Modern Atomic Physics

Experiments and Theory

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Motivation

You may ask: “I learned already atomic physics and quantum mechanics. What can I expect more from this course?”

What did we learn in “basic” quantum mechanics and atomic physics?

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Basics of quantum mechanics

In Quantum physics, Schrödinger equation describes how the quantum state of physical system evolves with time:

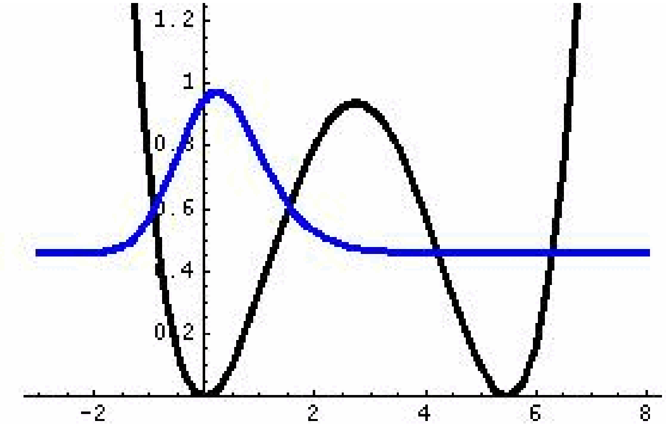
Erwin Schrödinger

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

Wave function

Hamiltonian operator

Define your system, define its initial state and you can find the state of the system in any moment of time *t*.



Schrödinger equation for single particle

For single particle Schrödinger equation reads:

$$i\hbar \frac{\partial \psi(\mathbf{r},t)}{\partial t} = \underbrace{-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r},t)}_{\text{kinetic term}} + \underbrace{U(\mathbf{r})\psi(\mathbf{r},t)}_{\text{potential term}}$$

If Hamiltonian does not depend on time, one can easily derive time-independent Schrödinger equation:

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

We have to solve eigenproblem!

Schrödinger equation in 1D case

Schrödinger equation (time-independent):

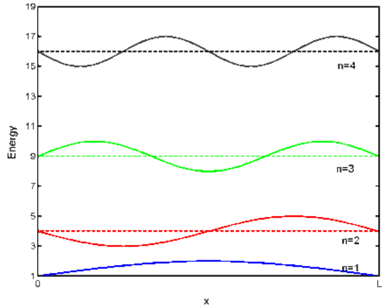
$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x)+U(x)\psi(x)=E\psi(x)$$

Potential

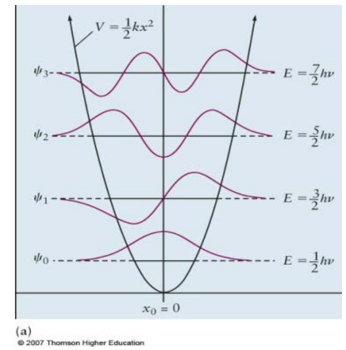
Wavefunction

Schrödinger equation opened a way of systematic analysis of quantum phenomena:

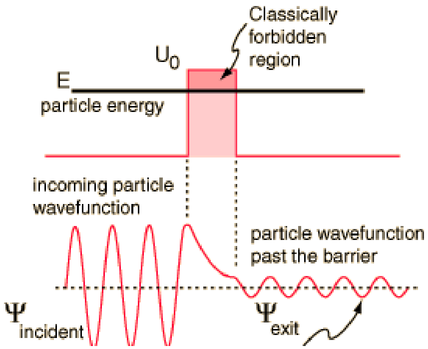
- tunneling
- particle confinement
- molecular vibrations
- hydrogen structure
- many-electron ions
- ….



$$U(x) = \begin{cases} 0 & 0 \le x \le L \\ \infty & otherwise \end{cases}$$



$$U(x) = \frac{kx^2}{2}$$



$$U(x) = \begin{cases} U_0 & 0 \le x \le L \\ 0 & otherwise \end{cases}$$

Pictures from HyperPhysics

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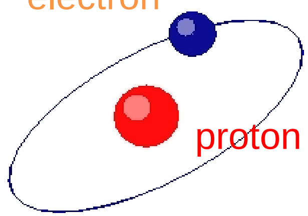
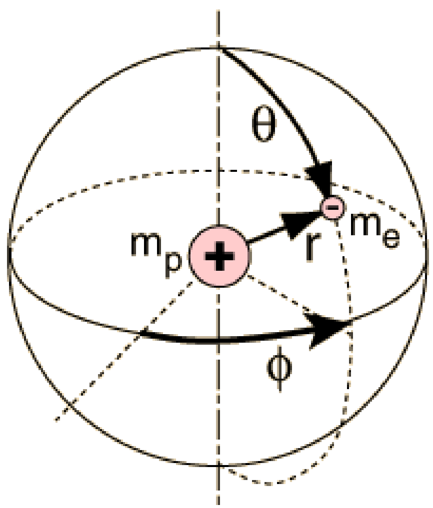
"Hydrogen atom" model

A textbook example of "hydrogen atom" – one of the basis models of quantum mechanics.





- 3D Schrödinger equation (time-independent):

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

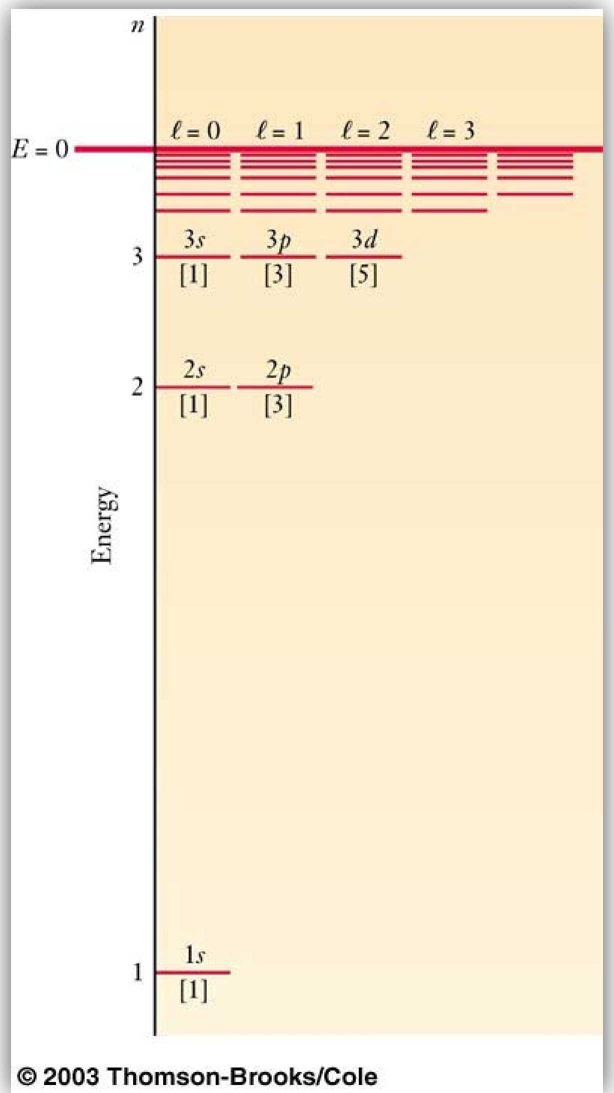
- Where Coulomb potential is:

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

- Indeed, we know how to find solutions (wavefunctions and energies) of this system.

