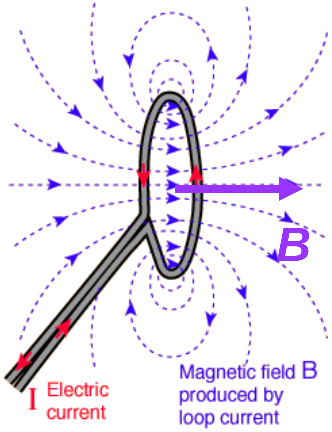
Spin-orbit interaction (2)

(qualitative and rather rough derivation)



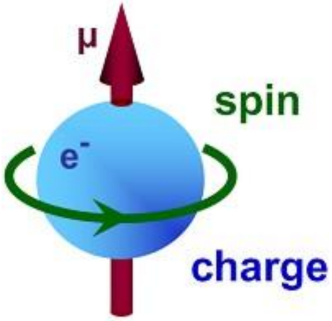
- In the rest frame of electron there is a magnetic filed caused by the relative motion of the nucleus (magnetic field of current loop)!

$$\boldsymbol{B} = \frac{\mu_0 Ze\boldsymbol{L}}{4\pi r^3 m} = \xi(r)\,\boldsymbol{L}$$



- Electron has spin (intrinsic moment) and, hence, spin magnetic moment:

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



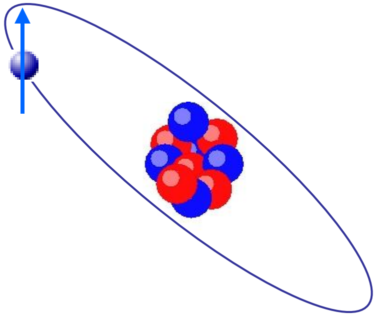
- Which interacts with external field as:

$$\hat{H}' = -\hat{\boldsymbol{\mu}}_s \cdot \boldsymbol{B} = \zeta(r)\,\hat{\boldsymbol{L}} \cdot \hat{\boldsymbol{S}}$$

Spin-orbit term! (A more rigorous derivation requires detailed analysis of Dirac equation.)

Spin-orbit interaction (3)

(qualitative and rather rough derivation)



- Coming back to Dirac equation for the hydrogen-like ions:

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

- Which should include the spin-orbit term: $\hat{H}^{'}=-\hat{\boldsymbol{\mu}}_s\cdot\boldsymbol{B}=\zeta(r)\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}}$

- Now it becomes clear why the wavefunction

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

is not adequate for Dirac’s case and, hence, *l*, m_l, *s*, m_s are “bad” quantum numbers.

- The reason is: $\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}}$ does not commute with L_z or S_z.

What to do?

Obviously: we have to build from *L* and *S* operator which commutes with *LS*.

Total angular momentum

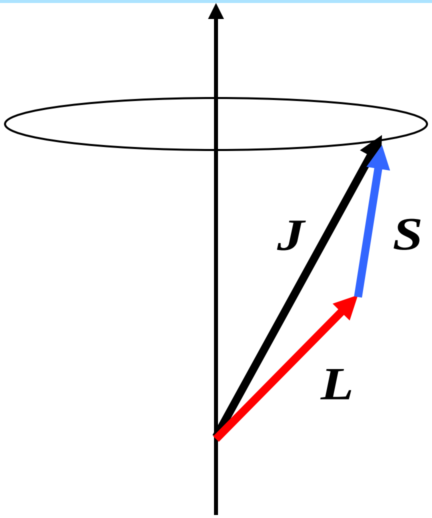
- **We shall introduce the total angular momentum :**

$$\vec{J} = \vec{L} + \vec{S}$$

Total angular momentum

Orbital angular momentum

Spin



- **Operators J^2 and J_z commutes with *LS* and with Dirac Hamiltonian!**

$\hat{J}$ is a "right" observable for the Dirac equation!

- **Since like any other angular momentum it satisfies:**

$$\hat{J}^2 \Omega_{jm_j} = j(j+1)\hbar^2 \Omega_{jm_j} \qquad \hat{J}_z \Omega_{jm_j} = m_j \hbar \Omega_{jm_j}$$

Now we can describe the state of relativistic hydrogen atom (ion) by set of quantum numbers: *n, j,* m_j

… and by parity.

Task 5.2

Please, prove that operator $\hat{\boldsymbol{L}} \cdot \hat{\boldsymbol{S}}$ commute with $\hat{\boldsymbol{J}}^2, \hat{\boldsymbol{J}}_z$

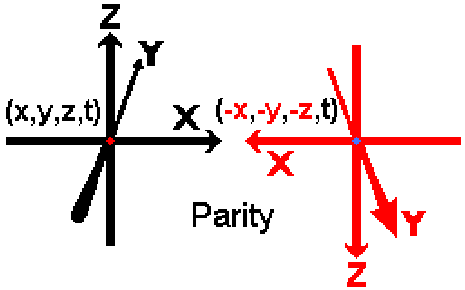
Plan of lecture

- **Reminder from the last lecture: Free-particle solution**
- **Dirac's spectroscopic notations**
  - **Integrals of motion**
  - **Parity of states**
- **Energy levels of the bound-state Dirac's particle**
- **Structure of Dirac's wavefunction**
- **Radial components of the Dirac's wavefunction**

Parity operator

- **Solutions of the Dirac (as well as Schrödinger) equation may be separated on the basis of their response to spatial coordinate inversion.**

- **Parity operator:**



$$\hat{P}\boldsymbol{r} = \hat{P}\begin{pmatrix} x \\ y \\ z \end{pmatrix} \rightarrow \begin{pmatrix} -x \\ -y \\ -z \end{pmatrix}$$

Cartesian coordinates

$$\hat{P}\boldsymbol{r} = \hat{P}\begin{pmatrix} r \\ \theta \\ \varphi \end{pmatrix} \rightarrow \begin{pmatrix} r \\ \pi-\theta \\ \varphi+\pi \end{pmatrix}$$

Spherical coordinates

- **For the Schrödinger case the parity operator commutes with Hamiltonian:**

$$\left[\hat{P}, \hat{H}_S\right] = 0$$ **where** $$\hat{H}_S = -\frac{\hbar^2}{2m}\nabla^2 - \frac{Ze^2}{r}$$

Parity is a good quantum number!

- **Hence, solutions of Schrödinger equation are - at the same time – eigenfunctions of permutation operator:**

$$\hat{P}\psi_{nlm_l}(\boldsymbol{r}) = \psi_{nlm_l}(-\boldsymbol{r}) = \varepsilon\psi_{nlm_l}(\boldsymbol{r})$$

Parity operator

- **For the Schrödinger case the parity operator commutes with Hamiltonian:**

$$\left[\hat{P},\hat{H}_S\right]=0 \quad \textbf{where} \quad \hat{H}_S=-\frac{\hbar^2}{2m}\nabla^2-\frac{Ze^2}{r}$$

Parity is a good quantum number!

