

# 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?

# Basics of quantum mechanics

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

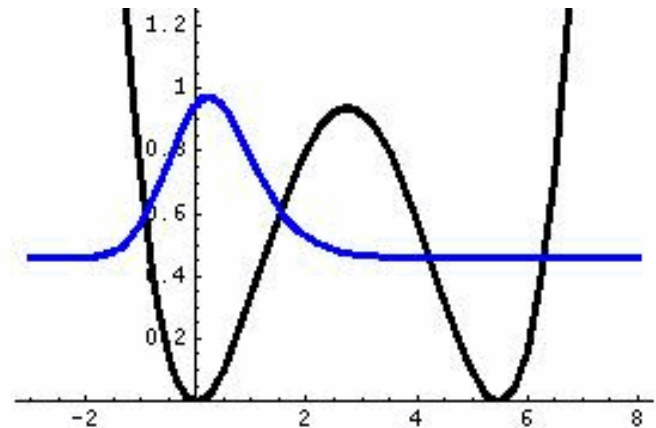
$$i\hbar \frac{\partial \psi(\mathbf{r}, t)}{\partial t} = \hat{H} \psi(\mathbf{r}, t)$$

Wave function Hamiltonian operator



Erwin Schrödinger

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

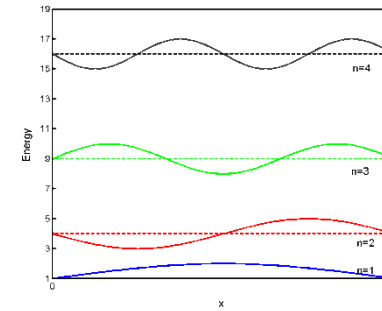
Schrödinger equation (time-independent):

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

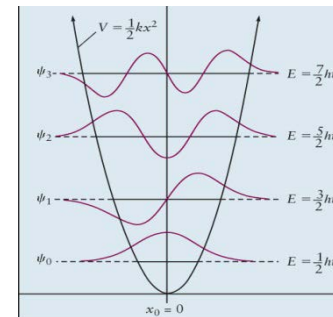
↑ Potential
↑ Wavefunction

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

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

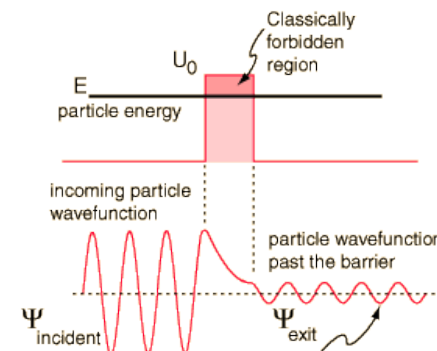


$$U(x) = \begin{cases} 0 & 0 \leq x \leq L \\ \infty & \text{otherwise} \end{cases}$$



(a) © 2007 Thomson Higher Education

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

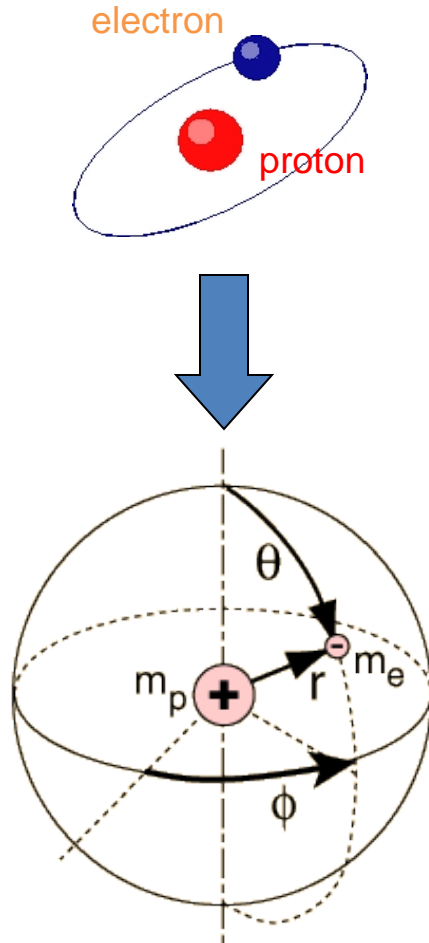


$$U(x) = \begin{cases} U_0 & 0 \leq x \leq L \\ 0 & \text{otherwise} \end{cases}$$

Pictures from HyperPhysics

# “Hydrogen atom” model

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



- ◆ 3D Schrödinger equation (time-independent):

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

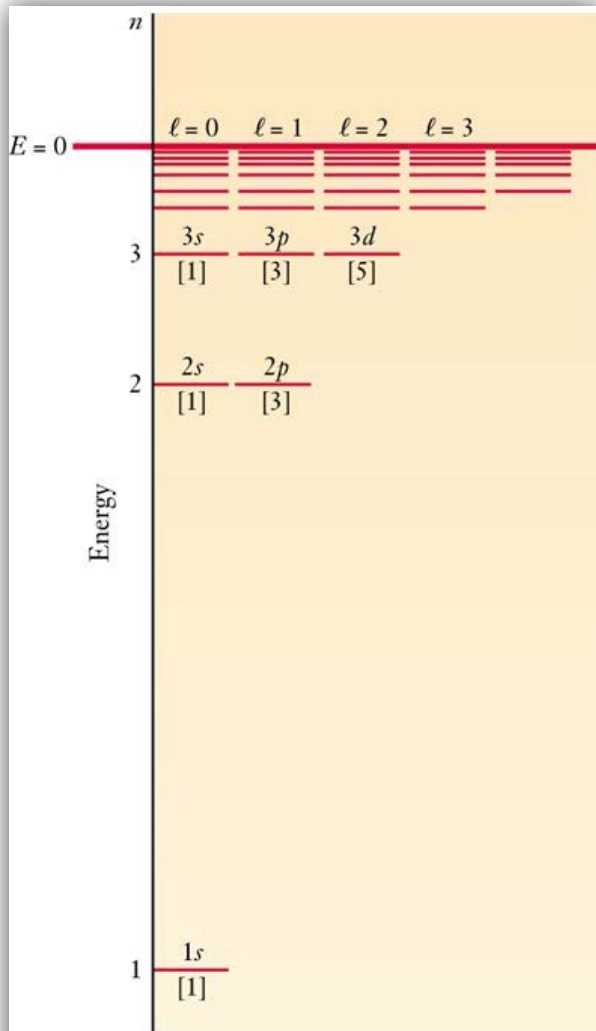
- ◆ Where Coulomb potential is:

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

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



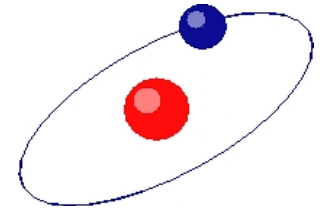
# “Hydrogen atom” model: Solutions



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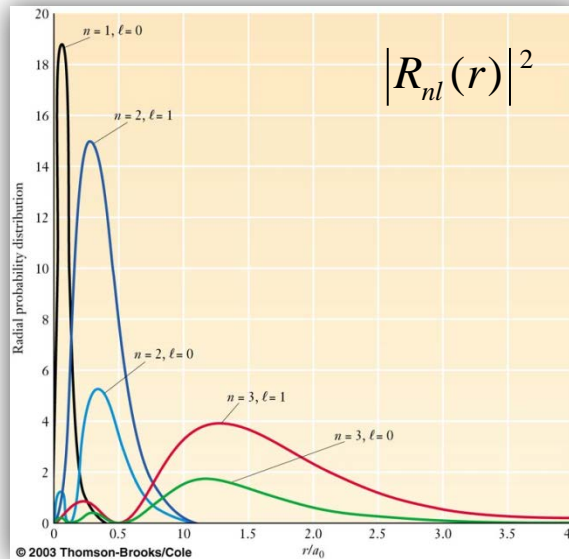
- ▶ Energy values of “hydrogen atom” are given by:

$$E_n = -\frac{\epsilon_0 Z^2}{2n^2}$$

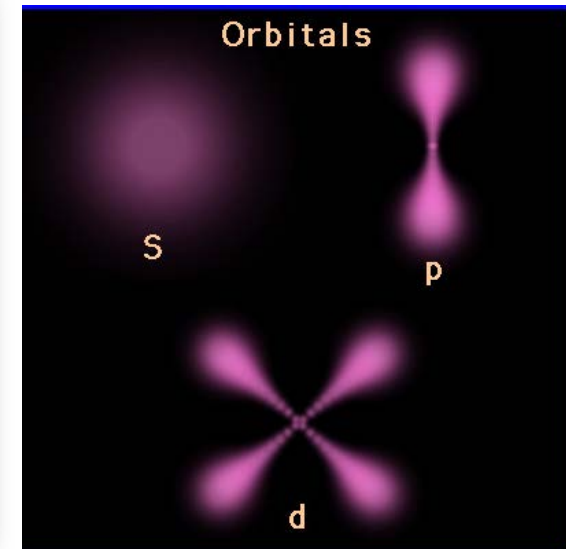


- ▶ ... and wavefunctions:

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



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Pictures from HyperPhysics

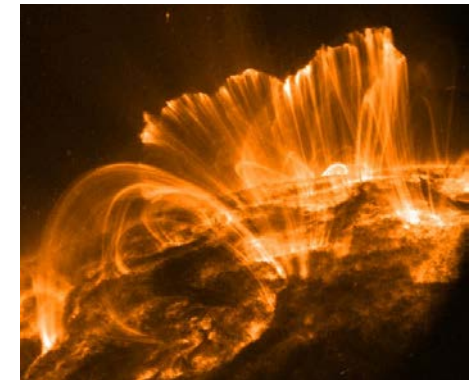
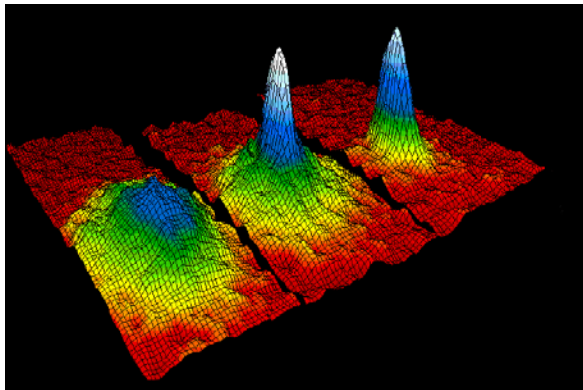
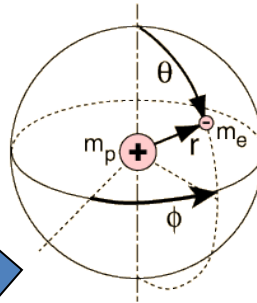
# Motivation

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!

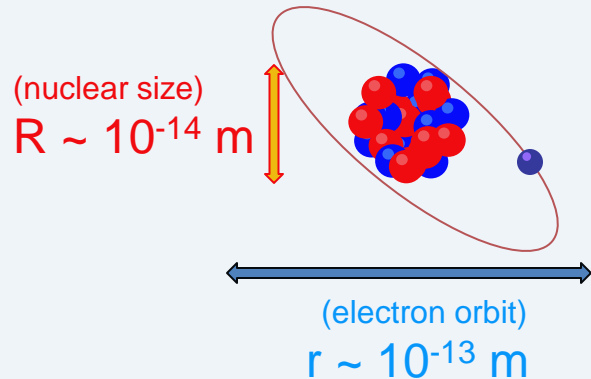


In our course we shall focus mainly on the high-energy (temperature, field-strength,...) part of the modern atomic physics.