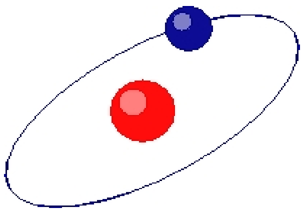
Pictures from HyperPhysics

“Hydrogen atom” model: Solutions



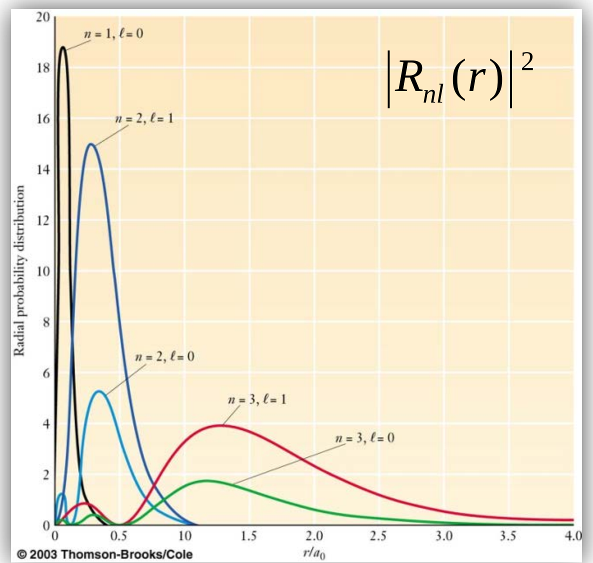
- Energy values of “hydrogen atom” are given by:

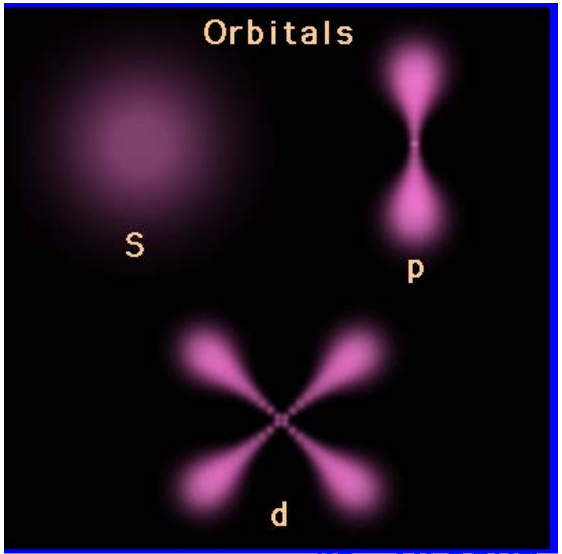
$$E_n = -\frac{\varepsilon_0 Z^2}{2n^2}$$



- … and wavefunctions:

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





Pictures from HyperPhysics

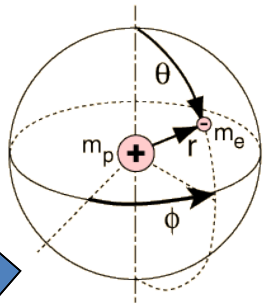
Motivation

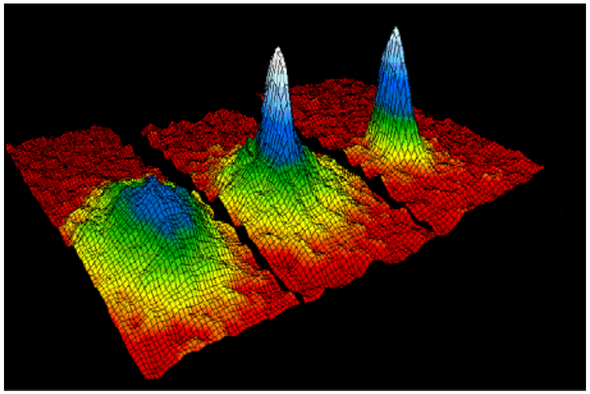
What is atomic physics today?

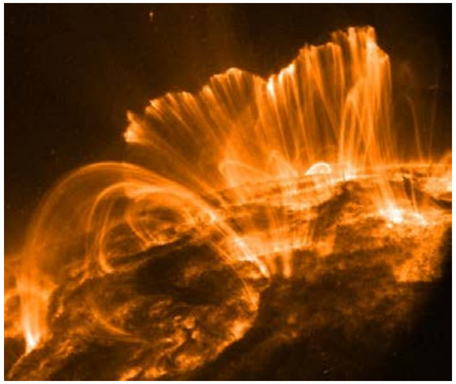
Modern atomic physics

Very roughly we can say that the present-day atomic physics focuses on extreme regimes: either very cold or very hot.

… and very precise!







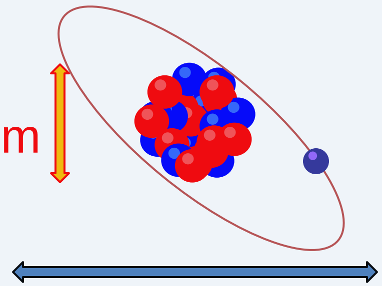
In our course we shall focus mainly on the high-energy (temperature, field-strength,…) part of the modern atomic physics.

Hydrogen-like ions: Properties

- What is so special about these ions?

- Size of the system

(nuclear size)
R ~ 10^{-14} m



(electron orbit)
r ~ 10^{-13} m

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

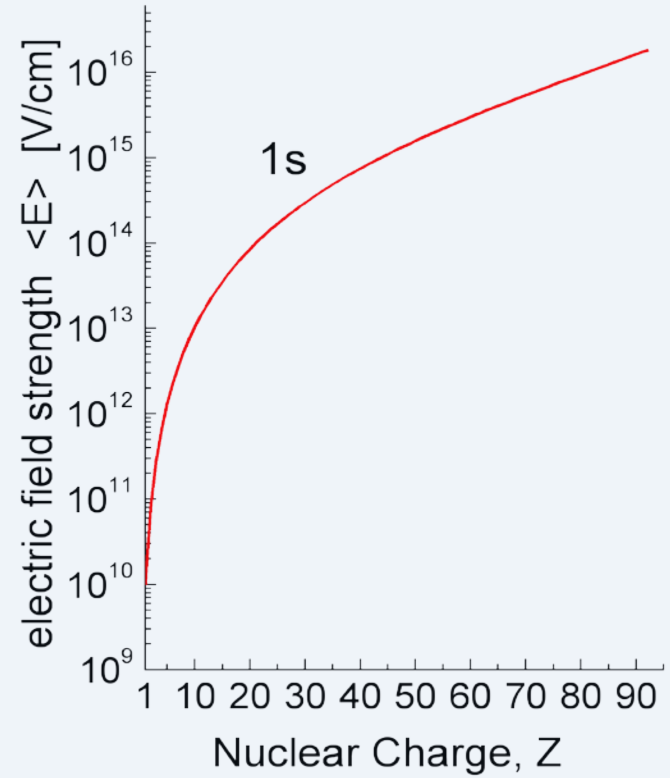
$$v_{el} \approx \alpha\, Z\, c$$

$$\alpha \approx 1/137$$

$$\alpha Z \approx 0.67$$

for H-like Uranium

- Electron is exposed to extremely strong EM filed.