- **Hence, solutions of Schrödinger equation are - at the same time – eigenfunctions of permutation operator:**

$$\hat{P}\psi_{nlm_l}(\mathbf{r})=\psi_{nlm_l}(-\mathbf{r})=\varepsilon\psi_{nlm_l}(\mathbf{r})$$

- **How to find eigenvalue ε?** $\hat{P}^2\psi_{nlm_l}(\mathbf{r})=\varepsilon\,\hat{P}\psi_{nlm_l}(\mathbf{r})=\varepsilon^2\psi_{nlm_l}(\mathbf{r})$

⇨ $\varepsilon=\pm 1$

Solutions of Schrödinger equation are either having even or odd parity! Why we usually don't use ε as an additional quantum number?

- **By employing properties of spherical harmonics we may find:**

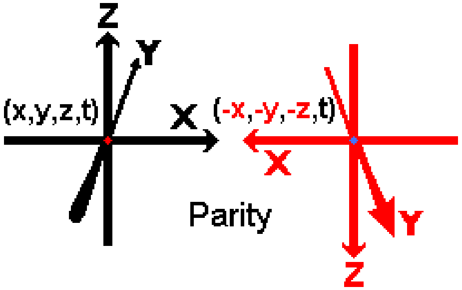
$$\hat{P}\psi_{nlm_l}(\mathbf{r})=\hat{P}\left[R_{nl}(r)Y_{lm_l}(\theta,\varphi)\right]=R_{nl}(r)Y_{lm_l}(\pi-\theta,\varphi+\pi)=(-1)^l R_{nl}(r)Y_{lm_l}(\theta,\varphi)=(-1)^l\psi_{nlm_l}(\mathbf{r})$$

Orbital momentum *l* defines also parity! **How it is for Dirac case?**

Parity of Dirac states

- **Solutions of the Dirac (as well as Schrödinger) equation may be separated on the basis of their response to spatial coordinate inversion.**

$$\hat{P}\boldsymbol{r} = \hat{P}\begin{pmatrix} r \\ \theta \\ \varphi \end{pmatrix} \rightarrow \begin{pmatrix} r \\ \pi - \theta \\ \varphi + \pi \end{pmatrix}$$



$$\hat{P}\Psi(\boldsymbol{r}) = \Psi(-\boldsymbol{r})$$

- **Dirac equation:** $\hat{H}_D = -i\hbar c\boldsymbol{\alpha}\cdot\nabla - \frac{Ze^2}{r} + m_e c^2 \alpha_0$

- **Does not commute with non-relativistic parity operator:** $\left[\hat{H}_D, \hat{P}\right] \neq 0$

- **But:** $\left[\hat{H}_D, \boxed{\boldsymbol{\alpha}_0\ \hat{P}}\right] = 0$ **where** $\alpha_0 = \begin{pmatrix} \boldsymbol{I} & 0 \\ 0 & -\boldsymbol{I} \end{pmatrix}$

(Dirac's) parity is a good quantum number!
… but what does it mean?

Structure of Dirac wavefunctions

- **Stationary Dirac equation for particle in Coulomb field reads:**

$$\left(-i\hbar c\boldsymbol{\alpha}\cdot\nabla-\frac{Ze^{2}}{r}+m_{e}c^{2}\alpha_{0}\right)\psi(\boldsymbol{r})=E\psi(\boldsymbol{r})$$

- **The four-spinor** $\psi(\boldsymbol{r})=\begin{pmatrix}\varphi_1(\boldsymbol{r})\\\varphi_2(\boldsymbol{r})\\\varphi_3(\boldsymbol{r})\\\varphi_4(\boldsymbol{r})\end{pmatrix}$ **is more convenient to write as:** $\psi(\boldsymbol{r})=\begin{pmatrix}g(\boldsymbol{r})\\f(\boldsymbol{r})\end{pmatrix}$

- **In this case:** $\boldsymbol{\alpha}_0\,\hat{P}\psi(\boldsymbol{r})=\boldsymbol{\alpha}_0\hat{P}\begin{pmatrix}g(\boldsymbol{r})\\f(\boldsymbol{r})\end{pmatrix}=\boldsymbol{\alpha}_0\begin{pmatrix}g(-\boldsymbol{r})\\f(-\boldsymbol{r})\end{pmatrix}=\begin{pmatrix}g(-\boldsymbol{r})\\-f(-\boldsymbol{r})\end{pmatrix}$

  ⇦ large component

  ⇦ small component

- **Obviously, since the wavefunction** $\psi(\boldsymbol{r})$ **should have definite parity, its large and small components must have an opposite parities!**

For the spectroscopic notation one uses parity of the large component.

Structure of Dirac wavefunctions

- **We just found:** $\boldsymbol{\alpha}_0\,\hat{P}\psi(\mathbf{r}) = \boldsymbol{\alpha}_0\hat{P}\begin{pmatrix} g(\mathbf{r}) \\ f(\mathbf{r}) \end{pmatrix} = \boldsymbol{\alpha}_0\begin{pmatrix} g(-\mathbf{r}) \\ f(-\mathbf{r}) \end{pmatrix} = \begin{pmatrix} g(-\mathbf{r}) \\ -f(-\mathbf{r}) \end{pmatrix}$ ⇦ large component ⇦ small component

- **We shall remember from the nonrelativistic quantum mechanics that parity is related to the orbital angular momentum *l*:**

$$\hat{P}\psi_{nlm_l}(\mathbf{r}) = \hat{P}\left[R_{nl}(r)Y_{lm_l}(\theta,\varphi)\right] = R_{nl}(r)Y_{lm_l}(\pi-\theta,\varphi+\pi) = (-1)^l\psi_{nlm_l}(\mathbf{r})$$

- **We can attribute to the large and small components their (individual) angular momenta *l*:**

one *j* (good quantum number) → *l* (and *p*=(-1)^{l}) for large component

one *j* (good quantum number) → *l'* (and *p*=(-1)$^{l'}$) for small component

Completely confused? OK, now it becomes easier....

Task 5.3

Consider an operator:

$H_W = f(\mathbf{r})\gamma_5$ where $\gamma_5 = \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix}$ and $f(\mathbf{r})$ is some even function.

Prove that matrix element of this operator:

$$\langle \boldsymbol{\psi_a} | \boldsymbol{H_w} | \boldsymbol{\psi_b} \rangle$$

is non-vanishing only if the functions $\boldsymbol{\psi_a}$ and $\boldsymbol{\psi_b}$ are opposite-parity functions (for example 2s and $2p_{1/2}$).

