
Physics of heavy multiply-charged ions:

Studies on the borderline of atomic and nuclear physics

Andrey Surzhykov

Technische Universität Braunschweig
Physikalisch-Technische Bundesanstalt (PTB)

Lecture 1

Introduction and motivation: What are multiply-charged ions? Why they are important? How they are produced and observed?

Plan of the lecture

- Organization questions: how the lecture will be structured
- Motivation: what you will learn at the lecture?
- Heavy multiply-charged ions: what is so special with them?
- Production and storage of multiply-charged ions
 - Accelerator and storage ring facilities
 - Ion trap devices
- Experimental “observation” of ions
 - Basic atomic processes
 - Detectors

Andrey Surzhykov

Technische Universität Braunschweig *and*
Fundamentale Physik für Metrologie @ Physikalisch-Technische Bundesanstalt (PTB)

E-mail: andrey.surzhykov@ptb.de

Web-page: <http://www.ptb.de/fpm>

How lectures will be organized?

Mostly transparencies (English)

If more detailed theory discussion is necessary we will switch to the blackboard

Properties of Wigner's matrix

- From the explicit form of rotation operator:
$$R(\phi) = \exp[-i\alpha \hat{J}_z] \exp[-i\beta \hat{J}_y] \exp[-i\gamma \hat{J}_z]$$
- And definition of the (elements of D-matrix):
$$D_{m'm}^{j}(\alpha, \beta, \gamma) = \langle jm' | \hat{R}(\alpha, \beta, \gamma) | jm \rangle$$

Eugene P. Wigner

Density matrix of spin-1/2 particles
Just a reminder

- We derived previously density matrix of 1/2-spin particle in the form:
$$\langle m_z | \hat{\rho} | m_z' \rangle = \frac{1}{2} \begin{pmatrix} 1 + P_z & P_x - iP_y \\ P_x + iP_y & 1 - P_z \end{pmatrix}$$
- We obtained very important result: density matrix which describes a mixture of 1/2-spin particles can be parameterized in terms of observables (i.e. in terms of expectation values of Pauli matrices).

Wigner's small d function:
$$d_{m'm}^{j}(\beta) = \langle j m' | \exp(-i\beta \hat{J}_y) | j m \rangle$$

Infinitely small rotations

$\delta\phi \rightarrow 0$

- If rotation angle (call it $\delta\phi$ for the moment) tends to zero our transformation operator should become identity operator:
$$\hat{U} = \hat{I} + i\delta\phi \hat{S}$$
- Here \hat{S} is the so-called generator of infinitely small transformation. Obviously, this operator should be Hermitian:
$$\hat{U}^\dagger \hat{U} = \hat{I} \Rightarrow \hat{S}^\dagger = \hat{S}$$
- Finite rotation can be re-presented as a series of infinitely small rotations:
$$\hat{U} = [\hat{I} + i\delta\phi \hat{S}]^n \Rightarrow \hat{U} = \lim_{n \rightarrow \infty} \left[\hat{I} + i\frac{\phi}{n} \hat{S} \right]^n = \exp[i\phi \hat{S}]$$
- It is easy to prove that $[\exp[i\phi \hat{S}], \hat{S}] = 0$



The language of the lecture is Russian.

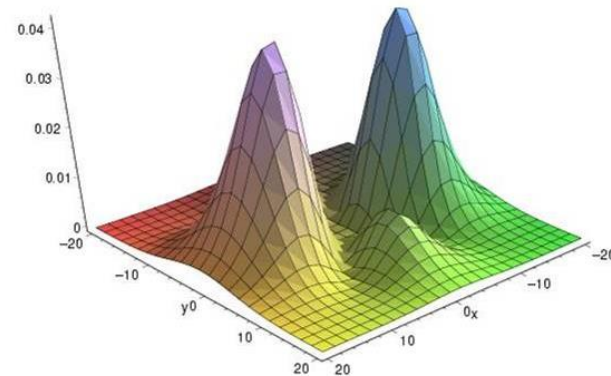
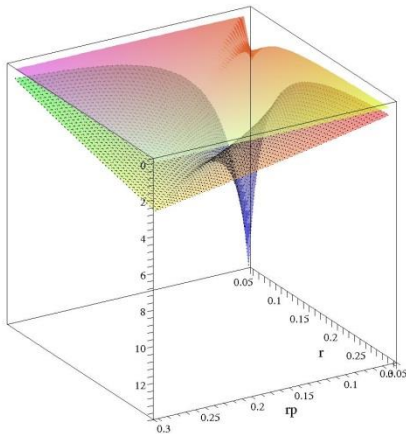
How lectures will be organized?

“Learning by playing with Mathematica!”



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:
www.ptb.de/fpm

Mathematica notebooks

`/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) :*

- $\kappa = -1$ corresponds to $j=1/2$, positive parity, i.e. $s_{1/2}$ state
- $\kappa = +1$ corresponds to $j=1/2$, negative parity, i.e. $p_{1/2}$ state
- $\kappa = -2$ 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[7.297352533000000000000000000000 / 1000, $MinPrecision];
alpha = FineStructureConstant;
```

Dirac spectroscopic notations

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

Output data: spectroscopic notation