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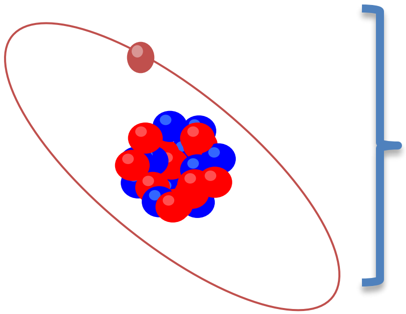
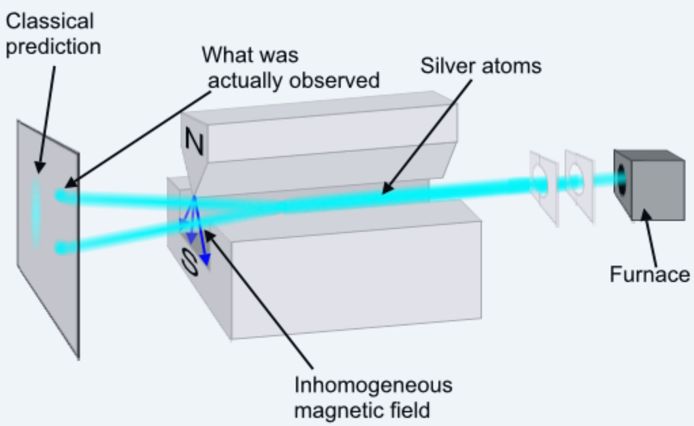
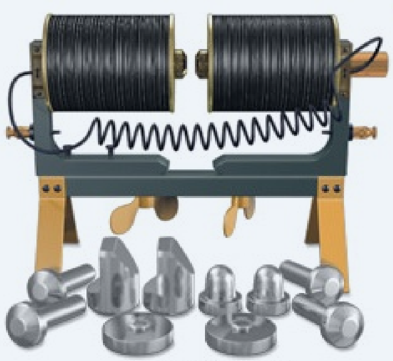
Heavy ions: Spin effects



- Relativistic electron, exposed to extremely strong electromagnetic filed as produced by the nucleus…
- … and having <u>spin</u>!





Zeeman Effect (circa 1896)

- Both, Stern-Gerlach and Zeeman experiment have suggested existence of *magnetic* properties of atomic systems!
- In classical electrodynamics magnetic moment interacts with B field as: $U = -\boldsymbol{\mu} \cdot \boldsymbol{B}$

Atomic physics of heavy ions

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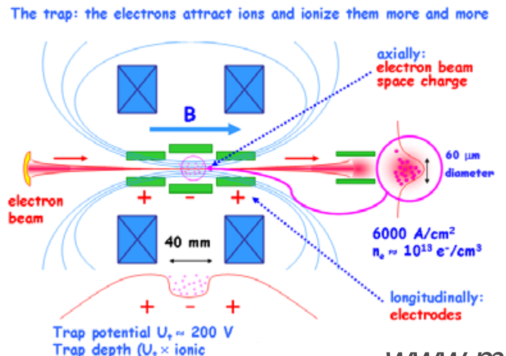

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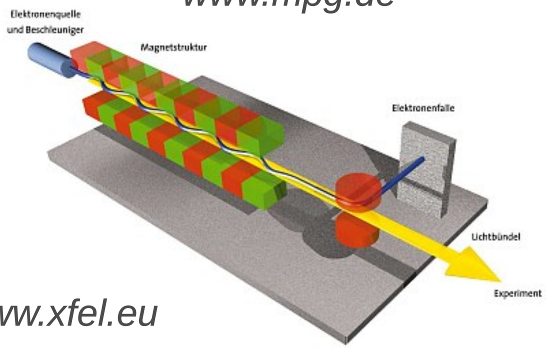

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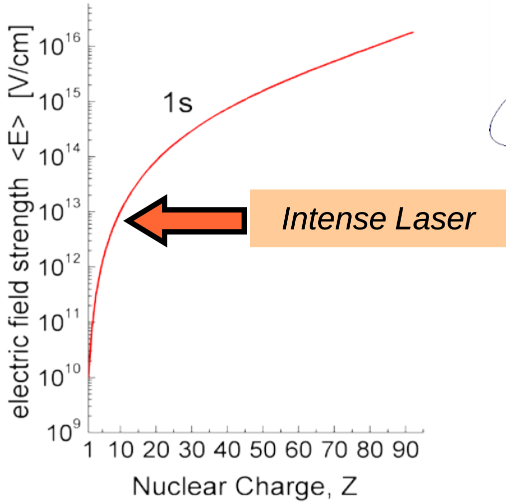
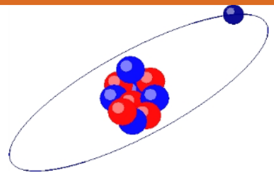
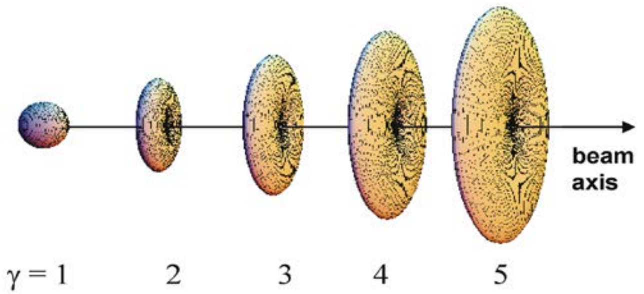




Studying of atomic systems
at extreme conditions:

- very strong fields
- very high velocities
- very short times



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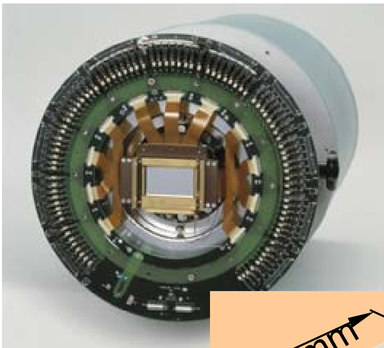
Atomic physics of heavy ions



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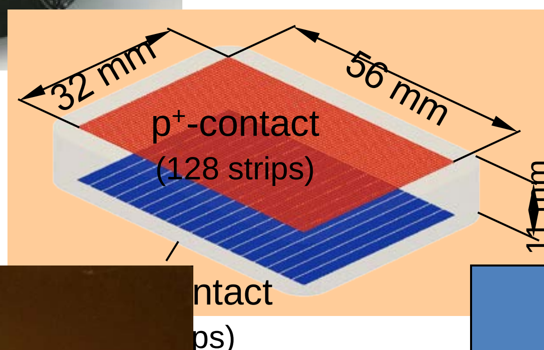
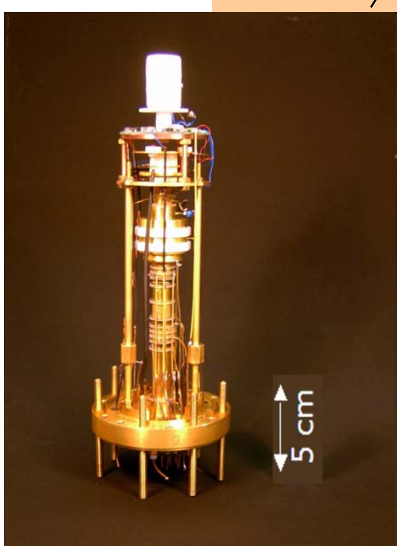
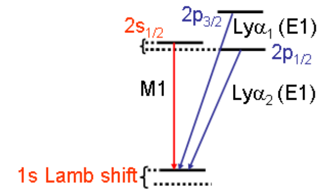
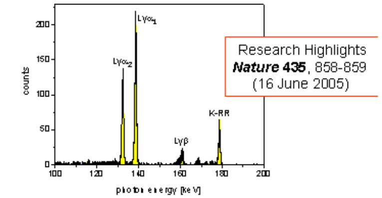
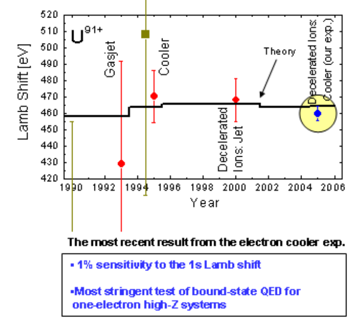