Dirac quantum number κ

- **To make relativistic notations of the bound-state Dirac's states more convenient a new quantum number κ is introduced (which combines together *j*, *l* (*l'*) and parity:)**

$$\kappa = -1, +1, -2, +2, -3, +3, \ldots$$

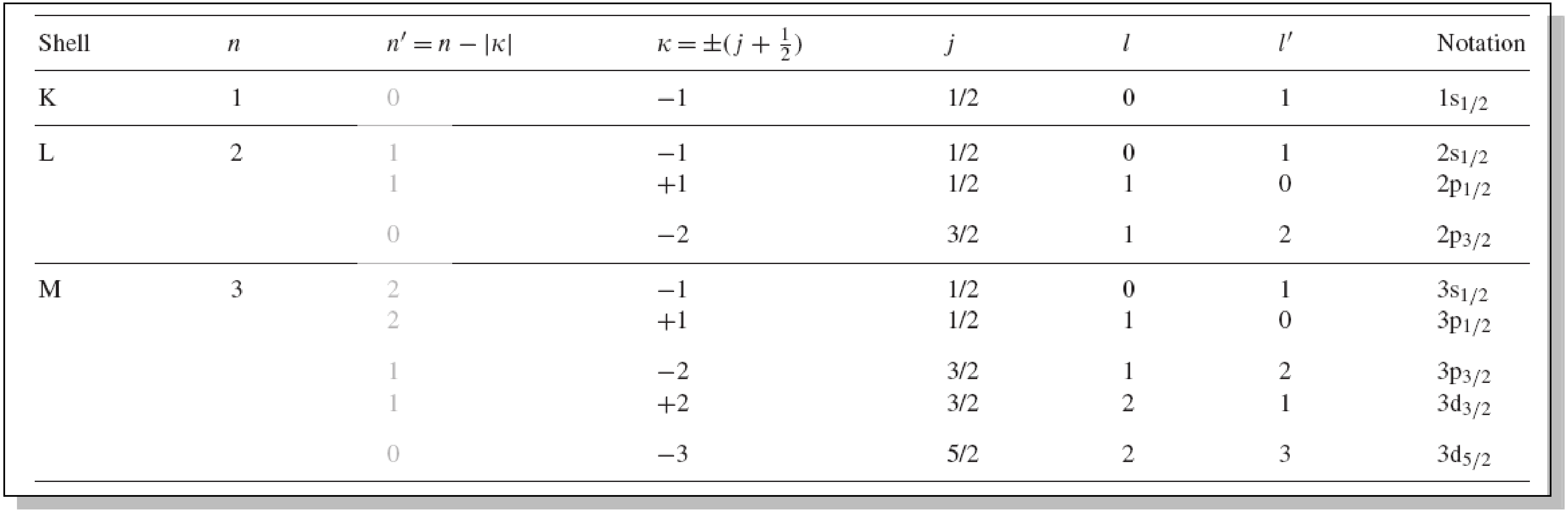
$$j = |\kappa| - 1/2$$

$$l = \begin{cases} \kappa & \kappa > 0 \\ -\kappa - 1 & \kappa < 0 \end{cases}, \quad l' = \begin{cases} -\kappa & \kappa < 0 \\ \kappa - 1 & \kappa > 0 \end{cases}$$

Finally: we shall describe Dirac's states by quantum numbers:

$$n \; \kappa \; m_j \Leftrightarrow n \; \kappa \; l \; l' \; j \; m_j$$

Spectroscopi notations



Shell	n	$n' = n - \|\kappa\|$	$\kappa = \pm(j + \frac{1}{2})$	j	l	l'	Notation
K	1	0	−1	1/2	0	1	$1s_{1/2}$
L	2	1	−1	1/2	0	1	$2s_{1/2}$
		1	+1	1/2	1	0	$2p_{1/2}$
		0	−2	3/2	1	2	$2p_{3/2}$
M	3	2	−1	1/2	0	1	$3s_{1/2}$
		2	+1	1/2	1	0	$3p_{1/2}$
		1	−2	3/2	1	2	$3p_{3/2}$
		1	+2	3/2	2	1	$3d_{3/2}$
		0	−3	5/2	2	3	$3d_{5/2}$

- **Finally, we know how to characterize bound states of (relativistic) hydrogen.**
- **What are the energies of these states?**

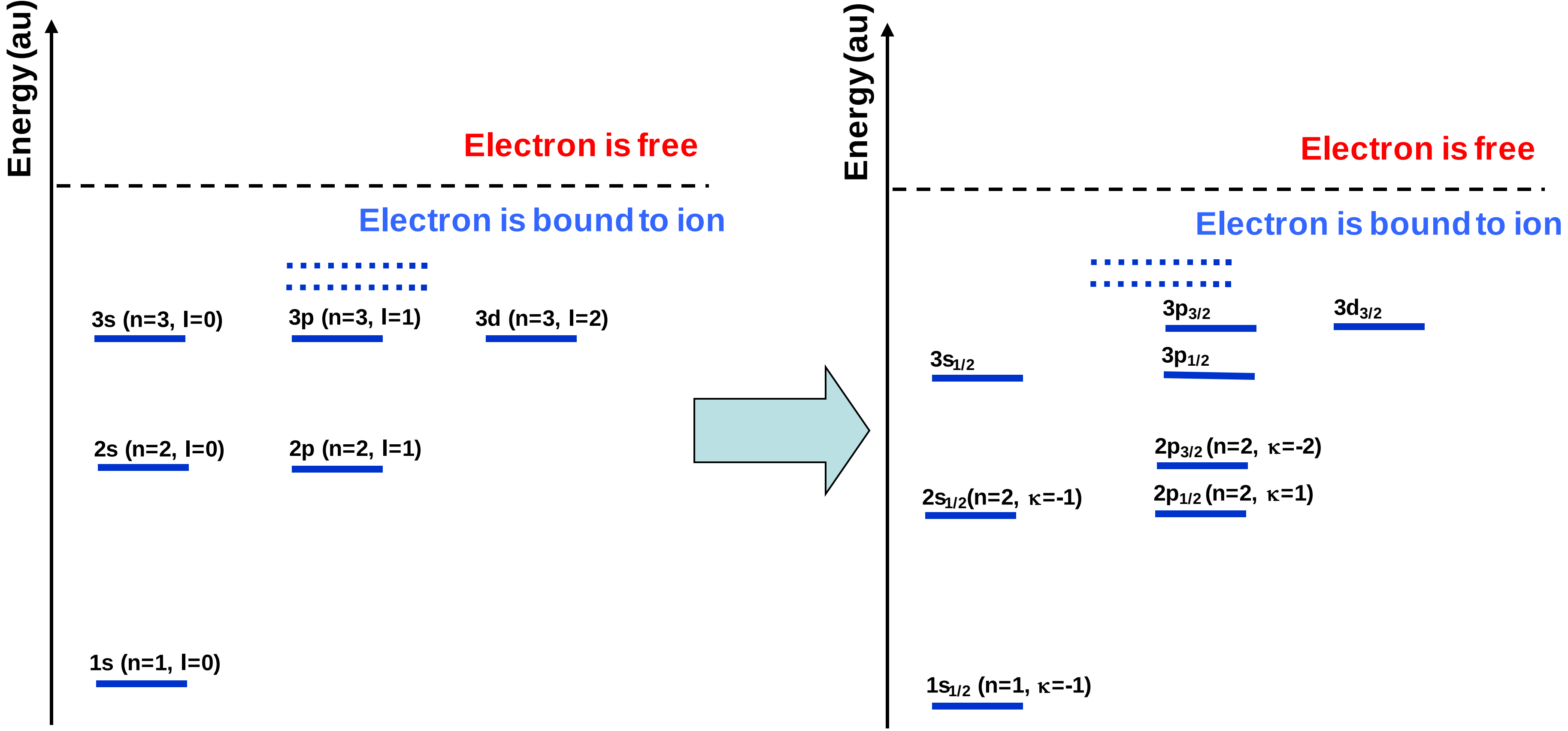
Plan of lecture

- **Reminder from the last lecture: Free-particle solution**
- **Dirac’s spectroscopic notations**
  - **Integrals of motion**
  - **Parity of states**
- **Energy levels of the bound-state Dirac’s particle**
- **Structure of Dirac’s wavefunction**
- **Radial components of the Dirac’s wavefunction**

Energy levels of hydrogen ion

$$E_n = -Z^2\varepsilon_0 \big/ 2n^2$$

$$E_{nj} = mc^2 \Bigg/ \sqrt{1+\left(\frac{Z\alpha}{n-|\,j+1/2\,|+\sqrt{(j+1/2)^2-(Z\alpha)^2}}\right)^2}$$



All state with the same n are degenerated!