# Hydrogen-like ions: Properties

## ► What is so special about these ions?

### ● Size of the system

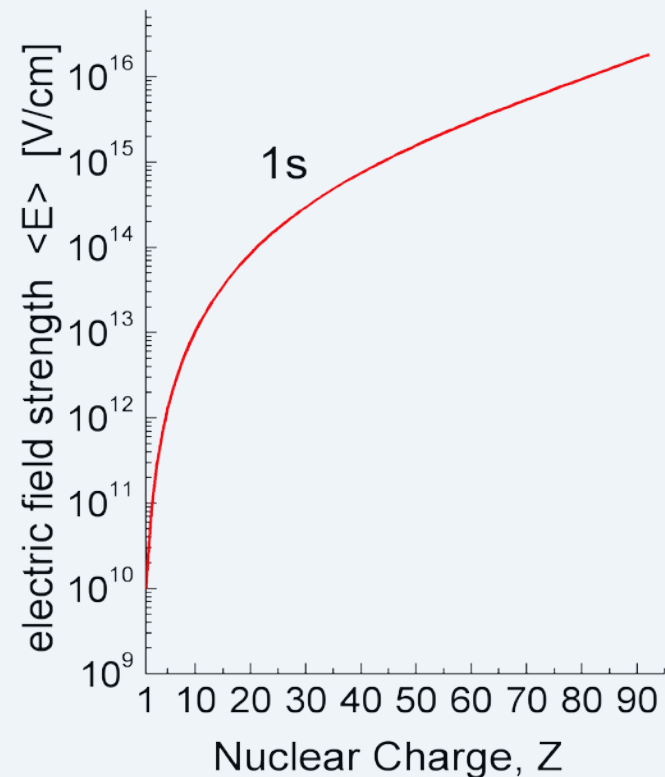


### ● From the simple model one can “estimate” the electron “velocity” in the ground state:

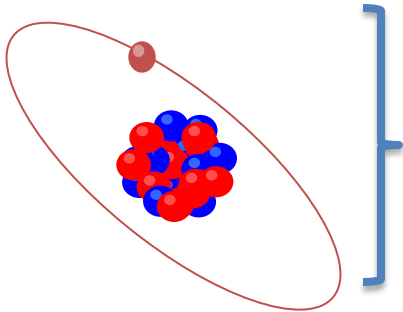
$$v_{el} \approx \alpha Z c$$
$$\alpha \approx 1/137 \quad \Rightarrow \quad \alpha Z \approx 0.67$$

for H-like Uranium

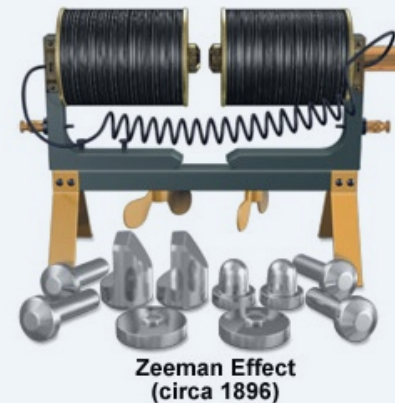
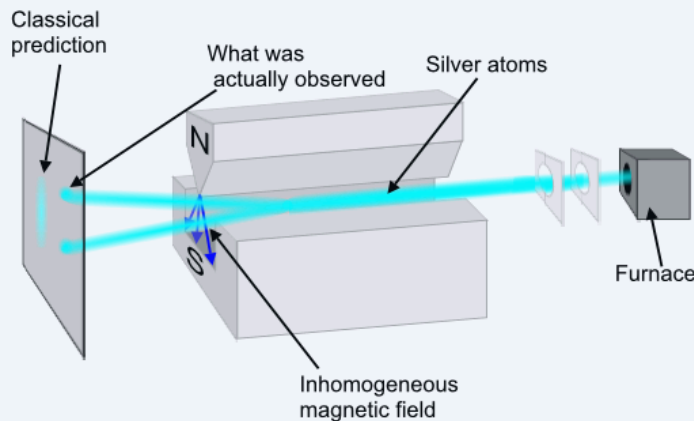
### ● Electron is exposed to extremely strong EM field.



# Heavy ions: Spin effects



- ▶ Relativistic electron, exposed to extremely strong electromagnetic field as produced by the nucleus...
- ▶ ... and having spin!



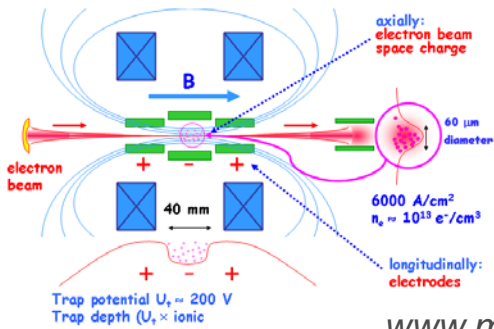
- ▶ Both, Stern-Gerlach and Zeeman experiment have suggested existence of *magnetic* properties of atomic systems!
- ▶ In classical electrodynamics magnetic moment interacts with B field as:  $U = -\boldsymbol{\mu} \cdot \mathbf{B}$

# Atomic physics of heavy ions

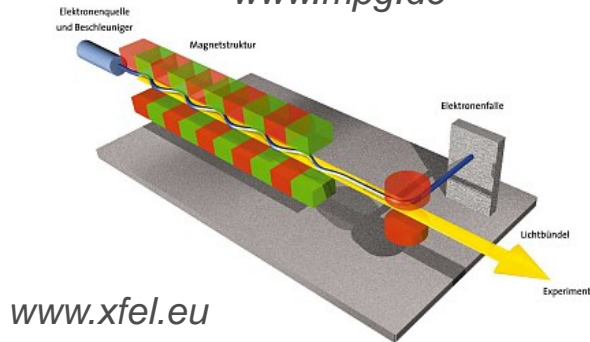


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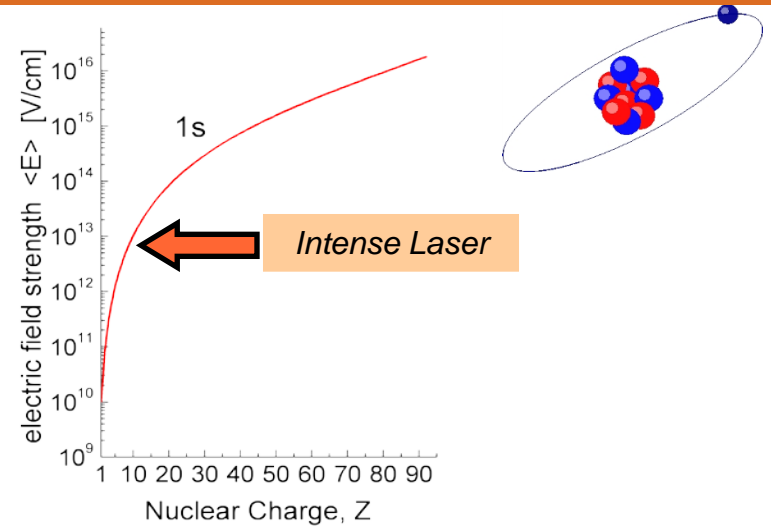
The trap: the electrons attract ions and ionize them more and more



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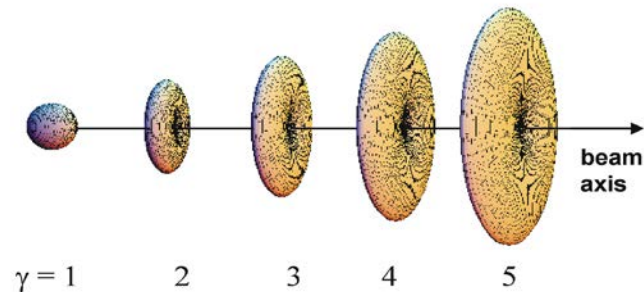