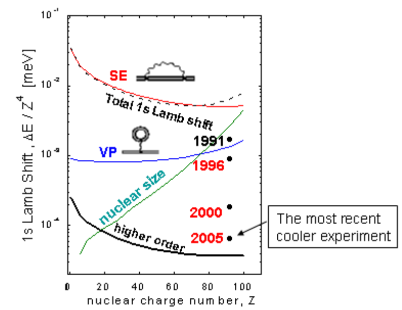


www.quantum.physik.uni-mainz.de

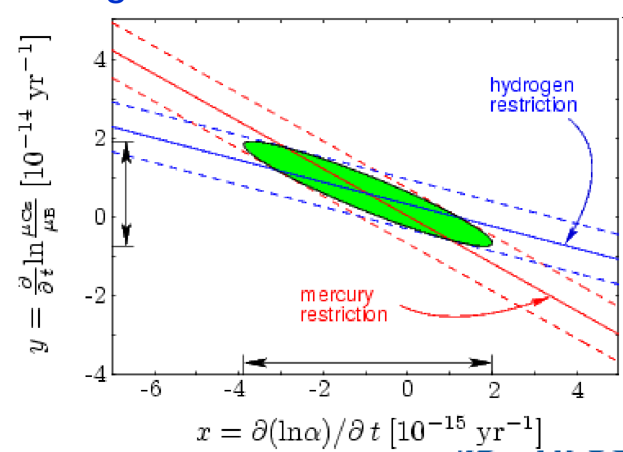


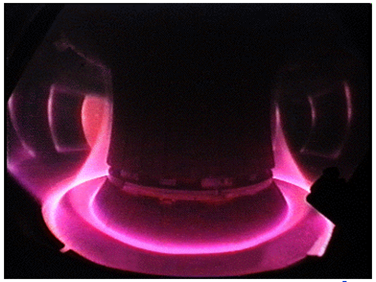






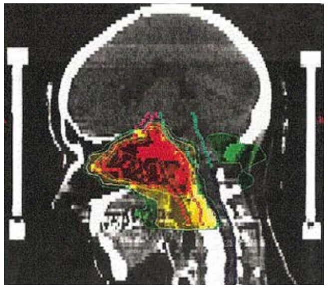
Extremely high precision experiments with ensembles of atoms/ions and even single ions!





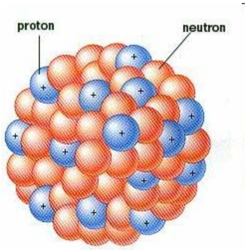
Plasma physics

Astrophysics

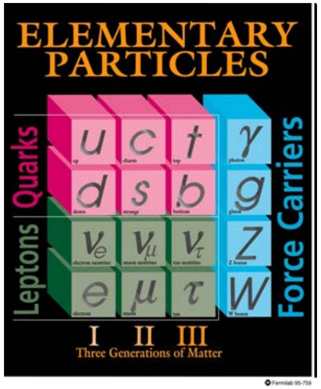


Medical research
and Biophysics

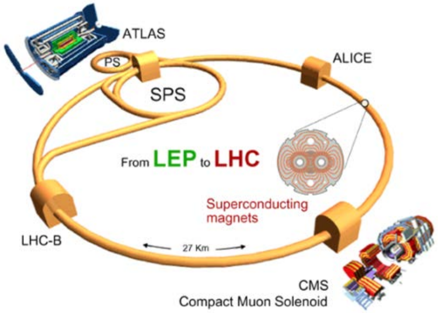
Atomic physics



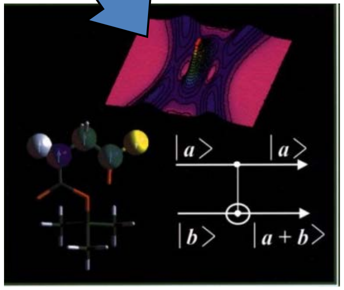
Nuclear physics



“New physics” beyond
the Standard Model



Accelerator physics



Quantum information

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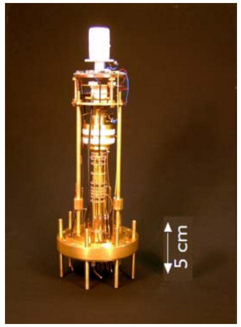
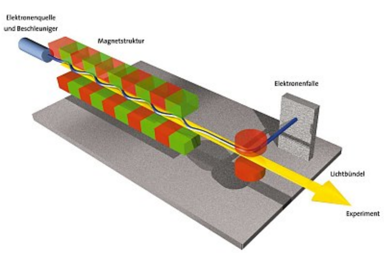
Modern atomic physics:
From experiment to theory and back



Studying of atomic systems
at <u>extreme</u> conditions:

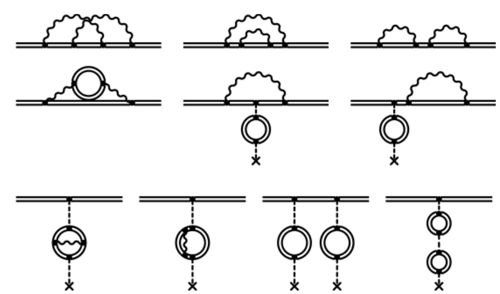
- very strong fields
- very high velocities
- very short times



$$\left(\alpha_0 mc^2+\sum_{j=1}^{3}\alpha_j p_j c\right)\psi(x,t)=i\hbar\frac{\partial\psi}{\partial t}(x,t)$$

One has to understand the:

- relativistic phenomena
- QED effects
- spin phenomena
- interelectronic interactions
- interplay with nuclear physics



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Preliminary plan of the lectures

- 1 15.04.2015 Preliminary Discussion / Introduction

- 2 22.04.2015 Experiments (discovery of the positron, formation of antihydrogen, ...)
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- 4 06.05.2015 Theory (from Schrödinger to Dirac equation, solutions with negative energy)
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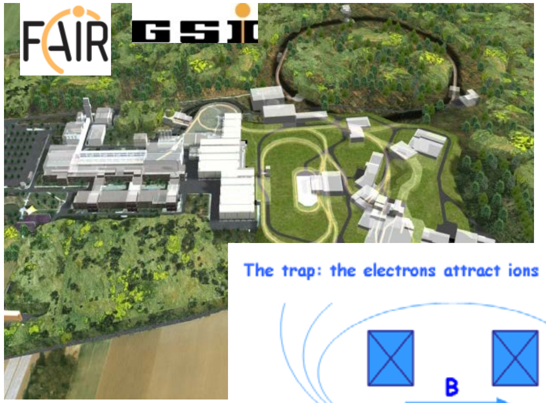
One electron heavy ions: Strong fields, relativity, QED