All state with the same n and j are degenerated!

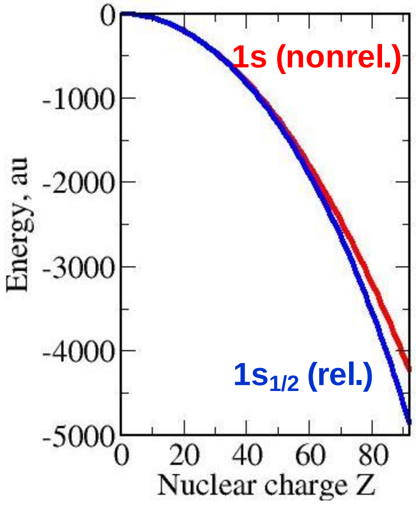
Energy levels of hydrogen ion

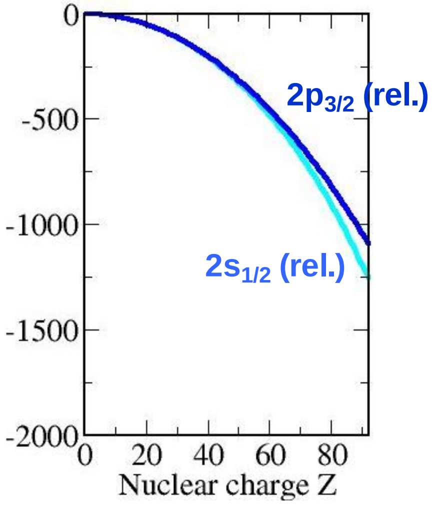
$$E_{nj} = mc^2 \Big/ \sqrt{1+\left(\frac{Z\alpha}{n-|\,j+1/2\,|+\sqrt{(j+1/2)^2-(Z\alpha)^2}}\right)^2}$$

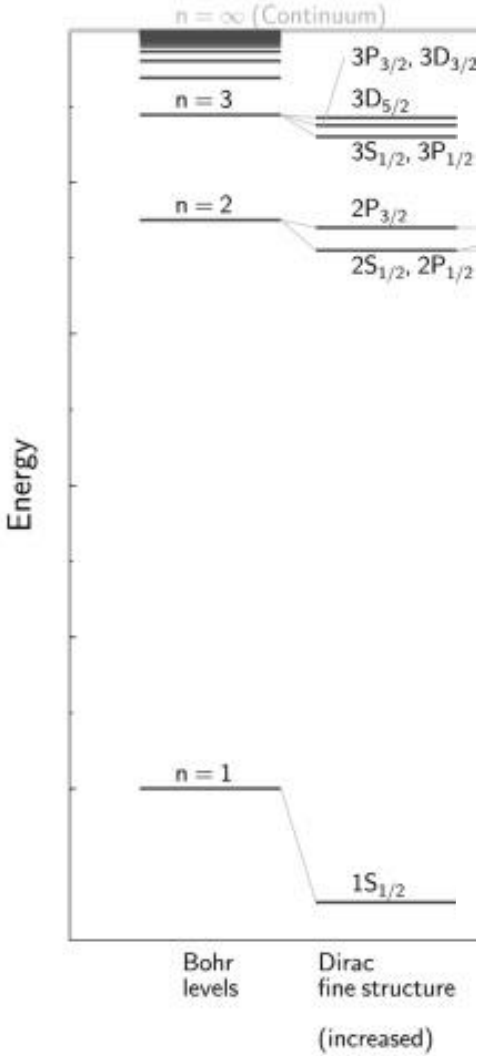
$$\approx mc^2\left(1-\frac{1}{2}\frac{(\alpha Z)^2}{n^2}-\frac{1}{2}\frac{(\alpha Z)^4}{n^3}\left(\frac{1}{j+1/2}-\frac{3}{4n}\right)-\dots\right)$$

Rest mass term **Nonrelativistic energy** **First relativistic correction**

- **Relativistic effects results both in shifting and splitting of energy levels.**

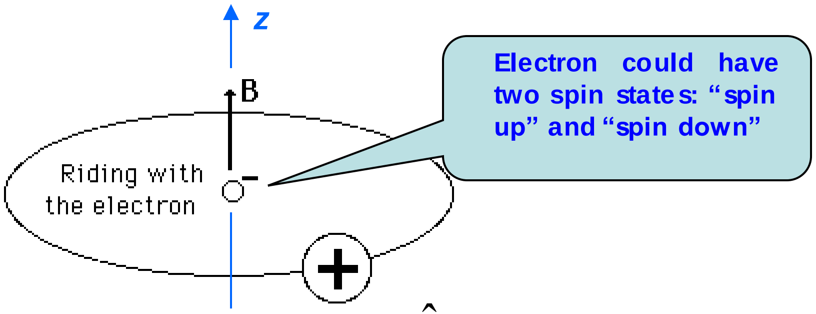






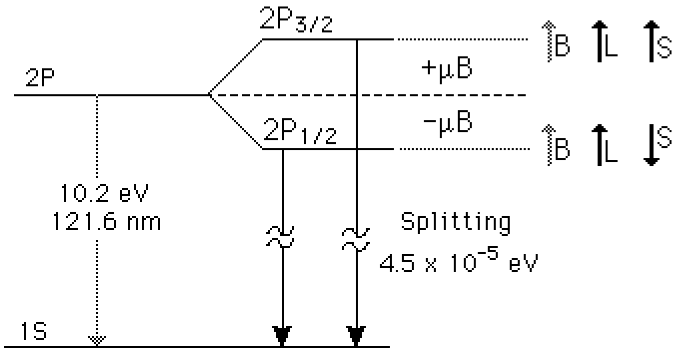
Splitting of energy levels

- **Splitting of energy levels with the same principal quantum number n but different total angular momenta j can be see as a results of spin-orbit interaction:**