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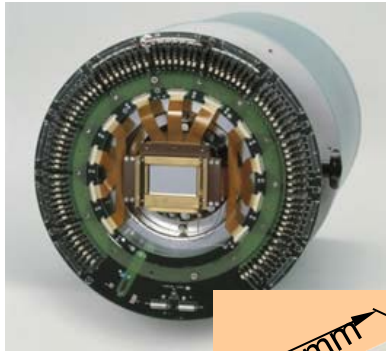


Studying of atomic systems at extreme conditions:

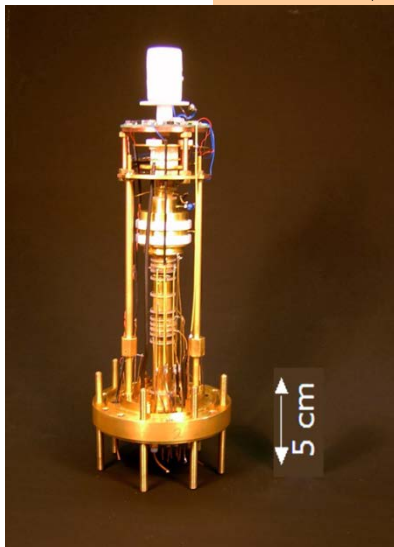
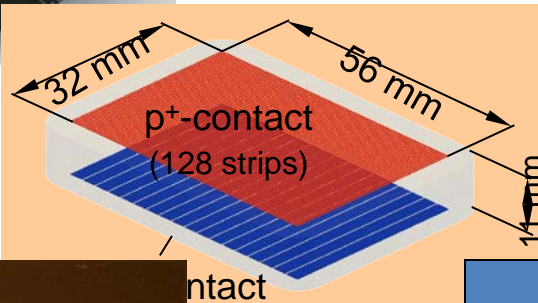
- very strong fields
- very high velocities
- very short times



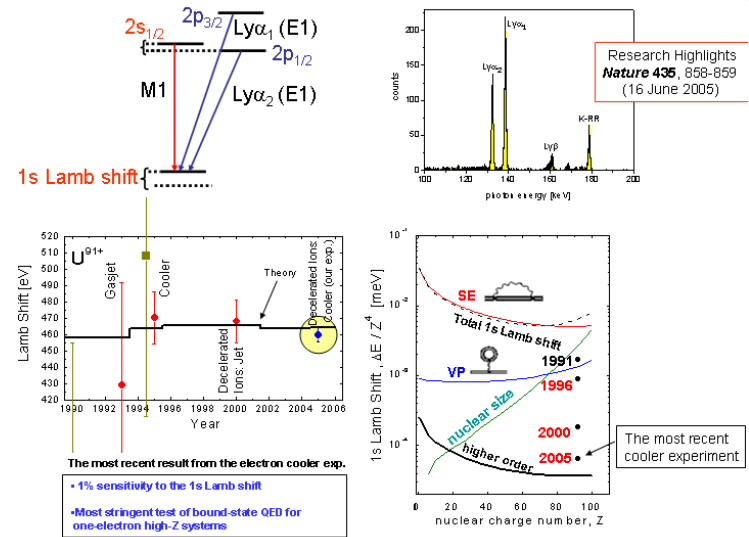
# Atomic physics of heavy ions



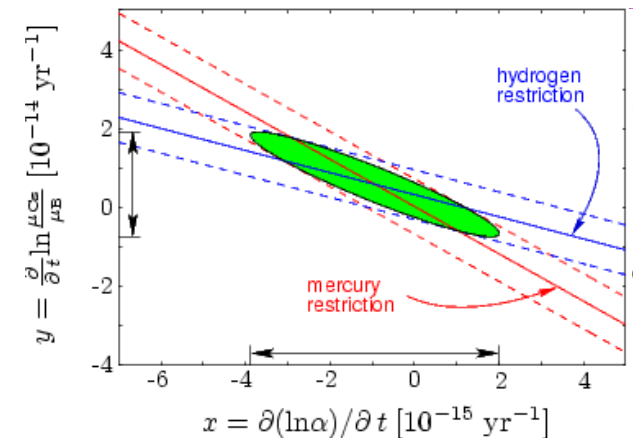
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[www.quantum.physik.uni-mainz.de](http://www.quantum.physik.uni-mainz.de)

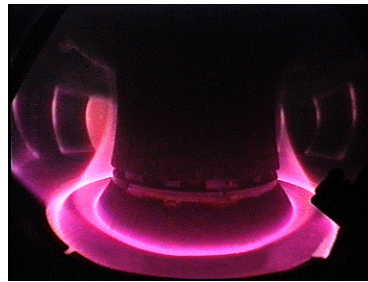


Extremely high precision experiments with ensembles of atoms/ions and even single ions!

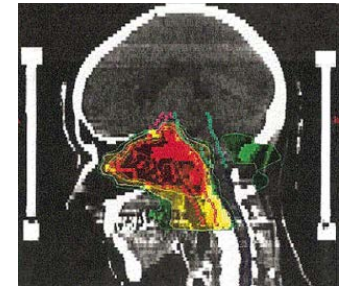




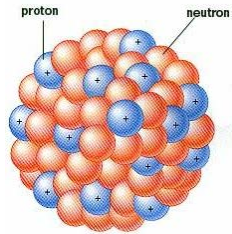
Astrophysics



Plasma physics

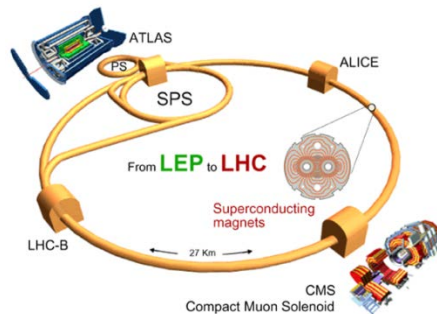


Medical research and Biophysics

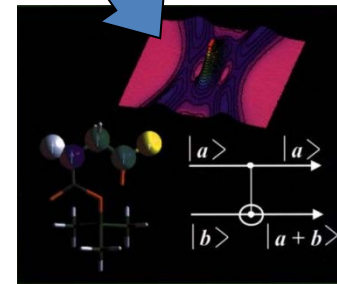


Nuclear physics

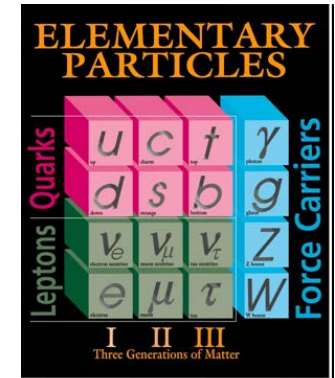
# Atomic physics



Accelerator physics



Quantum information



“New physics” beyond the Standard Model

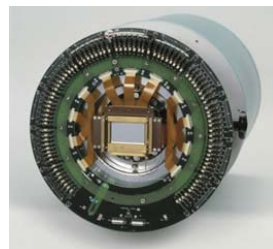
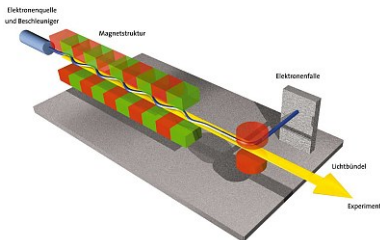