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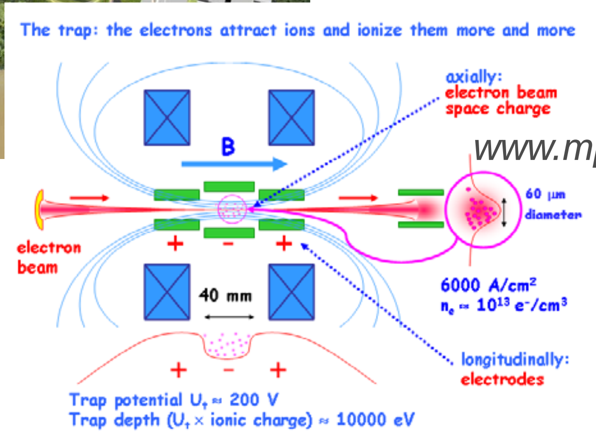

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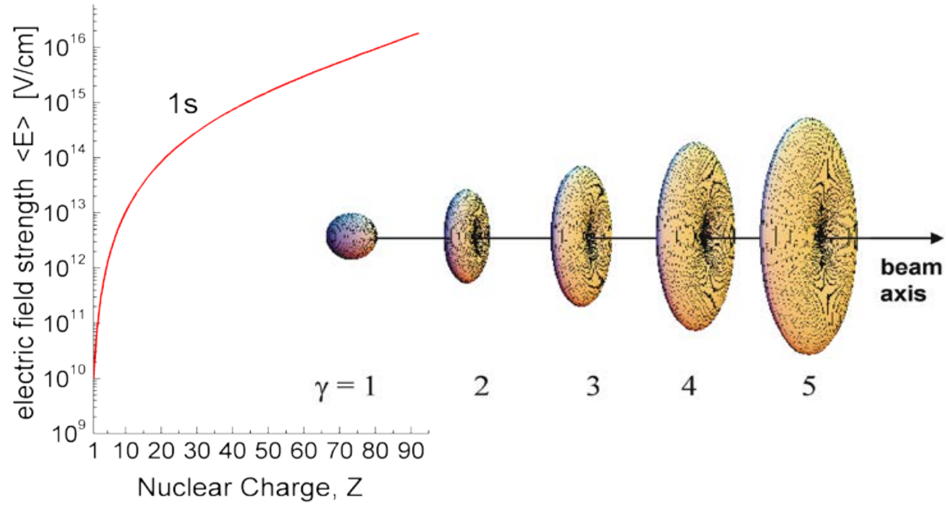

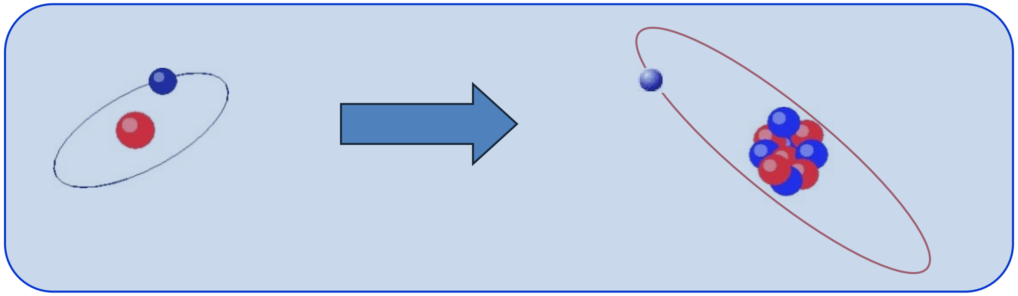

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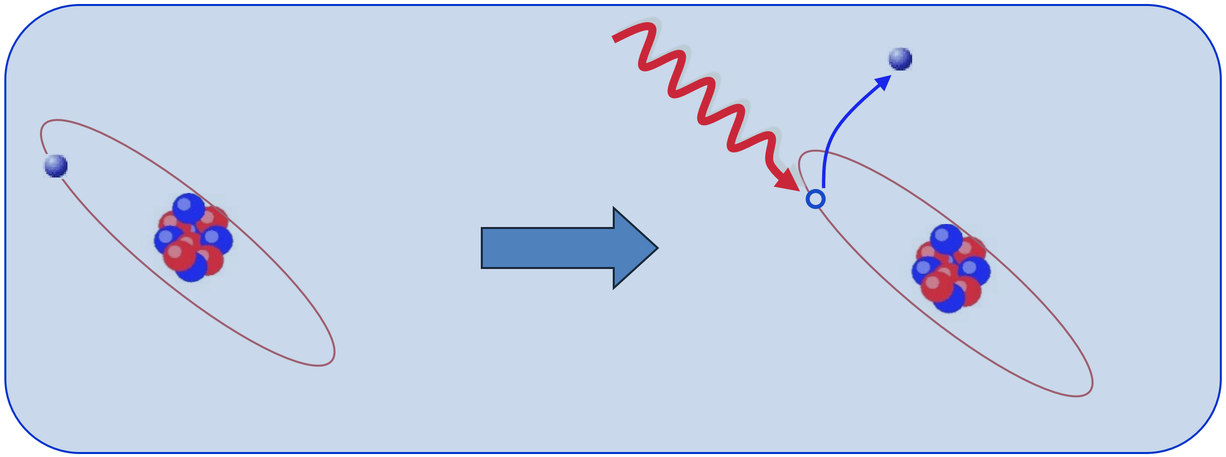
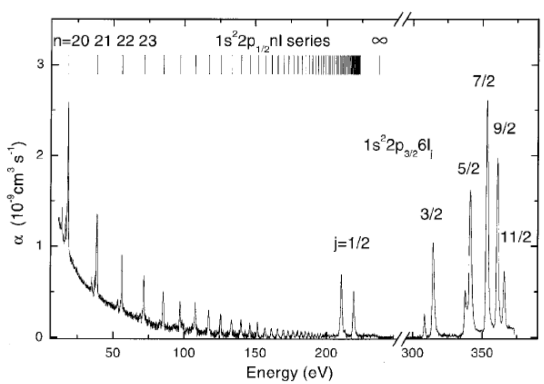
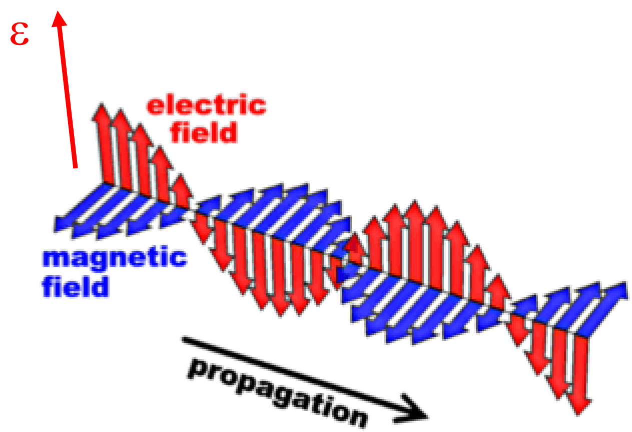
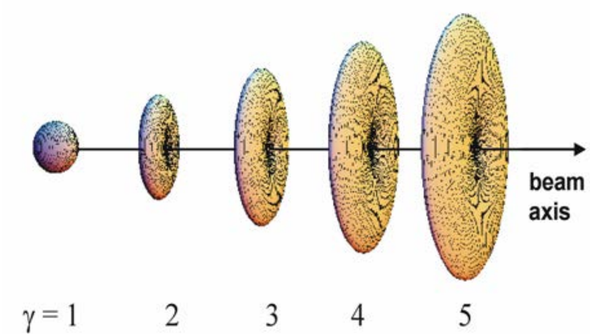
Atomic dynamics: Collisions, interaction with EM fields, penetration trough matter



$$M_{ab} = \left\langle \psi_b \middle| \boldsymbol{\alpha}\,\boldsymbol{\varepsilon}\, e^{i\mathbf{kr}} \middle| \psi_a \right\rangle \equiv \int \psi_b^{+}(\mathbf{r})\, \boldsymbol{\alpha}\,\boldsymbol{\varepsilon}\, e^{i\mathbf{kr}}\, \psi_a(\mathbf{r})\, d\mathbf{r}$$