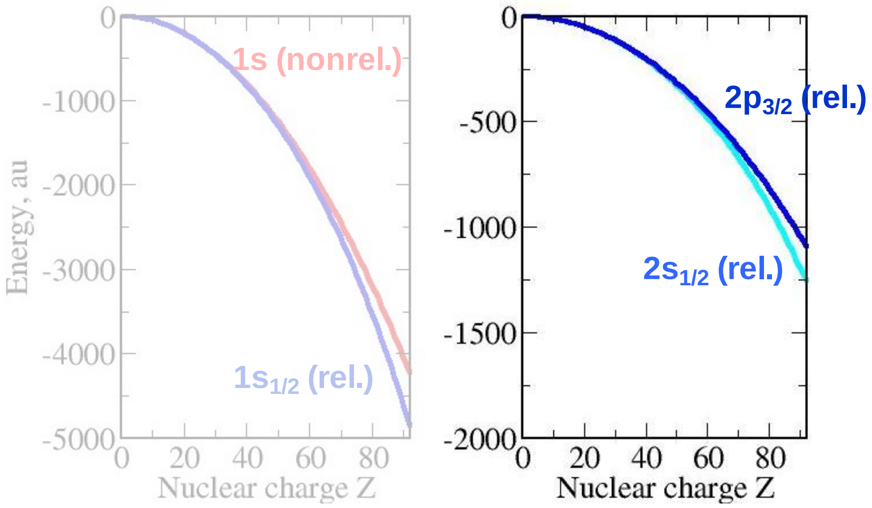


Electron could have two spin states: "spin up" and "spin down"

Spin-orbit interaction: $\hat{H}' = -\hat{\boldsymbol{\mu}}_s \cdot \boldsymbol{B} = \zeta(r)\,\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}}$



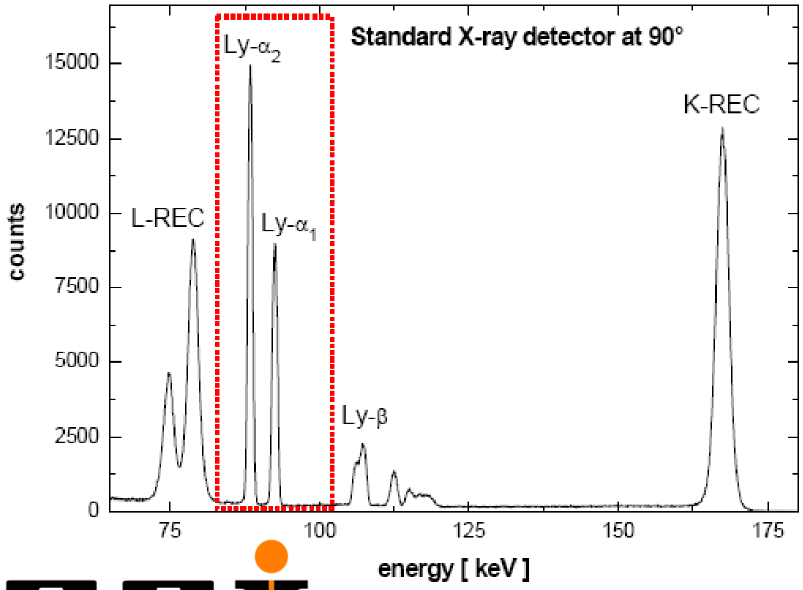
Pictures from: hyperphysics.phy-astr.gsu.edu



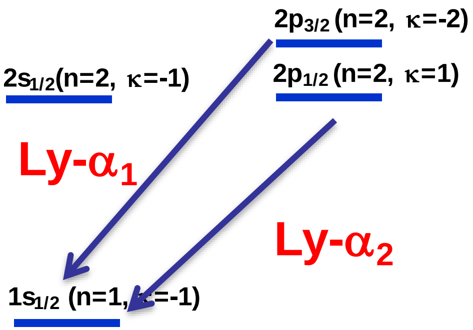
- **For neutral hydrogen fine structure splitting is very small but increases with nuclear charge Z.**

Splitting of energy levels

- **Can one observe fine-structure splitting of energy levels in experiment? Yes!**



- **Example: Fine-structure splitting in H-like uranium ion.**


$2p_{3/2}$ (n=2, κ=-2)

$2s_{1/2}$(n=2, κ=-1)

$2p_{1/2}$ (n=2, κ=1)

Ly-α_1

Ly-α_2

$1s_{1/2}$ (n=1, κ=-1)

- **Nowadays a fine-structure spectroscopy of heavy ions plays an important role in studying relativistic, QED and many-electron effects in atomic systems.**

Task 5.4

Calculate the energies of the Ly-α_1 and Ly-α_2 lines of hydrogen-like uranium. Compare with experimental findings presented on the previous transparency.

Plan of lecture

- Reminder from the last lecture: Free-particle solution
- Dirac's spectroscopic notations
    - Integrals of motion
    - Parity of states
- Energy levels of the bound-state Dirac's particle
- Structure of Dirac's wavefunction
- Radial components of the Dirac's wavefunction

Structure of Dirac wavefunctions

- **Stationary Dirac equation for particle in Coulomb field reads:**

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

- **The four-spinor** $\psi(\boldsymbol{r})=\begin{pmatrix}\varphi_1(\boldsymbol{r})\\ \varphi_2(\boldsymbol{r})\\ \varphi_3(\boldsymbol{r})\\ \varphi_4(\boldsymbol{r})\end{pmatrix}$ **is more convenient to write as:** $\psi(\boldsymbol{r})=\begin{pmatrix}g(\boldsymbol{r})\\ f(\boldsymbol{r})\end{pmatrix}$

What are the (large and small) components of wavefunction?

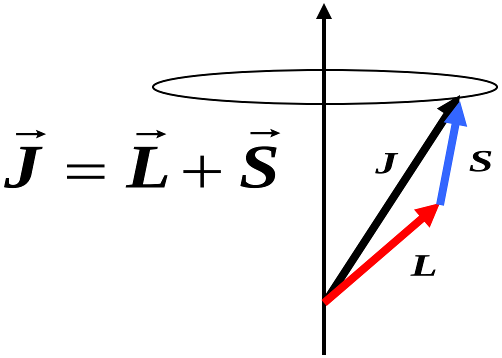
- **Please, remind yourself our (wrong) guess:**

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

What is wrong here? We already learned that *l* and *s* should be coupled together to form total angular momentum *j*.

Building Dirac spinor

- **We shall "couple" together angular momentum and spin to obtain total angular momentum:**



$$\vec{J} = \vec{L} + \vec{S}$$

$$Y_{lm_l}(\theta,\varphi)\,\chi_{sm_s}(\sigma)$$

$$\Omega_{ljm_j}(\hat{\boldsymbol{r}}) = \sum_{m_l m_s} \left(lm_l\ sm_s \middle| jm_j \right) Y_{lm_l}(\theta,\varphi)\,\chi_{sm_s}(\sigma)$$

Clebsch-Gordan coefficients
(more detailed discuss comes later)

- **Dirac spinors are the eigenfunctions of operators J^2 and J_z:**

$$\hat{\boldsymbol{J}}^2 \Omega_{jm_j} = j(j+1)\hbar^2 \Omega_{jm_j} \qquad \hat{J}_z \Omega_{jm_j} = m_j \hbar \Omega_{jm_j}$$

Structure of Dirac wavefunctions

- **Stationary Dirac equation for particle in Coulomb field reads:**

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

- **Wavefunctions can be written now as:** $\psi_{nljm_j}(\boldsymbol{r}) = \frac{1}{r} \begin{pmatrix} g_{nj}(r) \Omega_{ljm_j}(\hat{\boldsymbol{r}}) \\ i\, f_{nj}(r) \Omega_{l'jm_j}(\hat{\boldsymbol{r}}) \end{pmatrix}$