```
NN[nNN_, kappa_] :=
(
resNN = Switch[kappa, -4, "f_{7/2}", -3, "d_{5/2}", -2, "p_{3/2}", -1, "s_{1/2}", 1, "p_{1/2}", 2, "d_{3/2}", 3, "f_{5/2}"];
If[nNN == 1, {resNN} = {"1" resNN}];
If[nNN != 1, {resNN} = {nNN resNN}];
Return[resNN]
);
```

Dirac energy

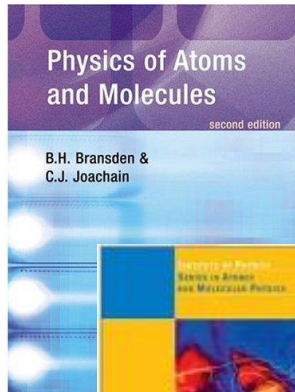
Input data: principal quantum number n , Dirac quantum number κ , nuclear charge Z

Output data: energy of the bound state in atomic units

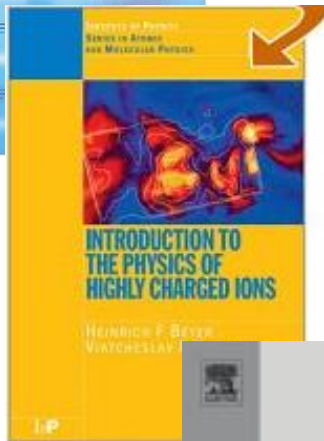
```
Energy[n, kappa_, Z] := 1/(FineStructureConstant^2 * Sqrt[1 + (FineStructureConstant * Z/(n - Abs[kappa] + Sqrt[kappa^2 - (Z * FineStructureConstant)^2]) )^2]) - 1/FineStructureConstant^2;
```

start | Fritzsche Ste... | 2 Windows ... | 2 Microsoft ... | 2 SSH Secu... | 2 Xming X.S... | Andrey Surz... | EN | 11:23 AM

Literature



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



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



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

J. Eichler
“Lectures on Ion-Atom Collisions”

Internet

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>