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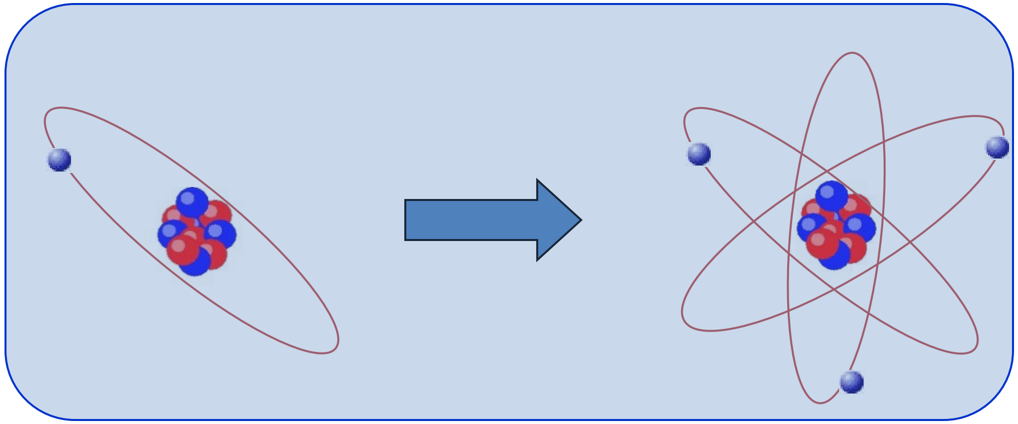
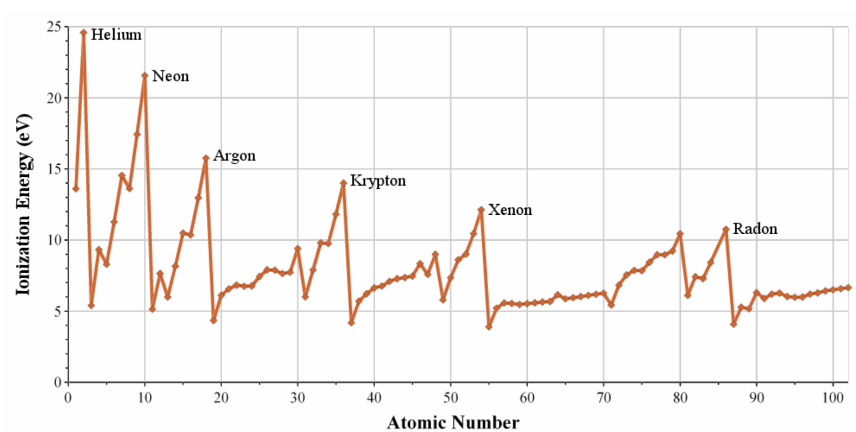
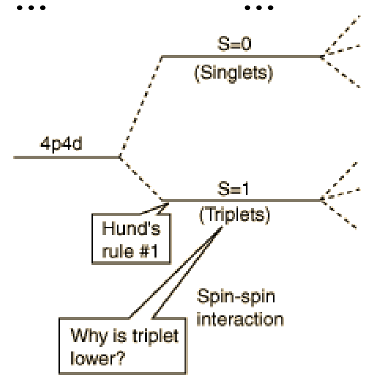
Many-electron ions and atoms: Interelectronic interaction effects



$$\Psi(\boldsymbol{r}_1,\boldsymbol{r}_2,\ldots)=\frac{1}{\sqrt{N!}}\sum_{\mu_a,\mu_b,\mu_c,\ldots} d(j_a\mu_a, j_b\mu_b, j_c\mu_c,\ldots : JM)\begin{vmatrix} \psi_{n_a j_a \mu_a}(\boldsymbol{r}_1) & \psi_{n_b j_b \mu_b}(\boldsymbol{r}_1) & \psi_{n_c j_c \mu_c}(\boldsymbol{r}_1) & \cdots \\ \psi_{n_a j_a \mu_a}(\boldsymbol{r}_2) & \psi_{n_b j_b \mu_b}(\boldsymbol{r}_2) & \psi_{n_c j_c \mu_c}(\boldsymbol{r}_2) & \cdots \\ \psi_{n_a j_a \mu_a}(\boldsymbol{r}_3) & \psi_{n_b j_b \mu_b}(\boldsymbol{r}_3) & \psi_{n_c j_c \mu_c}(\boldsymbol{r}_3) & \cdots \\ \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots \end{vmatrix}$$





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Preliminary plan of the lectures

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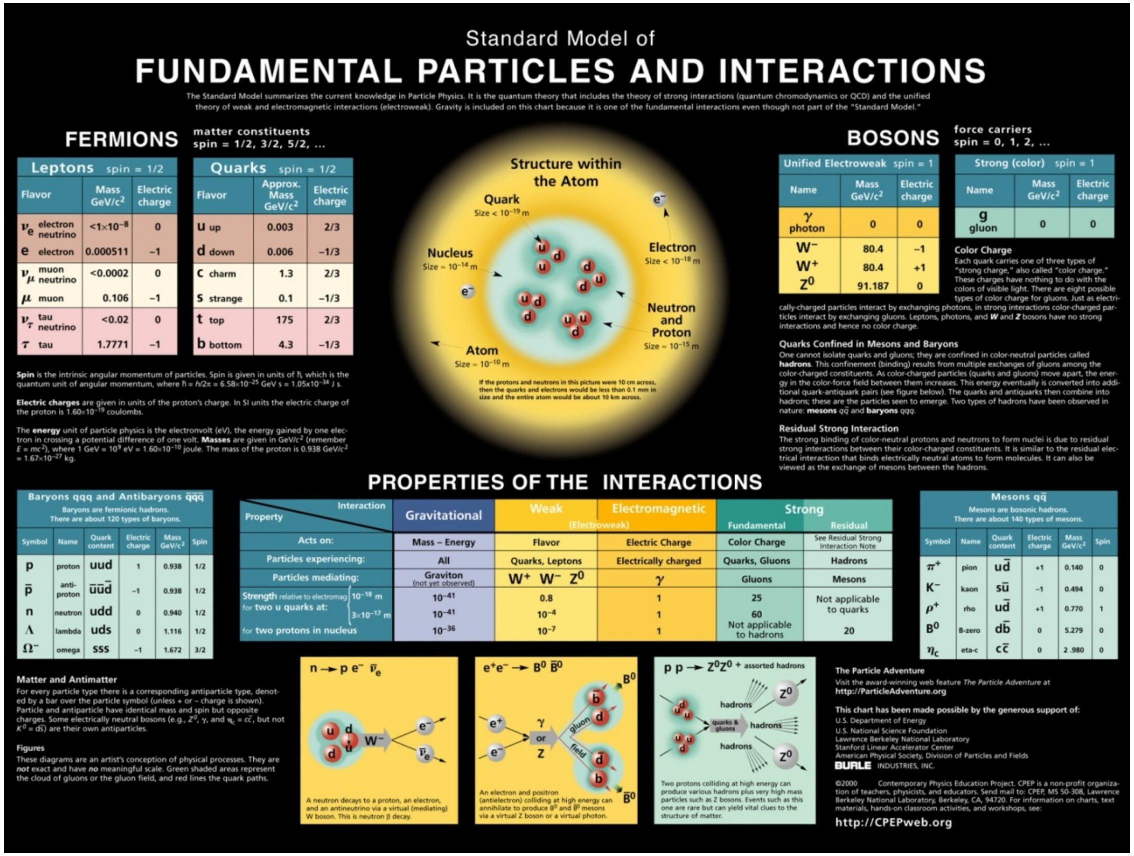
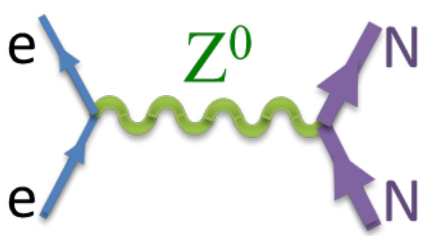
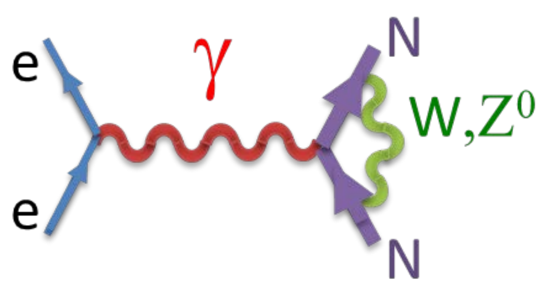
Atomic parity-violation experiments