- **Where the angular and spin dependence is in Dirac spinors:**

$$\Omega_{ljm_j}(\hat{\boldsymbol{r}}) = \sum_{m_l m_s} \left(l m_l \; s m_s \middle| j m_j \right) Y_{lm_l}(\theta, \varphi) \, \chi_{sm_s}(\sigma)$$

- **And *g(r)* and *f(r)* are the large and small radial components of the Dirac wavefunction.**

◆ **How to find these radial components?**

Plan of lecture

- **Reminder from the last lecture: Free-particle solution**
- **Dirac’s spectroscopic notations**
    - **Integrals of motion**
    - **Parity of states**
- **Energy levels of the bound-state Dirac’s particle**
- **Structure of Dirac’s wavefunction**
- **Radial components of the Dirac’s wavefunction**

Coupled radial equations

- **By substituting wavefunction** $\psi_{nljm_j}(\mathbf{r}) = \frac{1}{r}\begin{pmatrix} g_{n\kappa}(r)\Omega_{ljm_j}(\hat{\mathbf{r}}) \\ i\, f_{n\kappa}(r)\Omega_{l'jm_j}(\hat{\mathbf{r}}) \end{pmatrix}$

- **into Dirac's equation** $\left(-i\hbar c\boldsymbol{\alpha}\cdot\nabla - \frac{Ze^2}{r} + m_e c^2\alpha_0\right)\psi(\mathbf{r}) = E\psi(\mathbf{r})$

- **we obtain the coupled radial equations:**

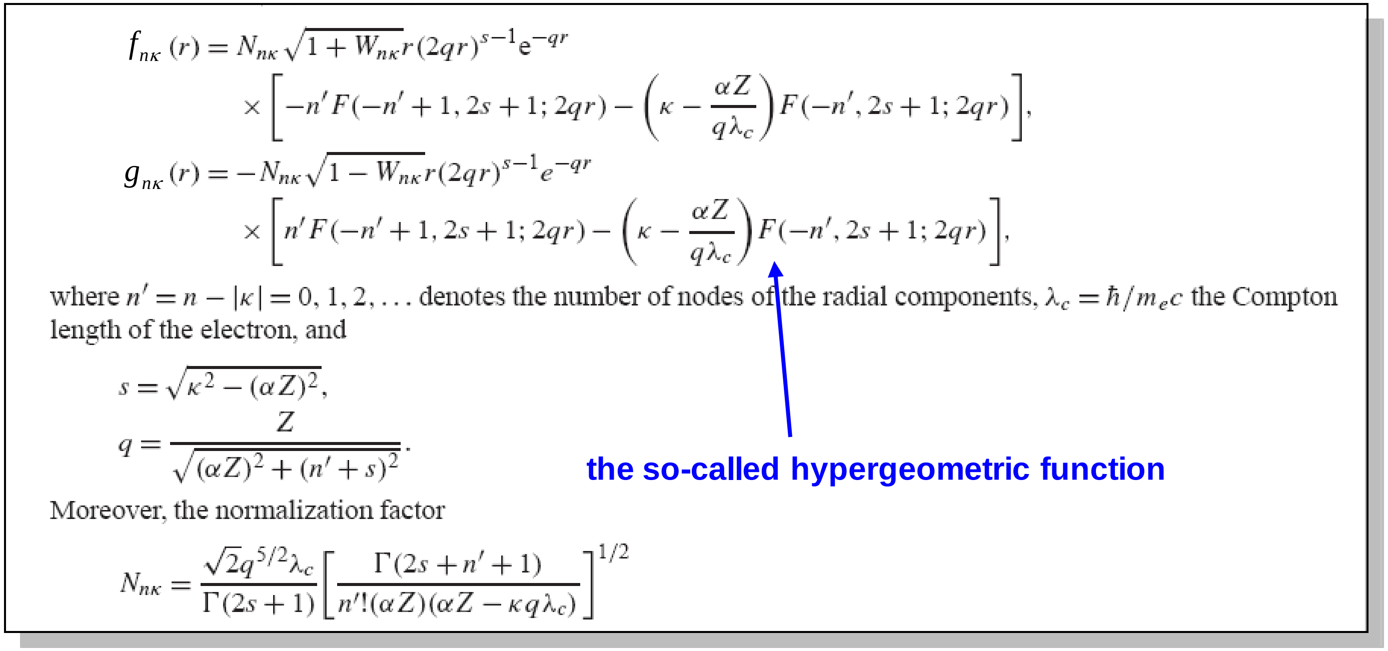
$$\left(\frac{d\ f_{n\kappa}(r)}{dr} - \frac{\kappa}{r} f_{n\kappa}(r)\right) = -\left(E - V(r) - m_e c^2\right) g_{n\kappa}(r)$$

$$\left(\frac{dg_{n\kappa}(r)}{dr} + \frac{\kappa}{r} g_{n\kappa}(r)\right) = \left(E - V(r) + m_e c^2\right) f_{n\kappa}(r)$$

- **which can be solved and ...**

Dirac‘s radial components

- **We finally may derive analytic expressions for the radial components of the Dirac’s equation (for point-like nucleus!):**



$$f_{n\kappa}(r) = N_{n\kappa}\sqrt{1+W_{n\kappa}}r(2qr)^{s-1}\mathrm{e}^{-qr} \times \left[-n'F(-n'+1, 2s+1; 2qr) - \left(\kappa - \frac{\alpha Z}{q\lambda_c}\right)F(-n', 2s+1; 2qr)\right],$$

$$g_{n\kappa}(r) = -N_{n\kappa}\sqrt{1-W_{n\kappa}}r(2qr)^{s-1}e^{-qr} \times \left[n'F(-n'+1, 2s+1; 2qr) - \left(\kappa - \frac{\alpha Z}{q\lambda_c}\right)F(-n', 2s+1; 2qr)\right],$$

where $n' = n - |\kappa| = 0, 1, 2, \ldots$ denotes the number of nodes of the radial components, $\lambda_c = \hbar/m_e c$ the Compton length of the electron, and

$$s = \sqrt{\kappa^2 - (\alpha Z)^2},$$

$$q = \frac{Z}{\sqrt{(\alpha Z)^2 + (n'+s)^2}}.$$

Moreover, the normalization factor

$$N_{n\kappa} = \frac{\sqrt{2}q^{5/2}\lambda_c}{\Gamma(2s+1)}\left[\frac{\Gamma(2s+n'+1)}{n'!(\alpha Z)(\alpha Z - \kappa q\lambda_c)}\right]^{1/2}$$

the so-called hypergeometric function

- **Radial components of the Dirac’s equation are implemented in many computer codes so there is usually no need to re-program these relations again.**