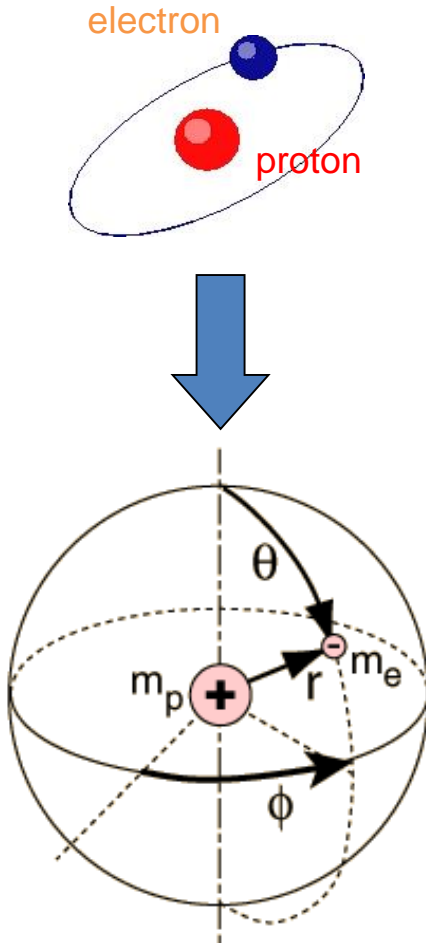
Motivation

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

To answer this question, let us discuss what is the modern atomic physics! What do we (you) know about atomic physics?

Hydrogen atom

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



- 3D Schrödinger equation (time-independent):

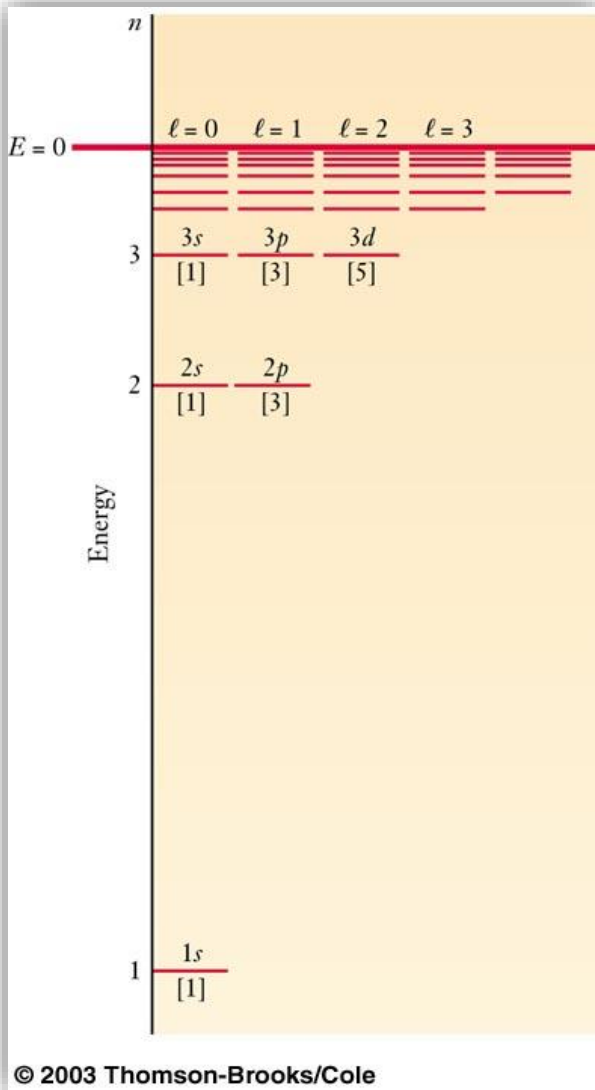
$$-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r}) + V(\mathbf{r})\psi(\mathbf{r}) = E\psi(\mathbf{r})$$

- Where Coulomb potential is:

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

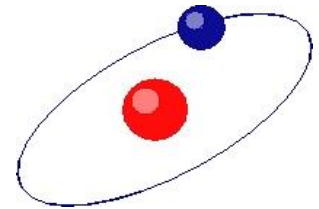
- Indeed, we know how to find solutions (wavefunctions and energies) of this system.

Hydrogen atom



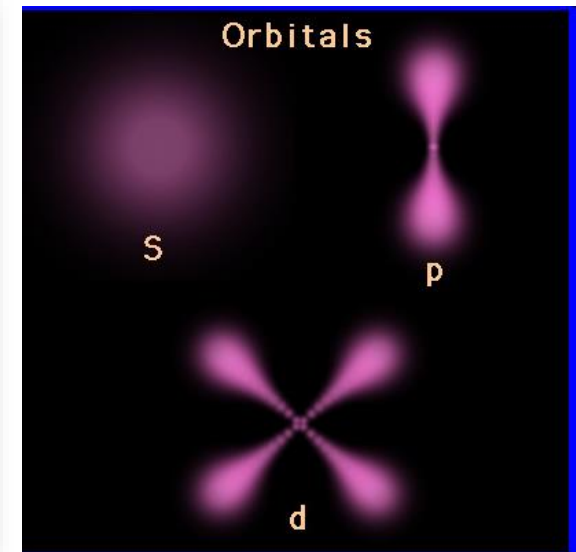
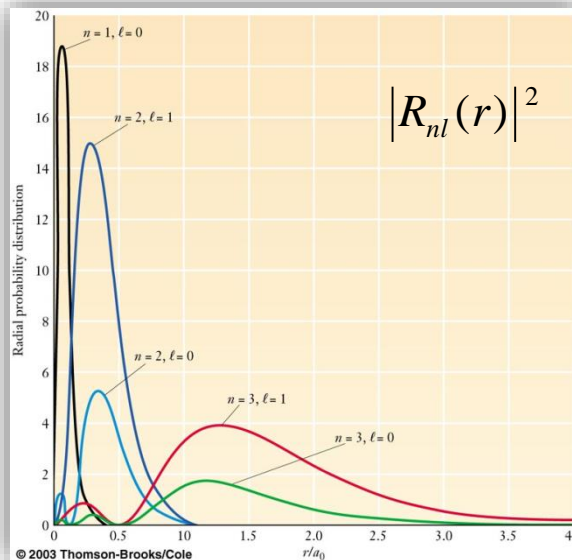
- Energy values of “hydrogen atom” are given by:

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



- ... and wavefunctions:

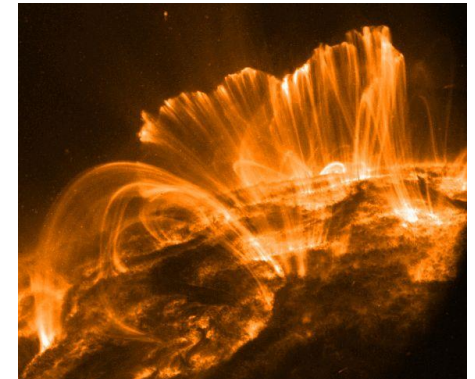
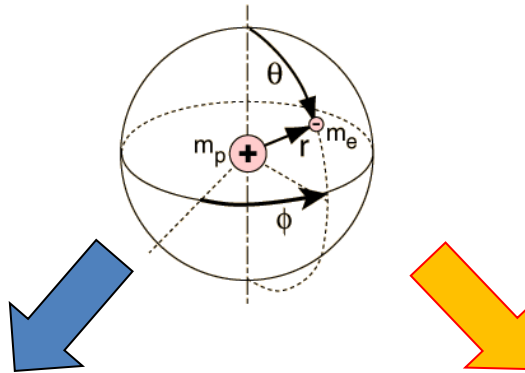
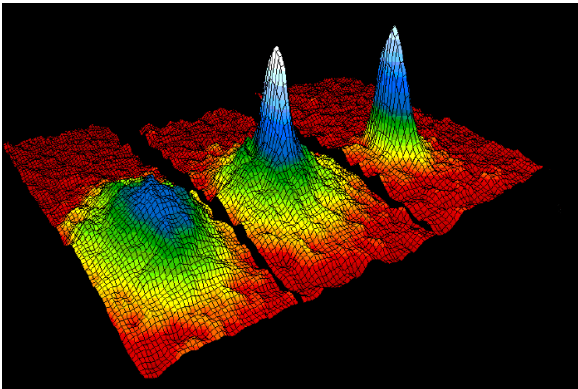