- Standard Model suggests the unified description of the electromagnetism and the weak interaction.
- Note that electromagnetic interaction preserves parity while weak interaction – not!





Literature and I-net sources

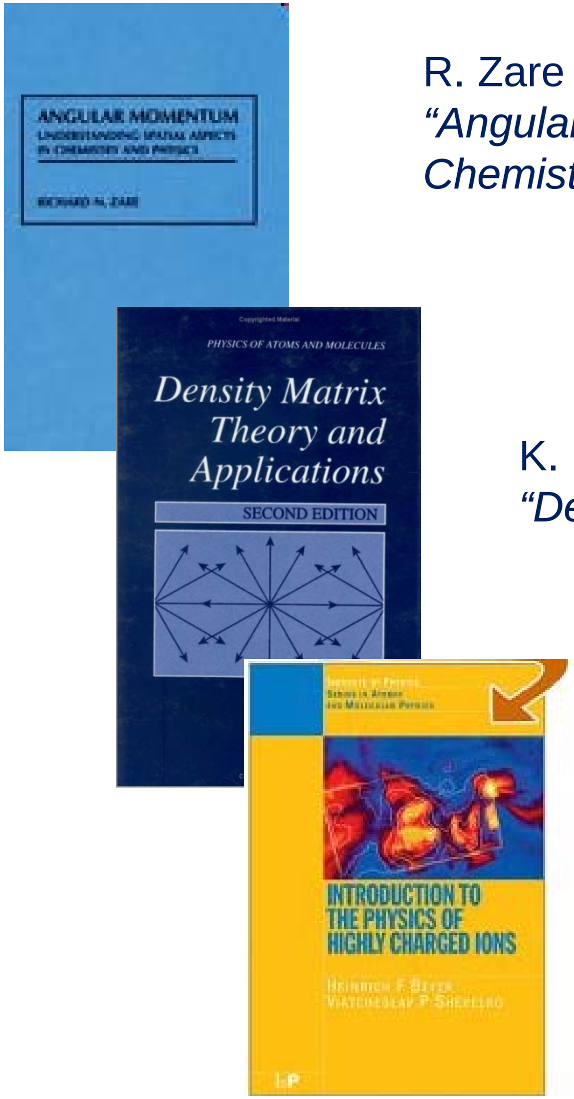
Basic literature

B.H. Bransden and C.J. Joachin
“Physics of Atoms and Molecules”

H. A. Bethe and E. E. Salpeter
“Quantum Mechanics of One- and Two-Electron Atoms”

J. Eichler and W. E. Meyerhof
“Relativistic Atomic Collisions”
Or
J. Eichler
“Lectures on Ion-Atom Collisions”

Additional literature



R. Zare
“Angular Momentum: Understanding Spatial Aspects in Chemistry and Physics”

K. Blum
“Density Matrix Theory and Applications”

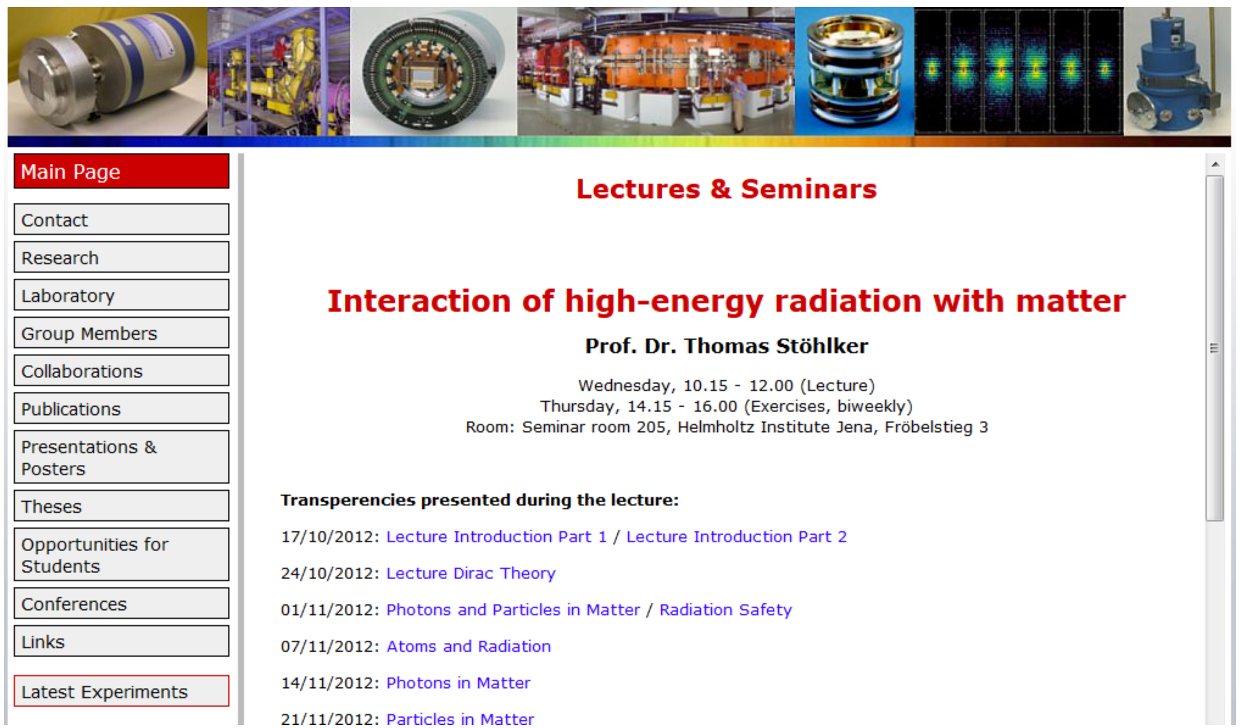
H.F. Beyer and V.P. Shevelko
“Introduction to Physics of Highly Charged Ions”