# Modern atomic physics: From experiment to theory and back

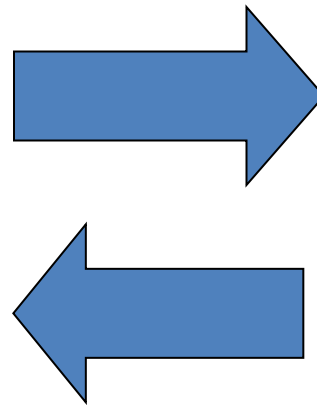


Studying of atomic systems at extreme conditions:

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

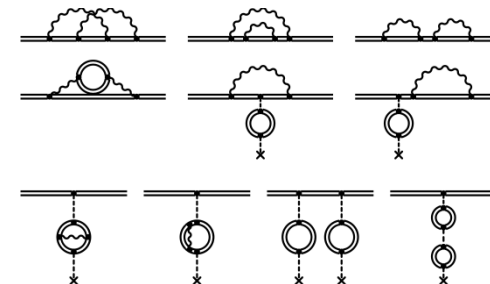


$$\left( \sum_{\alpha} c_{\alpha} \psi_{\alpha}(r, t) \right) = i \hbar \frac{\partial \psi}{\partial t} (\mathbf{x}, t)$$



One has to understand the:

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



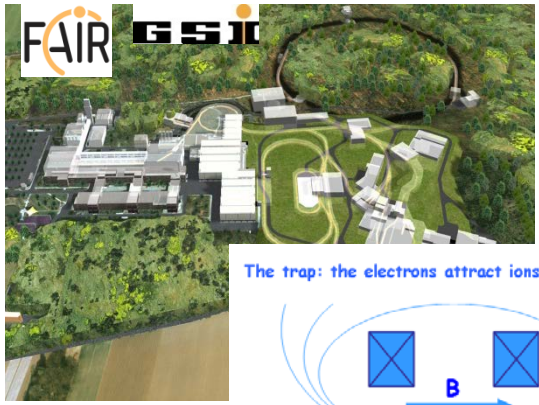
# Preliminary plan of the lectures

- 1 15.04.2015 Preliminary Discussion / Introduction
- 2 22.04.2015 Experiments (discovery of the positron, formation of antihydrogen, ...)
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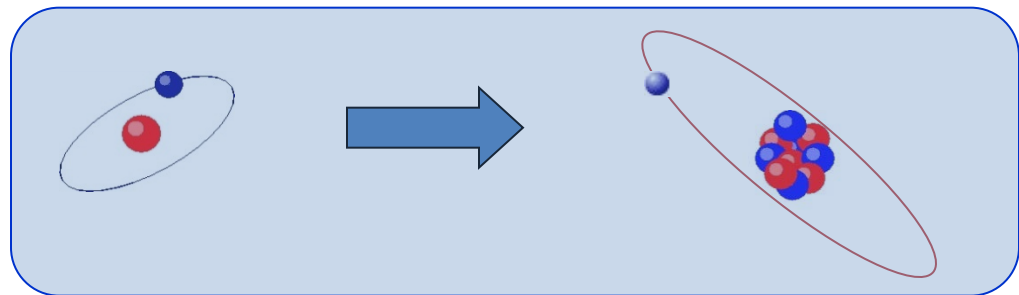
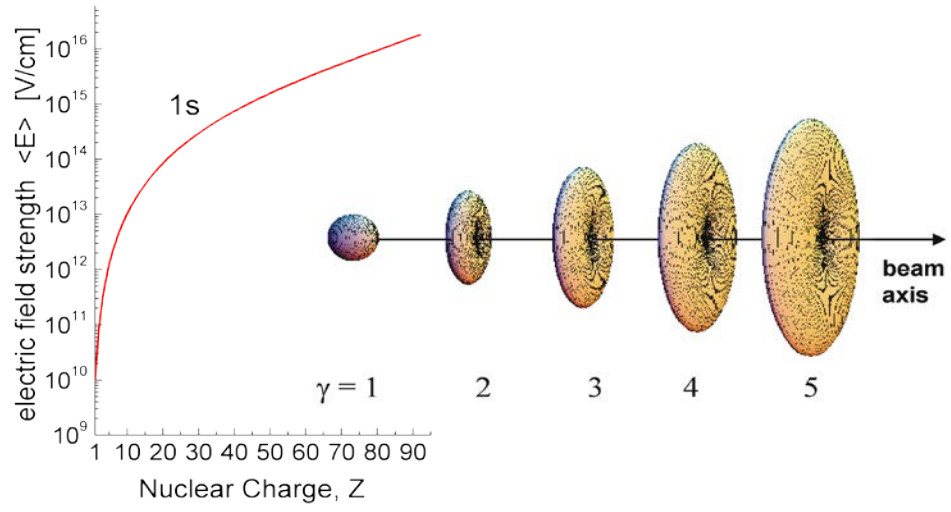
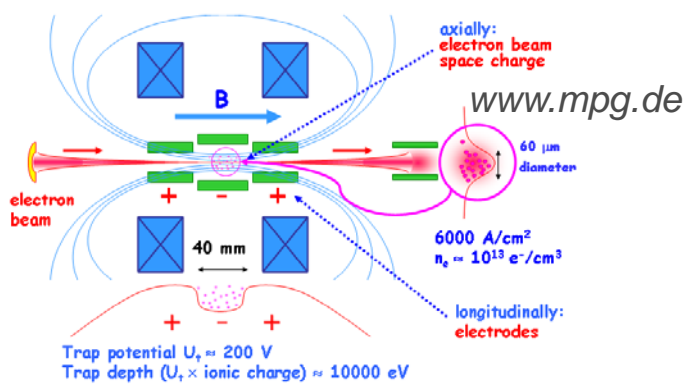
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# One electron heavy ions: Strong fields, relativity, QED