$$\psi(\mathbf{r}) = \psi(r, \theta, \varphi) = R_{nl}(r)Y_{lm_l}(\theta, \varphi)$$



Pictures from HyperPhysics


Modern atomic physics

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



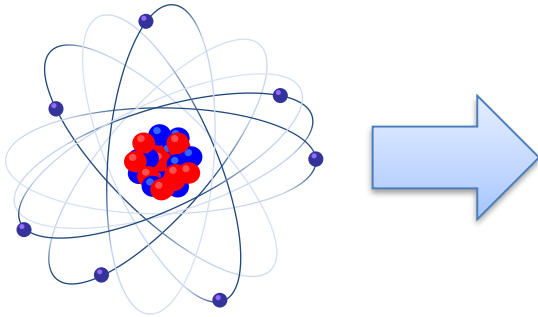
In our course we shall focus mainly on the high-energy (temperature, field-strength,...) part of the modern atomic physics.

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-  • Heavy multiply-charged ions: what is so special with them?
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Heavy multiply-charged ions

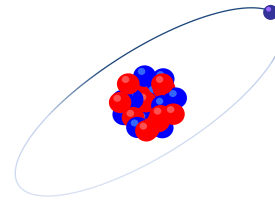
Neutral atom



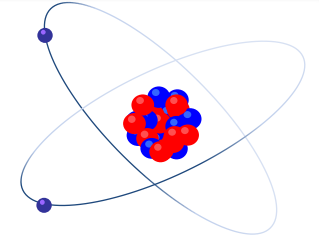
Highly-charged ions



bare



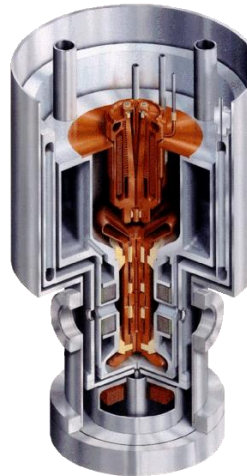
hydrogen-like



helium-like



Advanced particle acceleration facilities (e.g. GSI and FAIR, DESY)

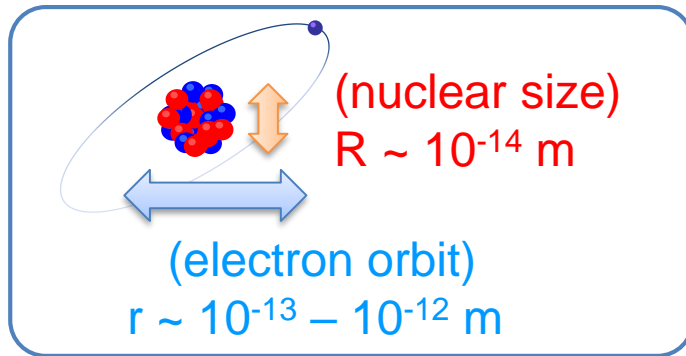


Electron beam ion traps (EBITs)
(e.g. MPI-K, Livermore)

During the last decades, a number of experimental facilities have been built (or designed) that are capable of producing and storing highly-charged ions.

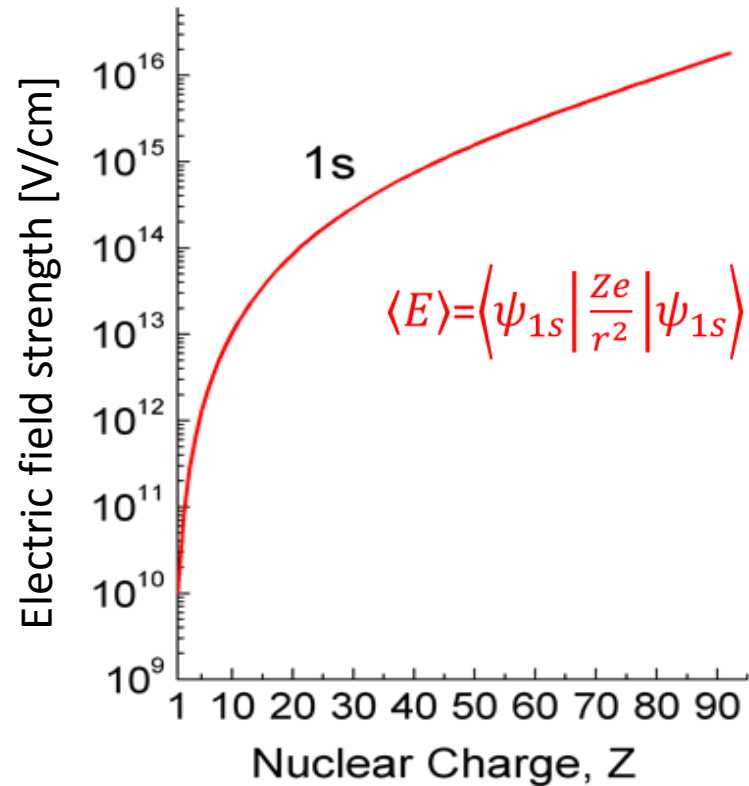