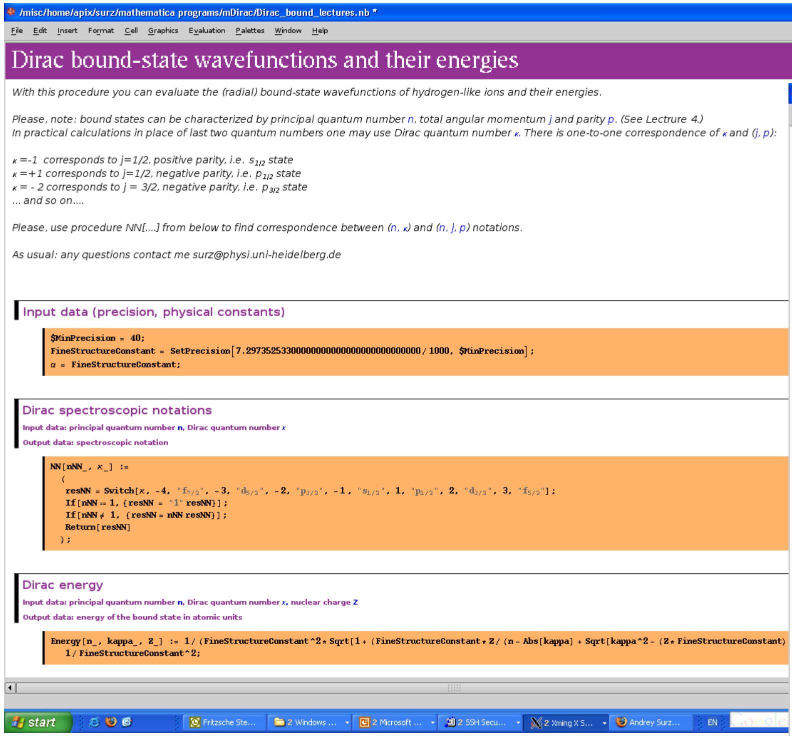
Dirac‘s radial components

(Mathematica package)

Please, find zipped .nb files with the Mathematic notebooks at:

http://www.physi.uni-heidelberg.de/Forschung/apix/TAP/lectures

(password: dirac2012)



/misc/home/apix/surz/mathematica programs/mDirac/Dirac_bound_lectures.nb *

Dirac bound-state wavefunctions and their energies

With this procedure you can evaluate the (radial) bound-state wavefunctions of hydrogen-like ions and their energies.

Please, note: bound states can be characterized by principal quantum number n, total angular momentum j and parity p. (See Lectrure 4.)
In practical calculations in place of last two quantum numbers one may use Dirac quantum number κ. There is one-to-one correspondence of κ and (j, p):

κ =-1 corresponds to j=1/2, positive parity, i.e. $s_{1/2}$ state
κ =+1 corresponds to j=1/2, negative parity, i.e. $p_{1/2}$ state
κ = - 2 corresponds to j = 3/2, negative parity, i.e. $p_{3/2}$ state
... and so on....

Please, use procedure NN[....] from below to find correspondence between (n, κ) and (n, j, p) notations.

As usual: any questions contact me surz@physi.uni-heidelberg.de

Input data (precision, physical constants)

```
$MinPrecision = 40;
FineStructureConstant = SetPrecision[7.2973525330000000000000000000000000 / 1000, $MinPrecision];
α = FineStructureConstant;
```

Dirac spectroscopic notations

Input data: principal quantum number n, Dirac quantum number ϰ

Output data: spectroscopic notation

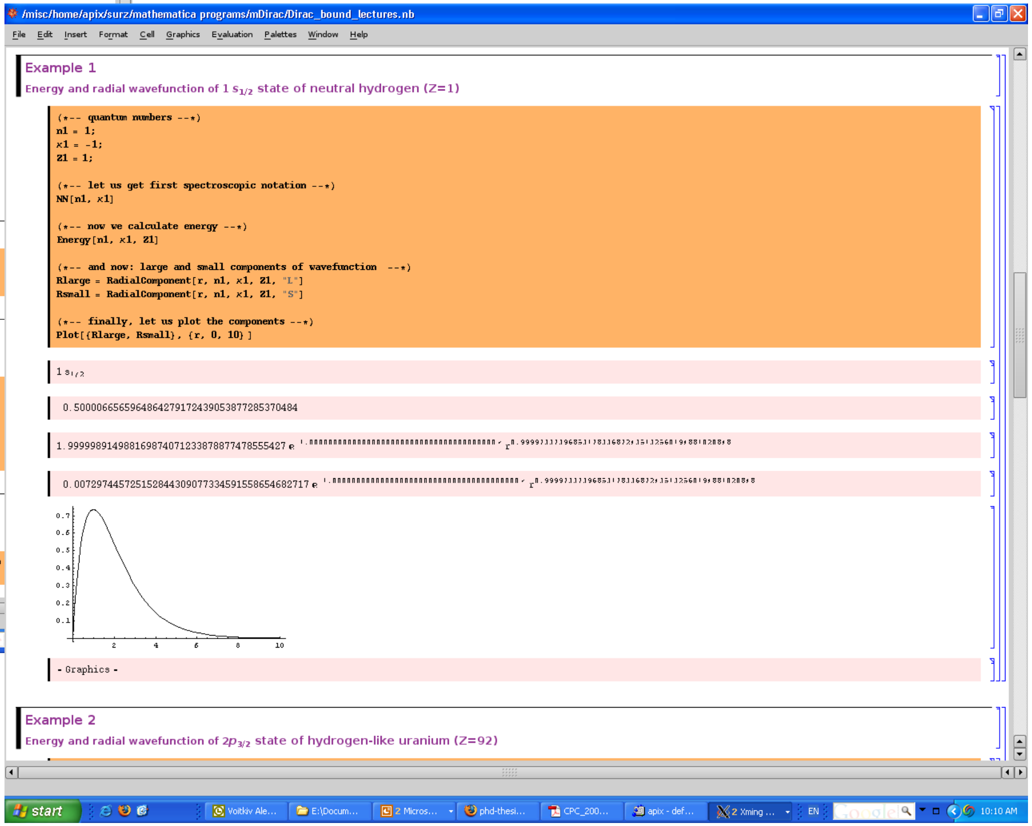
```
NN[nNN_, ϰ_] :=
  (
   resNN = Switch[ϰ, -4, "f7/2", -3, "d5/2", -2, "p3/2", -1, "s1/2", 1, "p1/2", 2, "d3/2", 3, "f5/2"];
   If[nNN == 1, {resNN = "1" resNN}];
   If[nNN ≠ 1, {resNN = nNN resNN}];
   Return[resNN]
  );
```

Dirac energy

Input data: principal quantum number n, Dirac quantum number ϰ, nuclear charge Z

Output data: energy of the bound state in atomic units

```
Energy[n_, kappa_, Z_] := 1/ (FineStructureConstant^2 * Sqrt[1 + (FineStructureConstant * Z / (n - Abs[kappa] + Sqrt[kappa^2 - (Z * FineStructureConstant)
   1 / FineStructureConstant^2;
```