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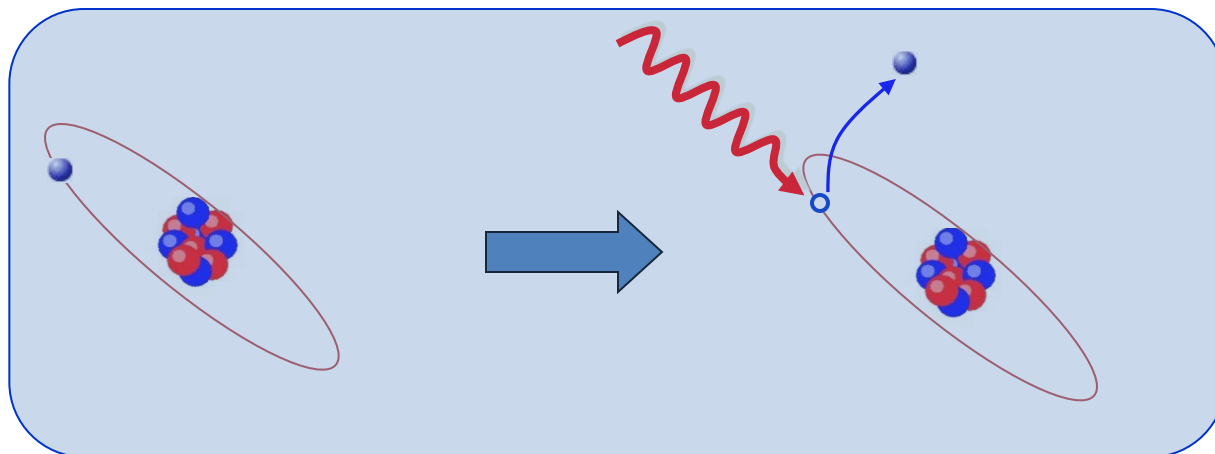
The trap: the electrons attract ions and ionize them more and more



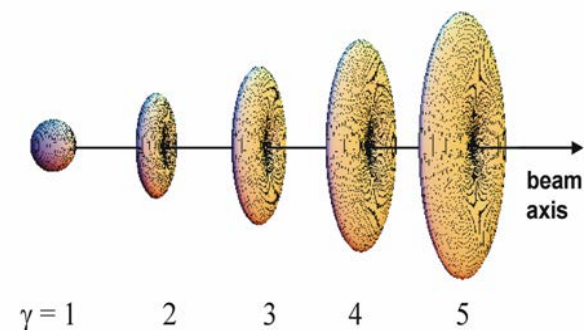
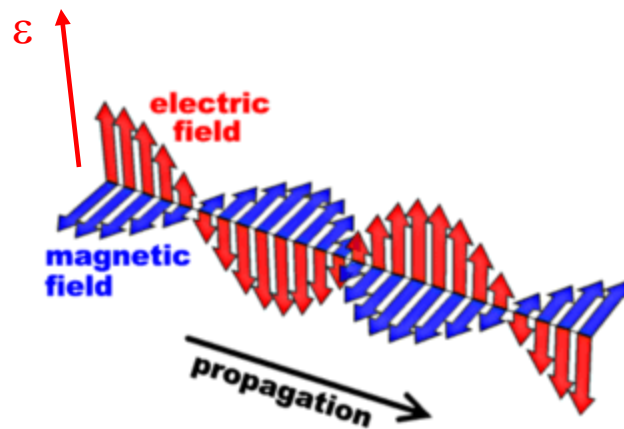
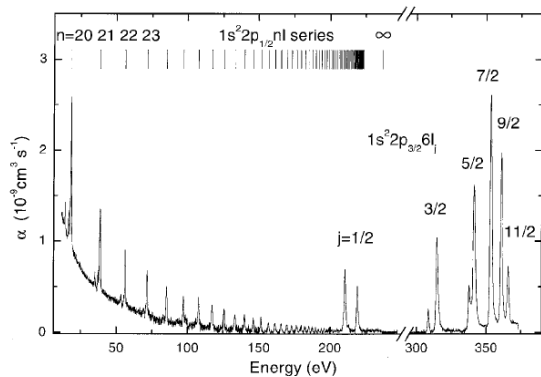
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# Atomic dynamics: Collisions, interaction with EM fields, penetration through matter



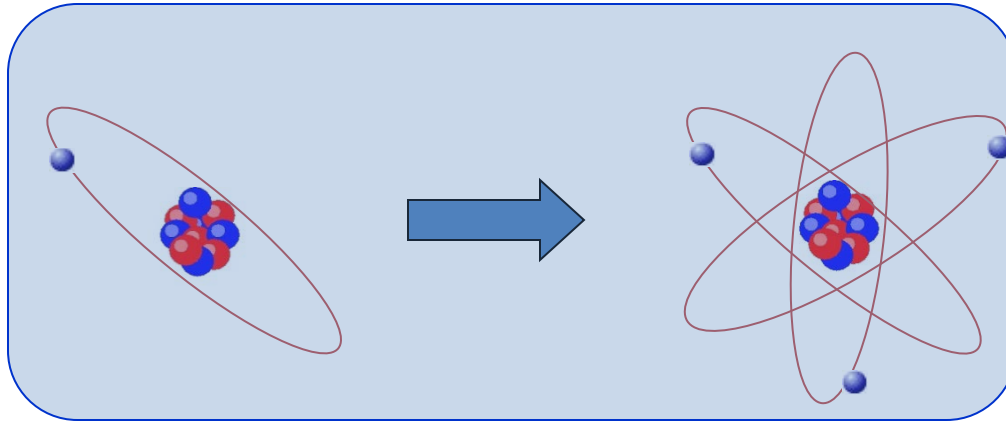
$$M_{ab} = \langle \psi_b | \alpha \varepsilon e^{ikr} | \psi_a \rangle \equiv \int \psi_b^+(\mathbf{r}) \alpha \varepsilon e^{ikr} \psi_a(\mathbf{r}) d\mathbf{r}$$