Heavy multiply-charged ions

What is so special about multiply-charged, heavy ions?



One can estimate the electron "velocity" in the ground state:

$$v_{el} \approx \alpha Z c \rightarrow v_{el} \approx 0.7c \quad (\text{for } \text{U}^{91+})$$

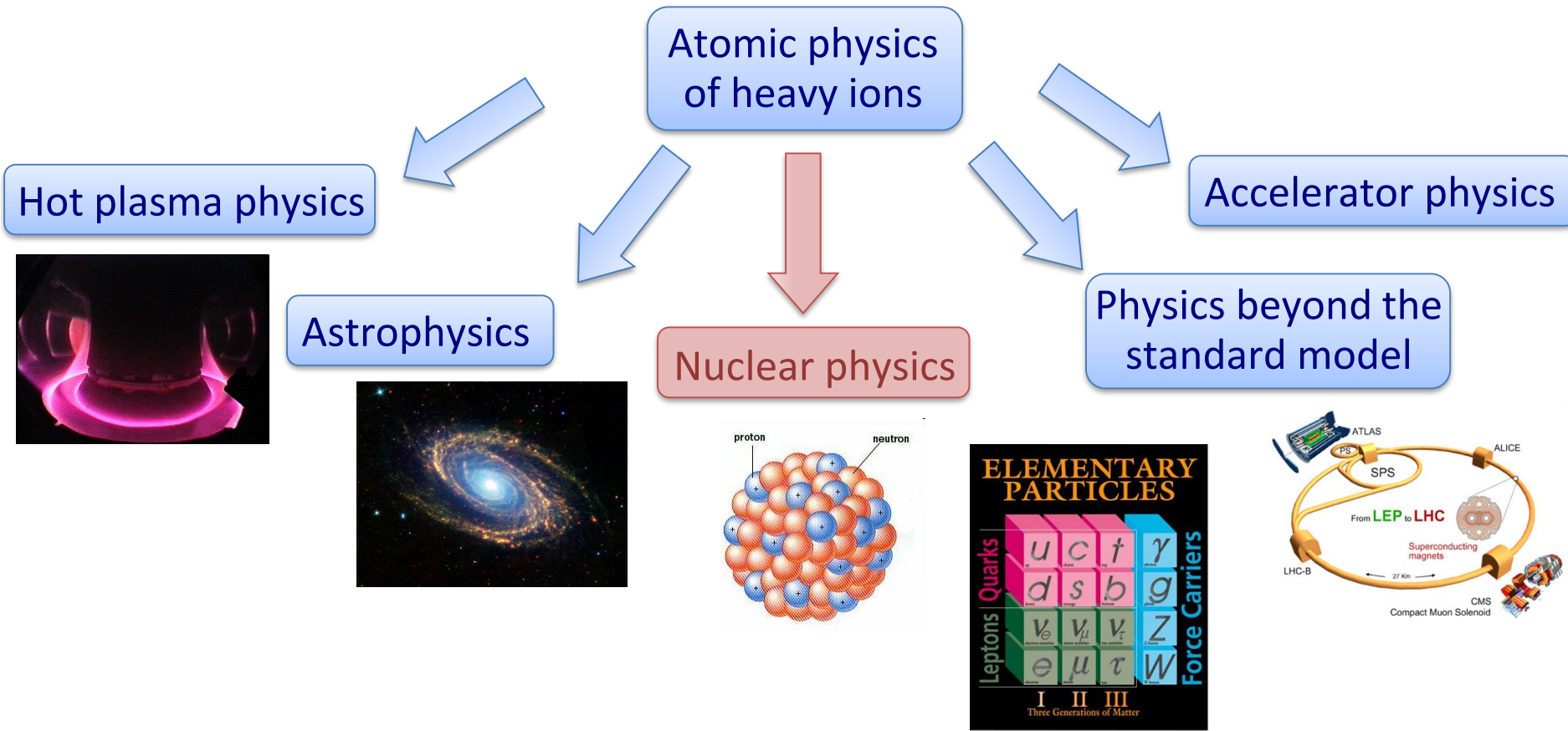


Electron is exposed to huge fields (of microscopic) dimensions.


These ions are natural "laboratories" for studying simple atomic systems under critical conditions.

Multiply-charged ions

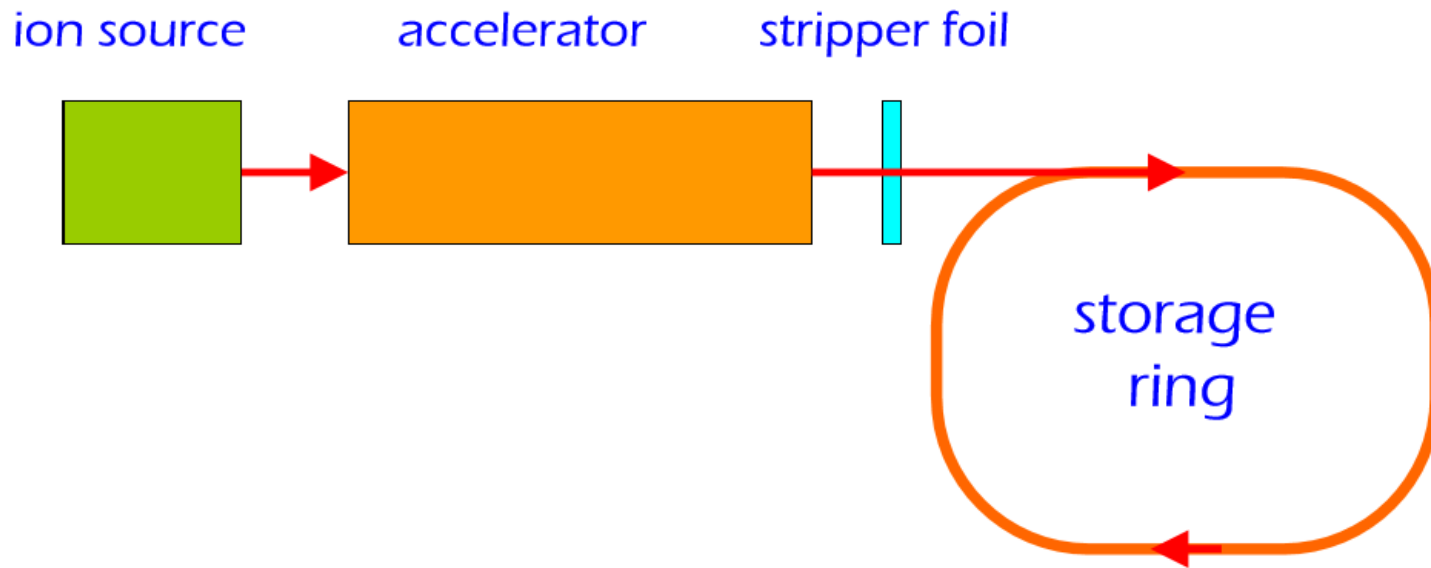
- Multiply-charged, heavy ions provide “natural laboratories” to investigate the structure and dynamics of few-electron systems in strong electromagnetic fields.
- The importance of studies with highly-charged, heavy ions goes far beyond atomic physics.



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Accelerator and storage ring facilities



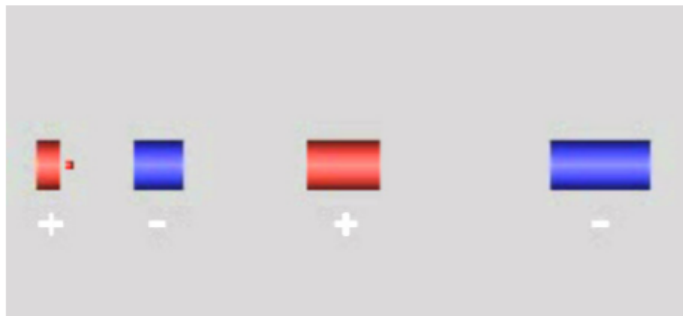
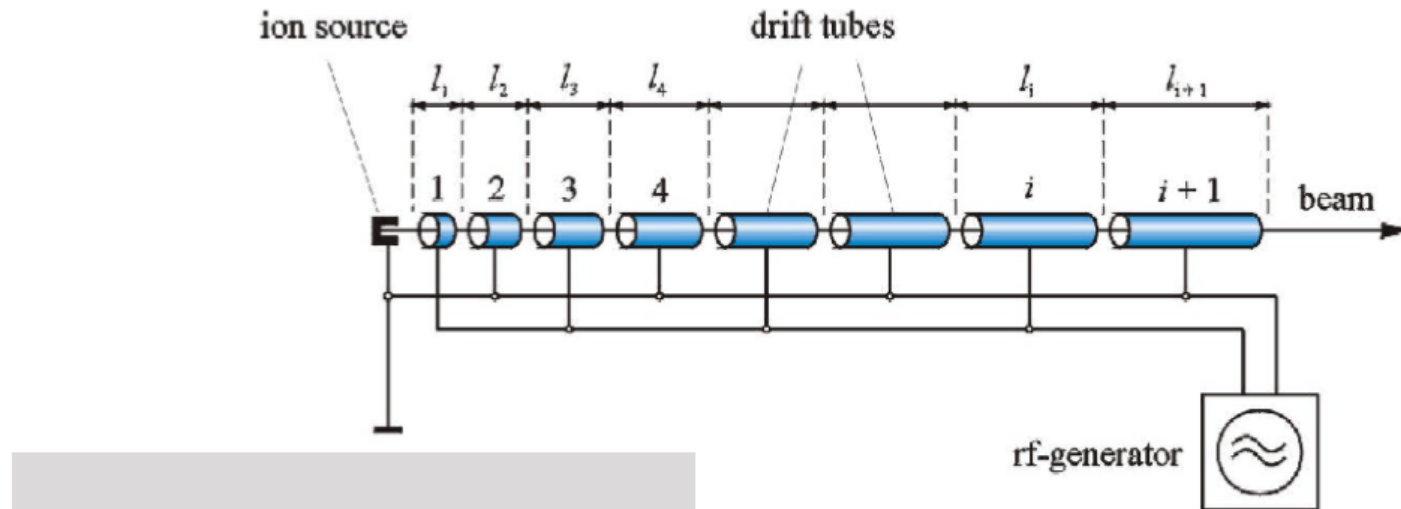
Storage ring = synchrotron without acceleration