Lectures in Internet

Find zipped .PPT & .PDF files with the lectures at:

http://web-docs.gsi.de/~stoe_exp/lectures/lectures.php

(password: dirac2015)



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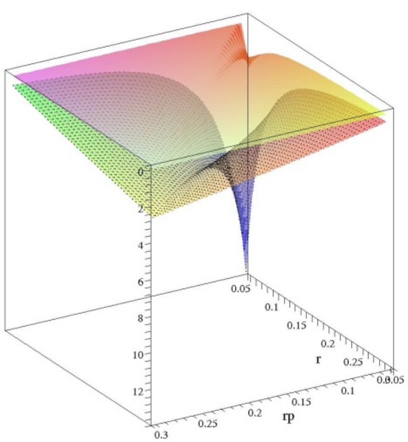
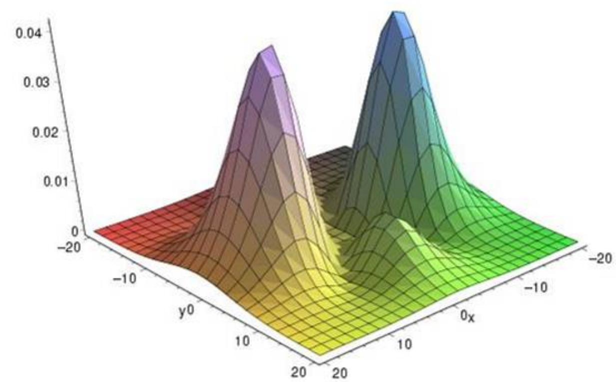
Mathematica library

Set of Mathematica programs will be provided for:

- Calculation of the energy levels
- Evaluation of the nonrelativistic as well as relativistic wavefunctions
- Cross section calculations
- ….





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Mathematica library

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

File Edit Insert Format Cell Graphics Evaluation Palettes Window Help

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 Lecture 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[7.297352533000000000000000000000000 / 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)^2]))^2]) -
   1/FineStructureConstant^2;
```

General

http://hyperphysics.phy-astr.gsu.edu/hbase/hframe.html

NIST Physical Reference Data - X-Ray and Gamma-Ray Data

http://physics.nist.gov/PhysRefData/contents-xray.html

Fundamental Physical Constants

http://physics.nist.gov/PhysRefData/contents-constants.html

Atomic Spectroscopic Data

http://physics.nist.gov/PhysRefData/contents-atomic.html

X-Ray World Wide Web Server

X-ray Emission Lines http://xray.uu.se/hypertext/XREmission.html
Electron Binding Energies http://xray.uu.se/hypertext/EBindEnergies.html

Berkeley National Laboratory

Table of Isotopes http://ie.lbl.gov/education/isotopes.htm
Atomic Data http://ie.lbl.gov/atomic/atom.htm
Elemental Physical Properties http://ie.lbl.gov/elem/elem.htm (pdf download possible)

CODATA Internationally recommended values of the Fundamental Physical Constants

http://physics.nist.gov/cuu/Constants/index.html

Institute of Chemistry, Free University Berlin

Fundamental Physical Constants http://www.chemie.fu-berlin.de/chemistry/general/constants_en.html
Conversion of Units http://www.chemie.fu-berlin.de/chemistry/general/units_en.html

Periodic tables (professional edition)

http://www.webelements.com/

Korea Atomic Energy Research Institute

Table of Nuclides http://atom.kaeri.re.kr/ton/nuc6.html

Center for Synchrotron Radiation Research and Instrumentation, Chicago, United States

Periodic Table of Elements - X-ray properties

http://www.csrri.iit.edu/periodic-table.html

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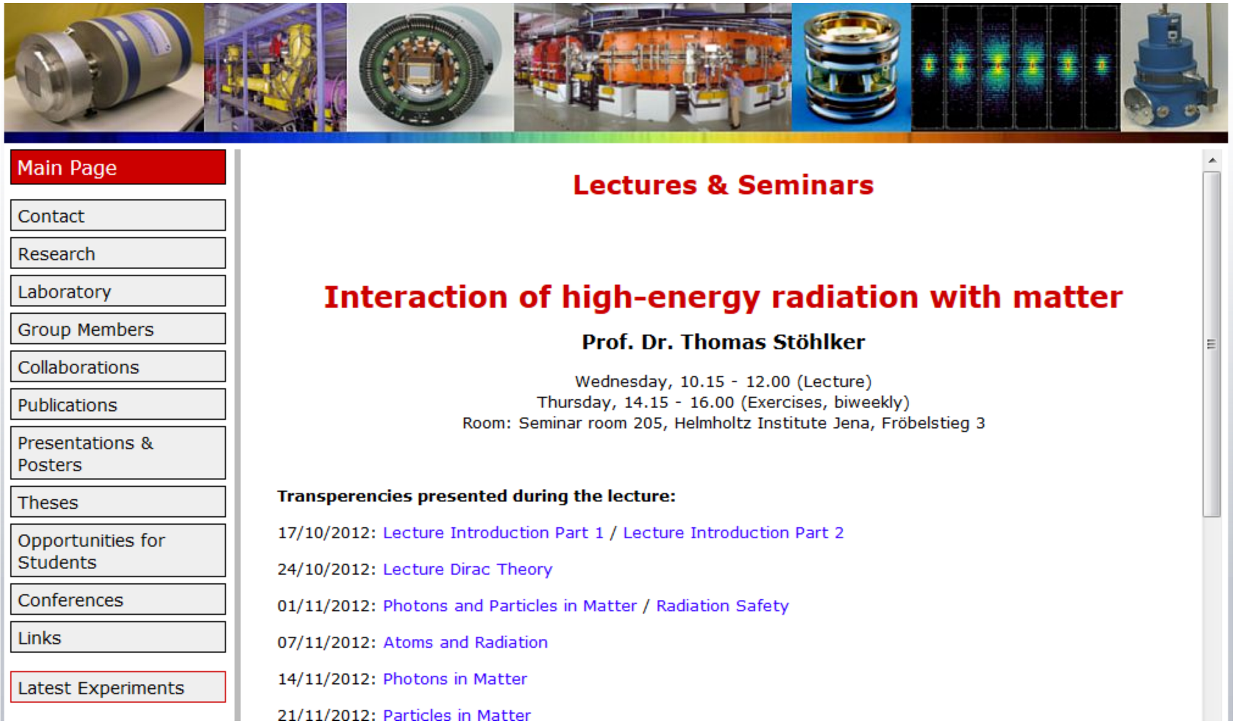

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Interaction of high-energy radiation with matter

Prof. Dr. Thomas Stöhlker

Wednesday, 10.15 - 12.00 (Lecture)
Thursday, 14.15 - 16.00 (Exercises, biweekly)
Room: Seminar room 205, Helmholtz Institute Jena, Fröbelstieg 3

Transperencies presented during the lecture:

17/10/2012: Lecture Introduction Part 1 / Lecture Introduction Part 2

24/10/2012: Lecture Dirac Theory

01/11/2012: Photons and Particles in Matter / Radiation Safety

07/11/2012: Atoms and Radiation

14/11/2012: Photons in Matter

21/11/2012: Particles in Matter