/misc/home/apix/surz/mathematica programs/mDirac/Dirac_bound_lectures.nb

Example 1

Energy and radial wavefunction of 1 $s_{1/2}$ state of neutral hydrogen (Z=1)

```
(*-- quantum numbers --*)
n1 = 1;
ϰ1 = -1;
Z1 = 1;

(*-- let us get first spectroscopic notation --*)
NN[n1, ϰ1]

(*-- now we calculate energy --*)
Energy[n1, ϰ1, Z1]

(*-- and now: large and small components of wavefunction  --*)
Rlarge = RadialComponent[r, n1, ϰ1, Z1, "L"]
Rsmall = RadialComponent[r, n1, ϰ1, Z1, "S"]

(*-- finally, let us plot the components --*)
Plot[{Rlarge, Rsmall}, {r, 0, 10} ]
```

```
1 s1/2

0.50000665659648642791724390538772853704 84

1.9999989149881698740712338788774785554 27 e

0.00729744572515284430907733459155865468 2717 e

- Graphics -
```

Example 2

Energy and radial wavefunction of $2p_{3/2}$ state of hydrogen-like uranium (Z=92)

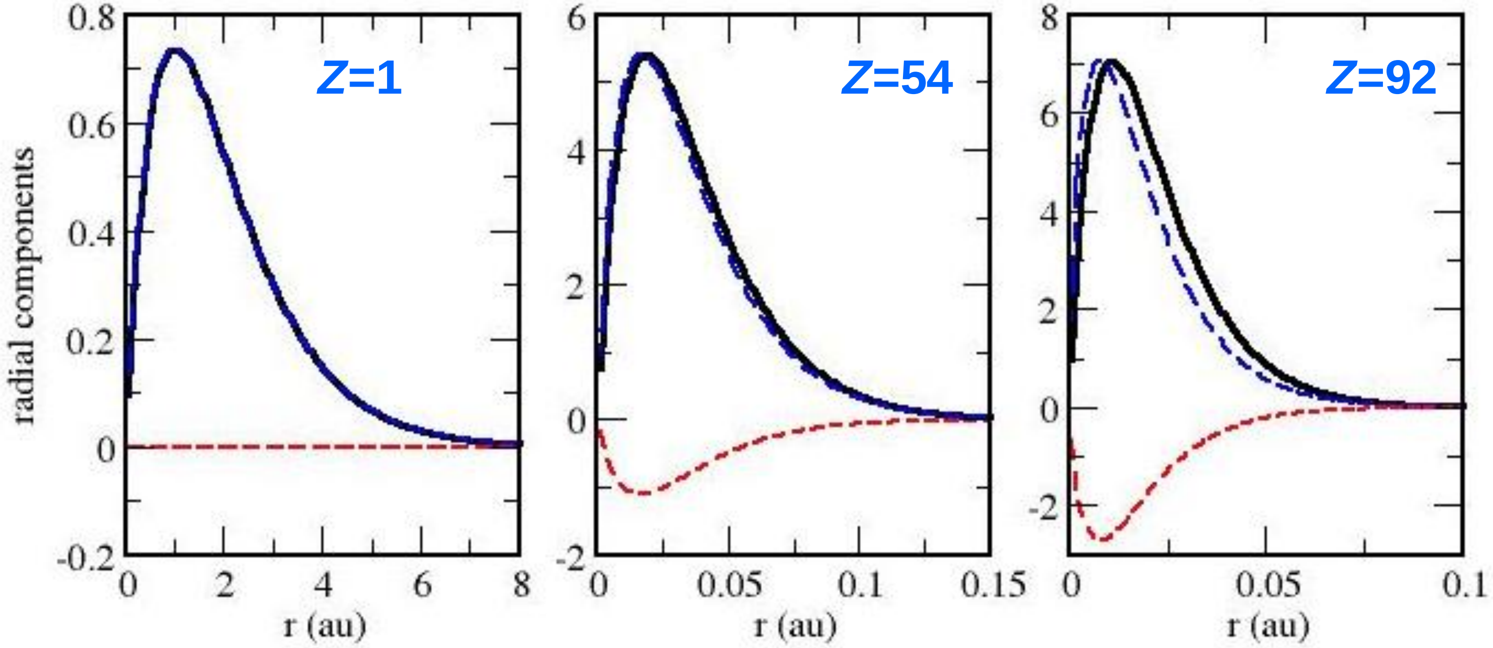
Dirac‘s radial components

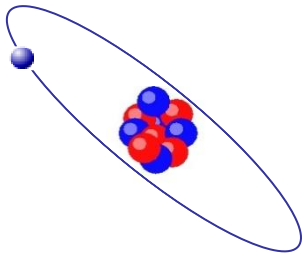
(...behaviour)

- **Let us consider radial components of the wavefunction**

$$\psi_{nljm_j}(\boldsymbol{r}) = \frac{1}{r}\begin{pmatrix} g_{nj}(r)\,\Omega_{ljm_j}(\hat{\boldsymbol{r}}) \\ i\,f_{nj}(r)\,\Omega_{l'jm_j}(\hat{\boldsymbol{r}}) \end{pmatrix}$$

for particular case of $1s_{1/2}$ ground state.

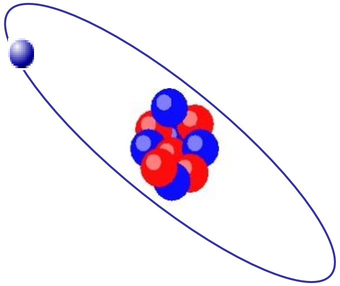




non-relativistic function
large component (rel)
small component (rel)

- **For low-Z regime: Dirac and Schrödinger wavefunctions basically coincides.**
- **For high-Z regime: small component becomes significant and ...**

Relativistic contraction of atomic orbitals



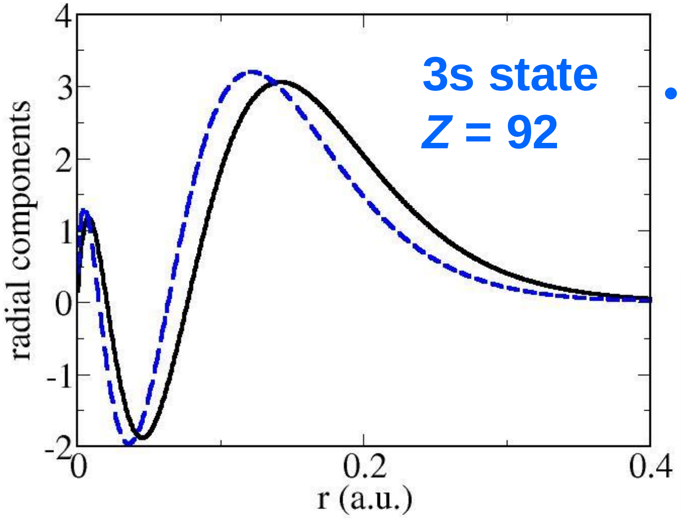
- **From the simple model one can "estimate" the electron "velocity" in the ground state:**

$$v = \boxed{(\alpha Z)}\, c$$

Speed of light

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

- **due to STR:** $\mathrm{m}_{\mathrm{el}} = \dfrac{\mathrm{m}^0_{\mathrm{el}}}{\sqrt{1-(v/c)^2}}$ **(electron becomes heavier)**
- **due to simple Bohr's model:** $r_n \propto \dfrac{n^2}{Z\,\mathrm{m}_{\mathrm{el}}}$



As the electron's mass increases, the radius of an orbit with constant angular momentum shrinks proportionately.

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)