To produce higher charge states in accelerators, ions in low charge states pass through a very thin foil where electrons are stripped.

Example:

- ion source produces a beam of 20 keV Ne²⁺
- accelerated to: 20 MeV Ne²⁺
- after passing stripper: 20 MeV Ne¹⁰⁺

HF linear accelerators

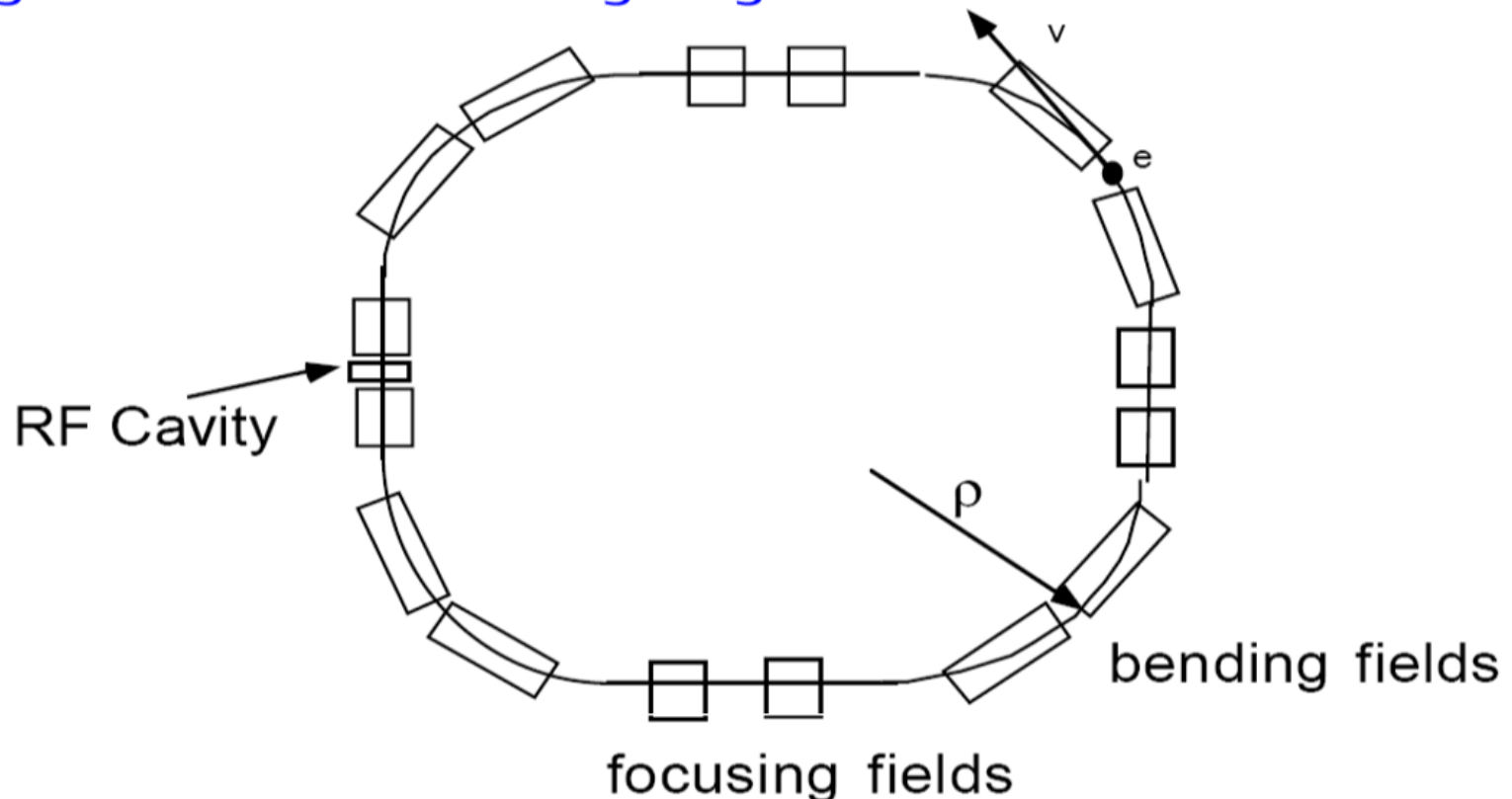


- Deliver bunched beams
- Use powerful RF generators
- High voltage generated by resonantly driven drift tubes

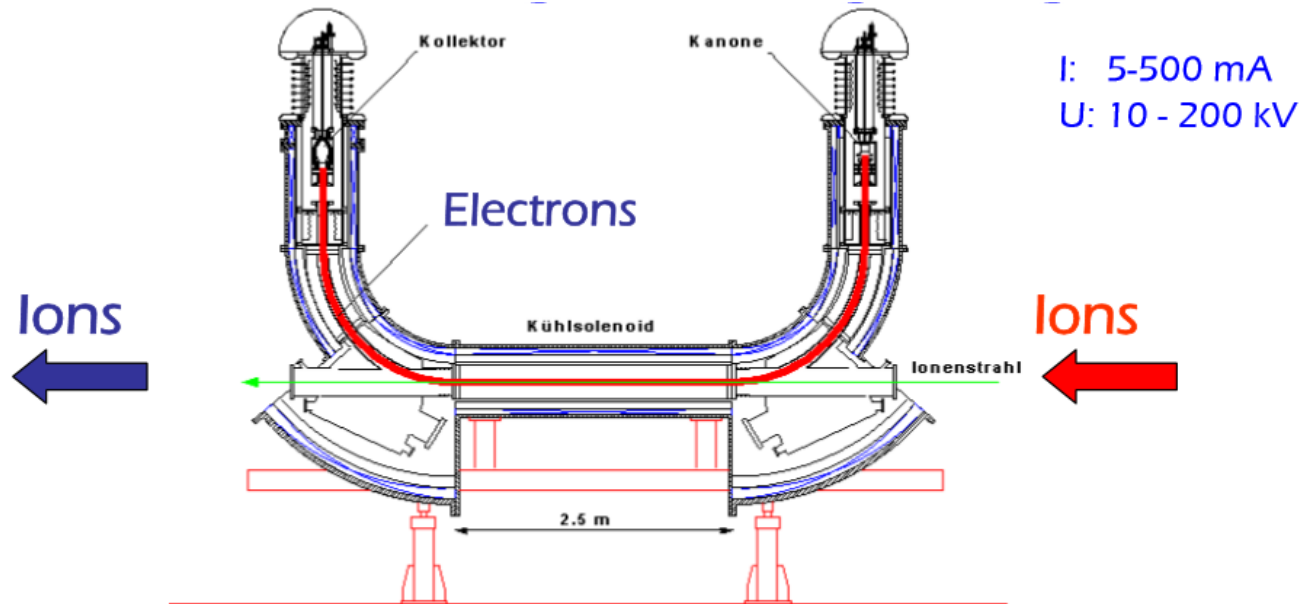
Wideröe (1928)

Synchrotron

- Ring with bending magnets and RF cavity synchronously accelerate particle bunches
- Magnetic focusing by quadrupoles and by radial field gradients in the bending magnets

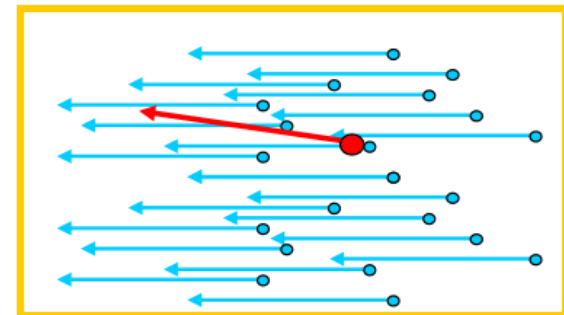


Ion cooling



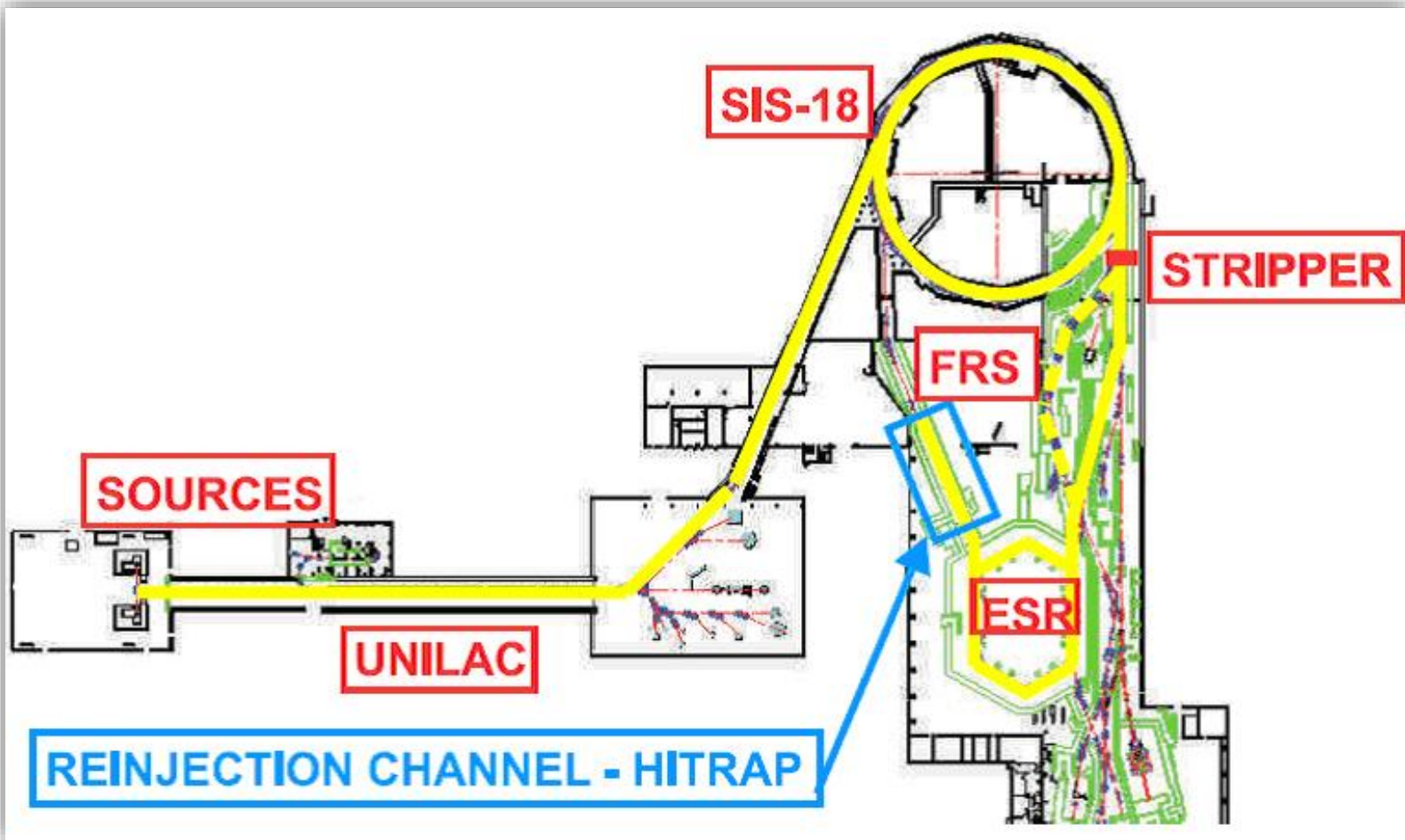
- Ions interact 10^6 times per second with a collinear beam of cold electrons at nearly the same speed.
- The transversal components of the ion motion are cooled.

- Momentum spread $\Delta p/p : 10^{-4} - 10^{-5}$
- Beam diameter : 2 mm

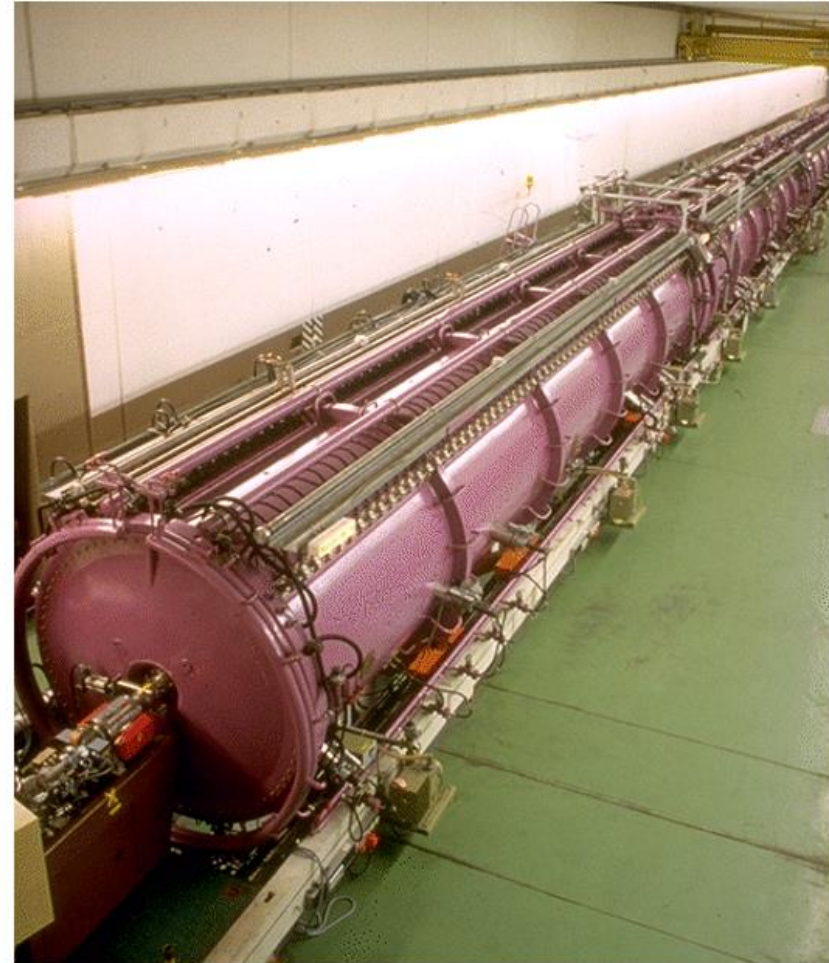


Accelerator and storage ring facilities

Let us consider the example of GSI facility. This is the heavy ion research facility in Darmstadt, Germany.