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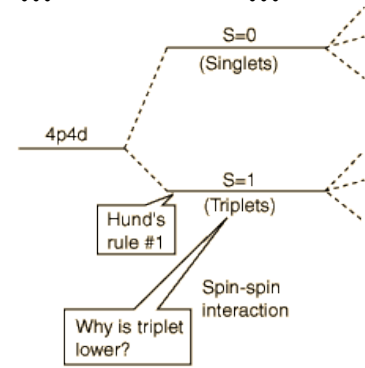
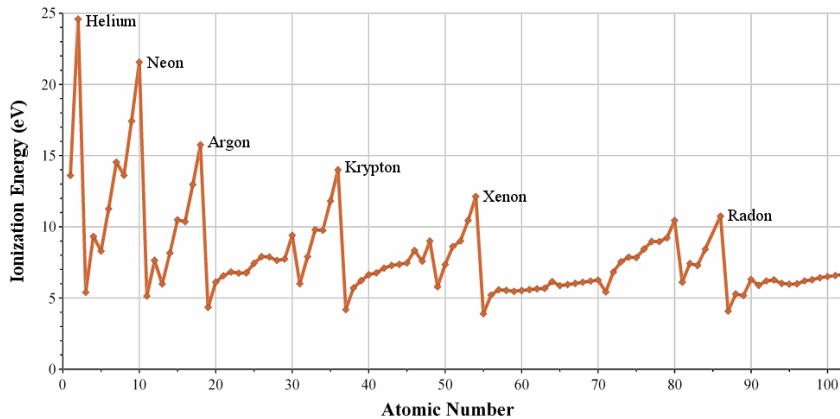
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# Many-electron ions and atoms: Interelectronic interaction effects



$$\Psi(\mathbf{r}_1, \mathbf{r}_2, \dots) = \frac{1}{\sqrt{N!}} \sum_{\mu_a, \mu_b, \mu_c, \dots} d(j_a \mu_a, j_b \mu_b, j_c \mu_c, \dots; JM)$$

$\psi_{n_a j_a \mu_a}(\mathbf{r}_1)$	$\psi_{n_b j_b \mu_b}(\mathbf{r}_1)$	$\psi_{n_c j_c \mu_c}(\mathbf{r}_1)$	...
$\psi_{n_a j_a \mu_a}(\mathbf{r}_2)$	$\psi_{n_b j_b \mu_b}(\mathbf{r}_2)$	$\psi_{n_c j_c \mu_c}(\mathbf{r}_2)$	...
$\psi_{n_a j_a \mu_a}(\mathbf{r}_3)$	$\psi_{n_b j_b \mu_b}(\mathbf{r}_3)$	$\psi_{n_c j_c \mu_c}(\mathbf{r}_3)$	...
...	...	...	...
...	...	...	...





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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!

## Standard Model of FUNDAMENTAL PARTICLES AND INTERACTIONS

The Standard Model summarizes the current knowledge in Particle Physics. It is the quantum theory that includes the theory of strong interactions (quantum chromodynamics or QCD) and the unified theory of weak and electromagnetic interactions (electroweak). Gravity is included on this chart because it is one of the fundamental interactions even though not part of the "Standard Model."

### FERMIONS

**Leptons** spin = 1/2

Flavor	Mass GeV/c <sup>2</sup>	Electric charge
$\nu_e$ electron neutrino	$<1 \cdot 10^{-8}$	0
$e^-$ electron	0.000511	-1
$\nu_\mu$ muon neutrino	$<0.0002$	0
$\mu^-$ muon	0.106	-1
$\nu_\tau$ tau neutrino	$<0.02$	0
$\tau^-$ tau	1.7771	-1

**Quarks** spin = 1/2

Flavor	Approx. Mass GeV/c <sup>2</sup>	Electric charge
$u$ up	0.003	2/3
$d$ down	0.006	-1/3
$c$ charm	1.3	2/3
$s$ strange	0.1	-1/3
$t$ top	175	2/3
$b$ bottom	4.3	-1/3

Structure within the Atom

### BOSONS

**Unified Electroweak** spin = 1

Name	Mass GeV/c <sup>2</sup>	Electric charge
$\gamma$ photon	0	0
$W^-$	80.4	-1
$W^+$	80.4	+1
$Z^0$	91.187	0

**Strong (color)** spin = 1

Name	Mass GeV/c <sup>2</sup>	Electric charge
$g$ gluon	0	0

**Color Charge**  
Each quark carries one of three types of "strong charge," also called "color charge." These charges have nothing to do with the color of visible light. There are eight possible types of color charge for gluons. Just as electrical particles interact by exchanging photons, in strong interactions color-charged particles interact by exchanging gluons. Leptons, photons, and  $W$  and  $Z$  bosons have no strong interactions and hence no color charge.

**Quarks Confined in Mesons and Baryons**  
One cannot isolate quarks and gluons. They are confined in color-neutral particles called hadrons. This confinement (binding) results from multiple exchanges of gluons among the color-charged constituents. As color-charged particles (quarks and gluons) move apart, the energy in the color-force field between them increases. This energy eventually is converted into additional quark-antiquark pairs (see figure below). The quarks and antiquarks then combine into hadrons. These are the particles seen to emerge. Two types of hadrons have been observed in nature: mesons  $q\bar{q}$  and baryons  $qqq$ .

**Residual Strong Interaction**  
The strong binding of color-neutral protons and neutrons to form nuclei is due to residual strong interactions between their color-charged constituents. It is similar to the residual electrical interaction that binds electrically neutral atoms to form molecules. It can also be viewed as the exchange of mesons between the hadrons.

### PROPERTIES OF THE INTERACTIONS

Property	Interaction	Weak (Electroweak)		Electromagnetic		Strong	
		Acts on:	Color Charge	Color Charge	Fundamental	Residual	
Acts on:		Mass - Energy	Flavor	Electric Charge	Quarks, Gluons	See Residual Strong Interaction Note	
Particles experiencing:	All	Quarks, Leptons	Electrically charged	Quarks, Gluons	Hadrons		
Particles mediating:	Graviton (not yet observed)	$W^+, W^-, Z^0$	$\gamma$	Gluons	Mesons		
Strength (relative to electrical for two u quarks at $10^{-16}$ m for two protons in nucleus $10^{-17}$ m)		$10^{-41}$	0.8	1	25	Not applicable to quarks	
		$10^{-41}$	$10^{-4}$	1	60		
		$10^{-36}$	$10^{-7}$	1	Not applicable to hadrons	20	

### Mesons $q\bar{q}$

Mesons are bosonic hadrons. There are about 180 types of mesons.

Symbol	Name	Quark content	Electric charge	Mass GeV/c <sup>2</sup>	Spin
$\pi^+$	pion	$u\bar{d}$	+1	0.140	0
$K^-$	kaon	$s\bar{u}$	-1	0.494	0
$\rho^+$	rho	$u\bar{d}$	+1	0.770	1
$B^0$	B-meson	$d\bar{b}$	0	5.279	0
$\eta_c$	eta-c	$c\bar{c}$	0	2.380	0

**Matter and Antimatter**  
For every particle type there is a corresponding antiparticle type, denoted by a bar over the particle symbol (unless + or - charge is shown). Particle and antiparticle have identical mass and spin but opposite charge. Some electrically neutral bosons (e.g.,  $Z^0$ ,  $\gamma$ , and  $\eta_c = c\bar{c}$ , but not  $K^0 = d\bar{s}$ ) are their own antiparticles.

**Figures**  
These diagrams are an artist's conception of physical processes. They are not exact and have no meaningful scale. Green shaded areas represent the cloud of gluons or the gluon field, and red lines the quark paths.

$n \rightarrow p + e^- + \bar{\nu}_e$

A neutron decays to a proton, an electron, and an antineutrino via a virtual (breasting)  $W^-$  boson. This is a neutron  $\beta$  decay.

$e^- + e^+ \rightarrow B^0 + \bar{B}^0$

An electron and positron (antilepton) colliding at high energy can annihilate to produce  $B^0$  and  $\bar{B}^0$  mesons via a virtual  $Z$  boson or a virtual photon.

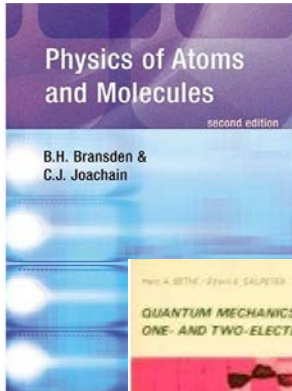
$p + p \rightarrow Z^0 + \text{assorted hadrons}$

Two protons colliding at high energy can produce various hadrons plus very high mass particles such as  $Z$  bosons. Events such as this one are rare but can yield vital clues to the structure of matter.

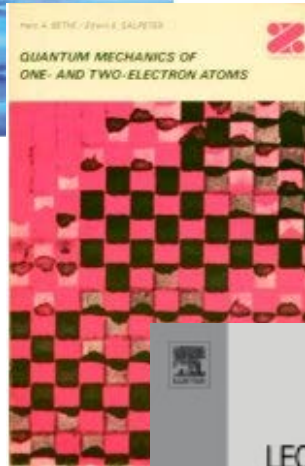
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# Literature and I-net sources

# Basic literature



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



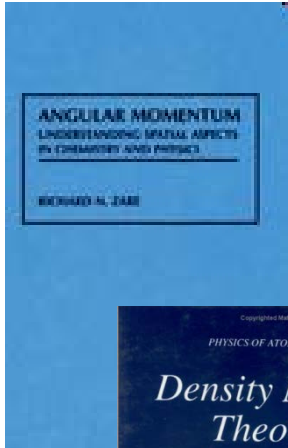
H. A. Bethe and E. E. Salpeter  
*“Quantum Mechanics of One- and Two-Electron Atoms”*



J. Eichler and W. E. Meyerhof  
*“Relativistic Atomic Collisions”*  
Or

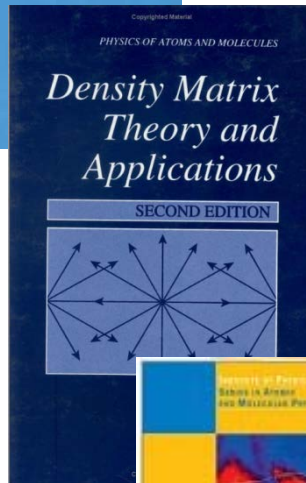
J. Eichler  
*“Lectures on Ion-Atom Collisions”*

# Additional literature



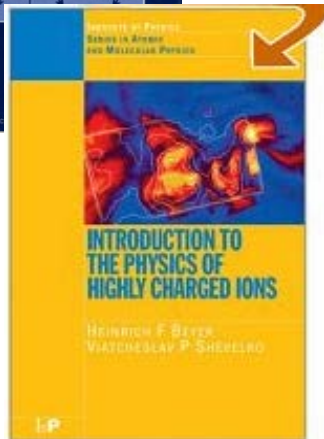
R. Zare

*“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](http://web-docs.gsi.de/~stoe_exp/lectures/lectures.php)

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## Lectures & Seminars

### 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

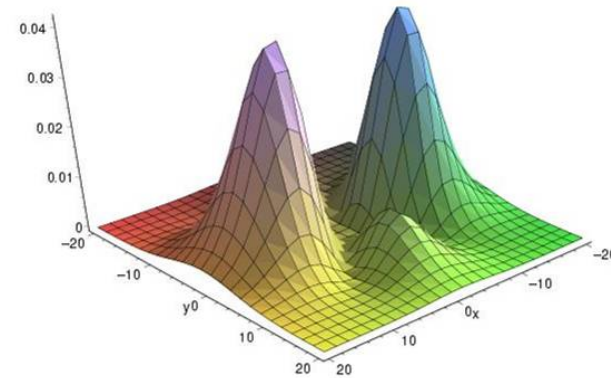
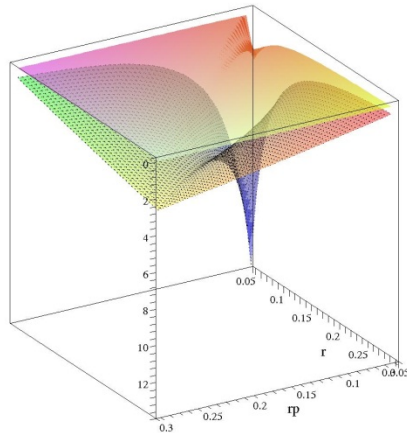
**Transparencies presented during the lecture:**

- 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](#)

# 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
- ....



The programs will be available for downloading from:

[http://web-docs.gsi.de/~stoe\\_exp/lectures/lectures.php](http://web-docs.gsi.de/~stoe_exp/lectures/lectures.php)





## General

**NIST Physical Reference Data - X-Ray and Gamma-Ray Data** <http://hyperphysics.phy-astr.gsu.edu/hbase/hframe.html>

<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](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](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.csriiit.edu/periodic-table.html>

# Preliminary plan of the 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 (photon, quantum field theory (just few words), Feynman diagrams, QED corrections)
- 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)

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