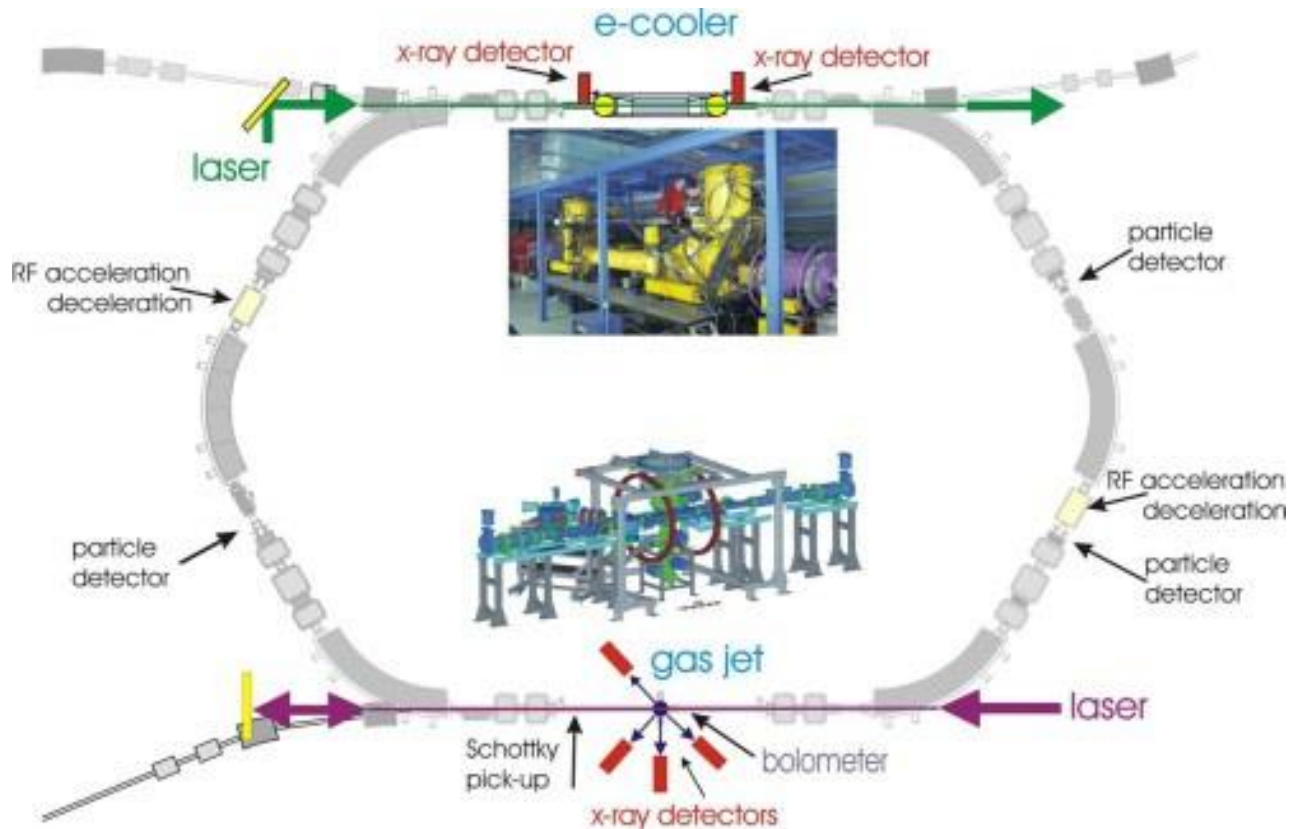


Linear accelerator at the GSI facility



Ion storage rings

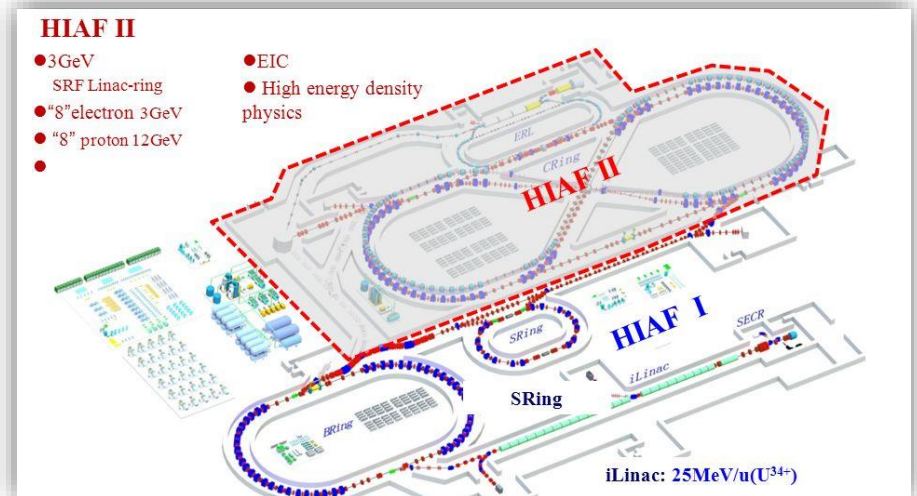
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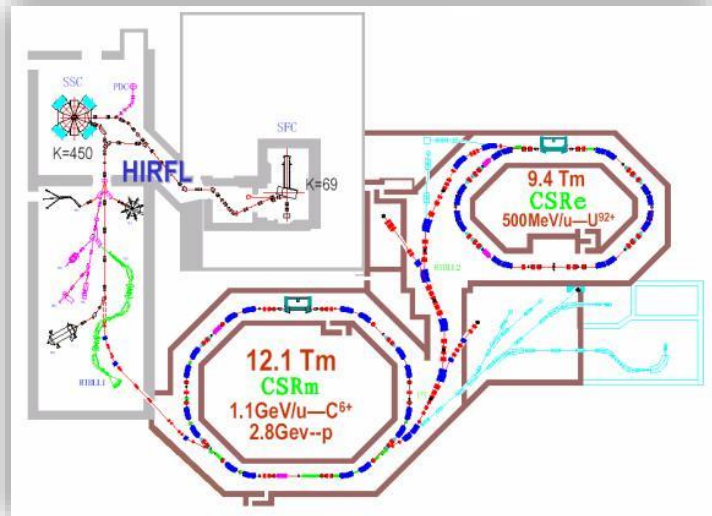
Present and future accelerators



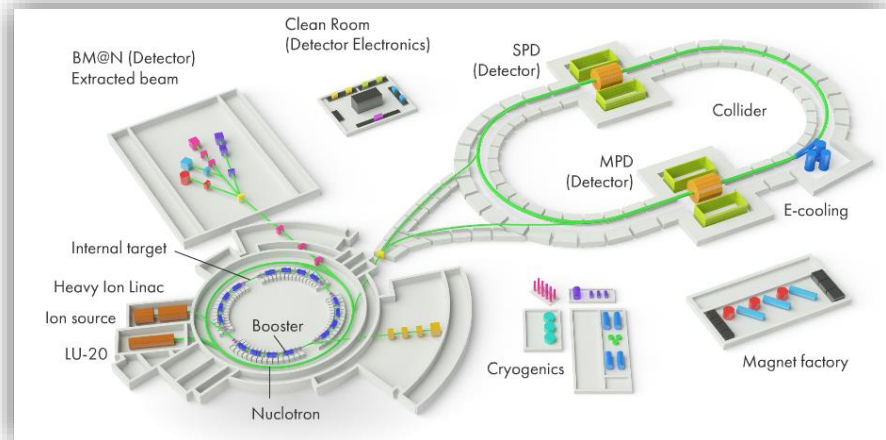
Facility for Antiproton and Ion Research



High Intensity heavy ion Accelerator Facility

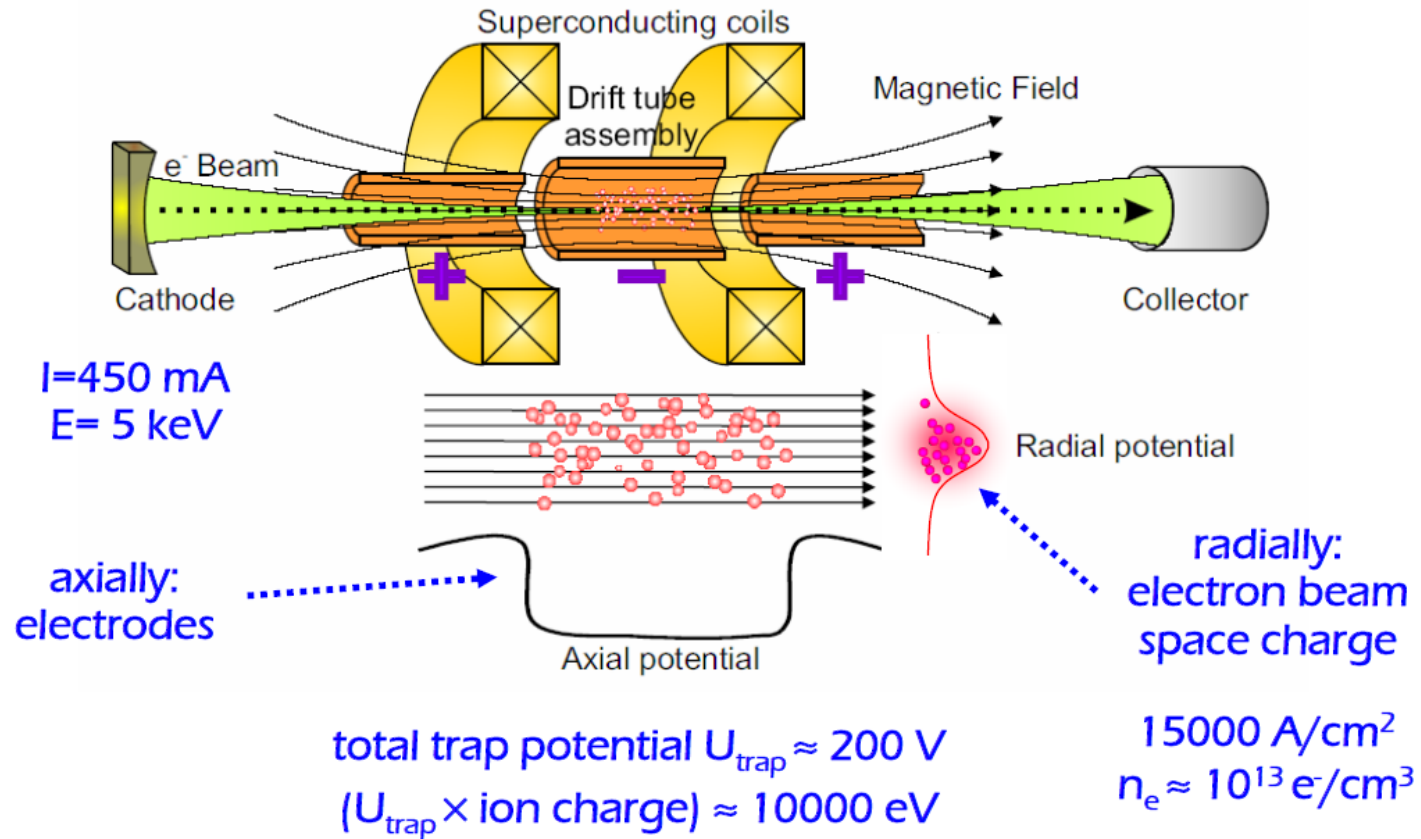


Heavy Ion Research Facility



Nuclotron-based Ion Collider fAcility

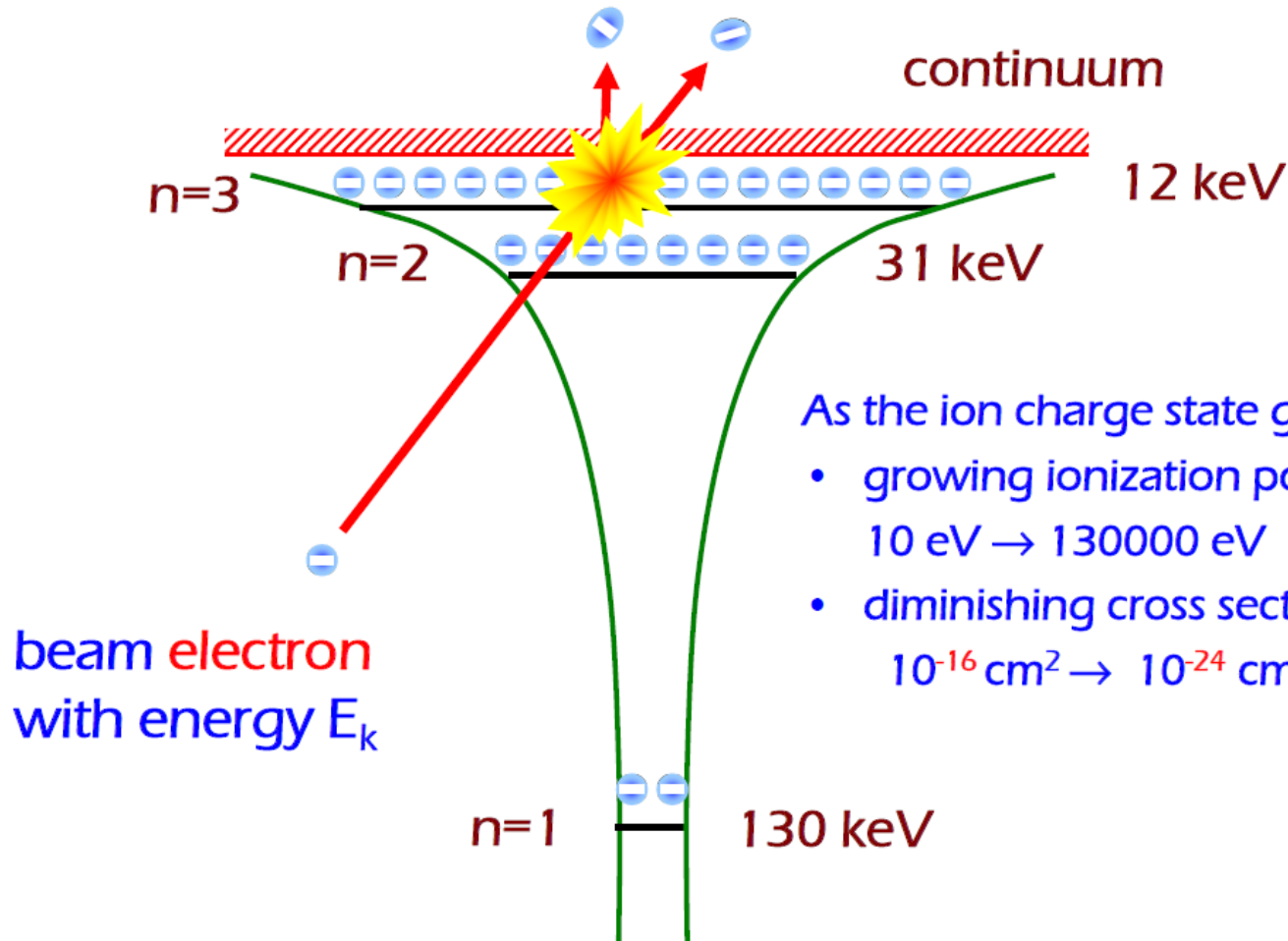
Electron-beam ion traps



The electron beam ion trap (EBIT) is a small-scale laboratory instrument which uses a tightly focused and energy-tunable electron beam to create, trap, and probe highly charged ions.

Electron-beam ion traps: Principles

As electrons collide with the ions in the beam, they strip off electrons until the energy required to remove the next electron is higher than the beam energy.

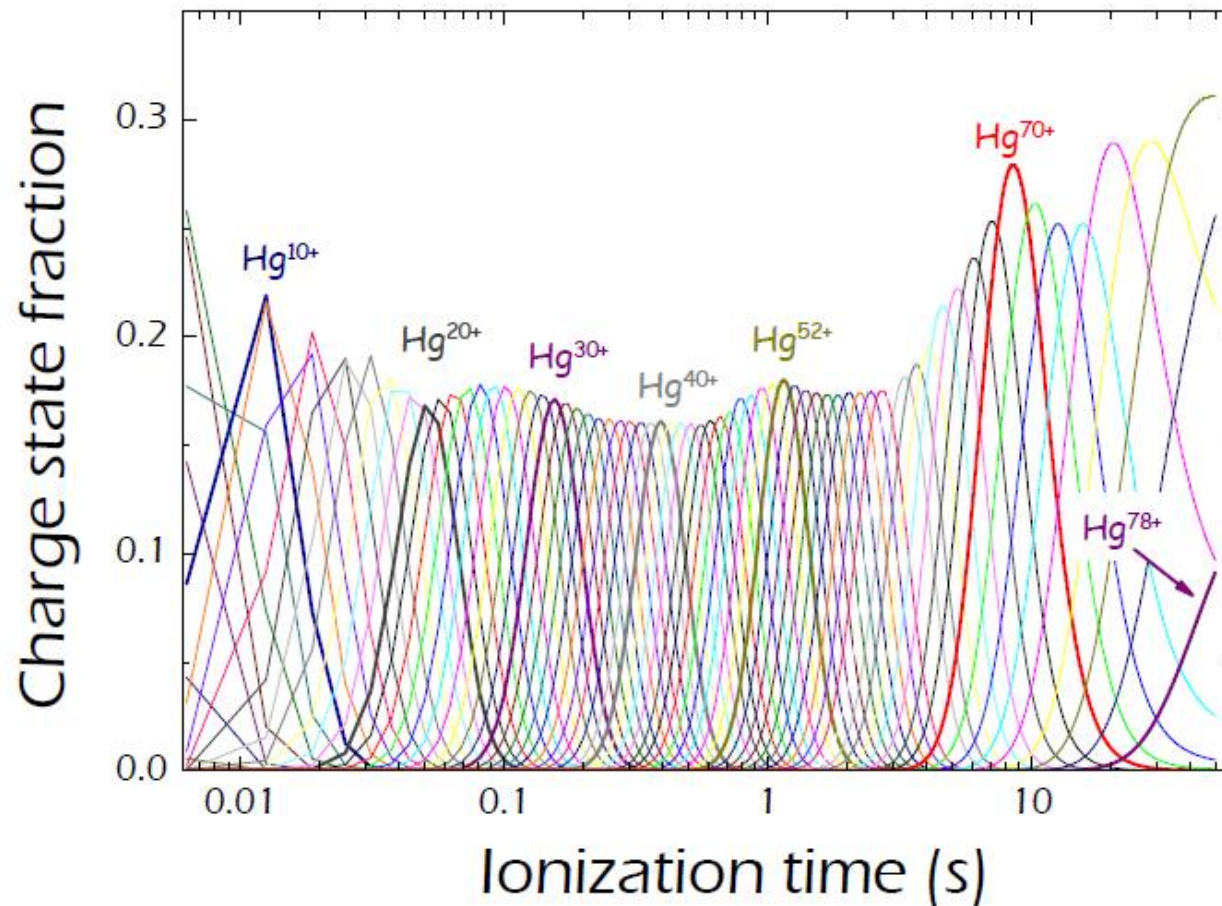


As the ion charge state goes up:

- growing ionization potential:
 $10 \text{ eV} \rightarrow 130000 \text{ eV}$
- diminishing cross section:
 $10^{-16} \text{ cm}^2 \rightarrow 10^{-24} \text{ cm}^2$

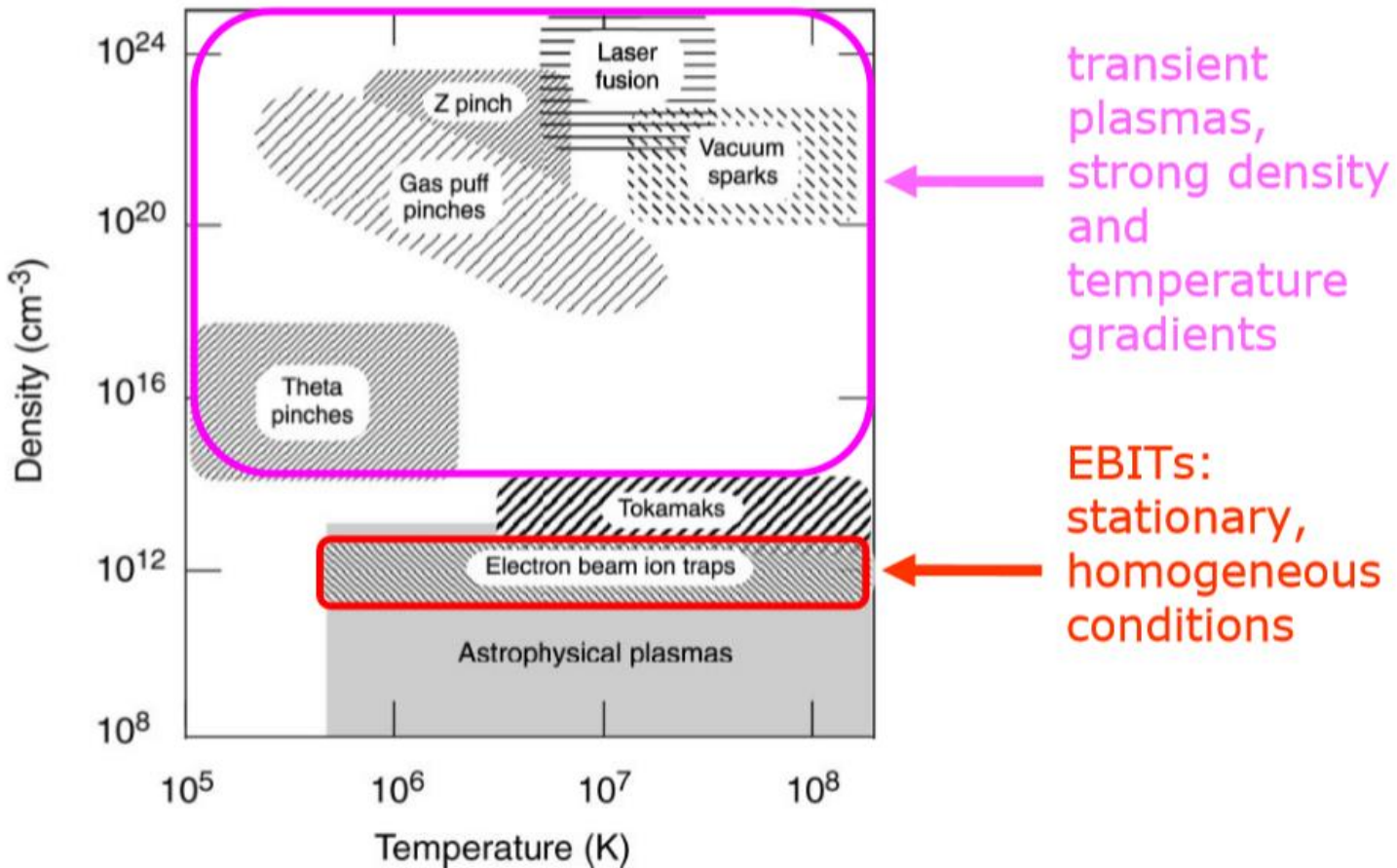
Charge state evolution

Calculated for Hg ions at 50 keV electron beam energy by solving a numerically a set of coupled differential equations for the ionization and recombination processes.



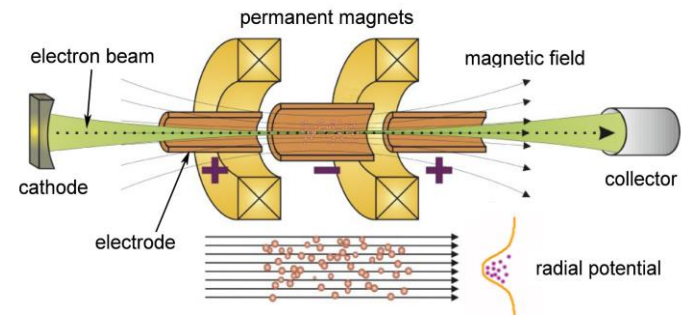
Electron-beam ion traps

EBITs are good to reproduce the conditions prevailing in astrophysical plasmas



Density and temperature space sampled by different spectroscopic light sources

Storage rings *versus* EBITs



Storage rings

Ions are in well-defined charged state (e.g. H-like, He-like...)

Ions are moving with energies from few eV/u up to few GeV/u

Ions up to hydrogen-like uranium U^{92+} can be produced and stored

Very large facilities

EBITs

A distribution of different charge states is produced in EBIT's


Ions are at “rest”

Usually medium-Z ions are produced in highly-charged states

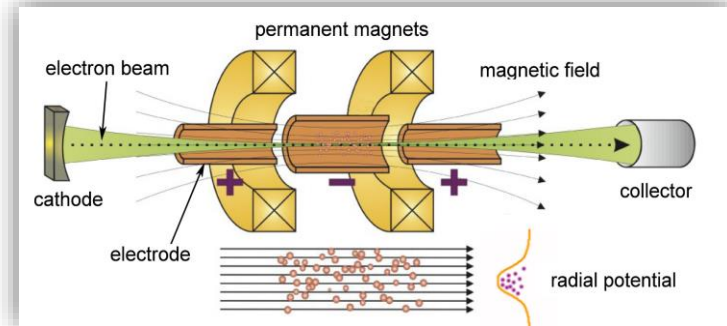
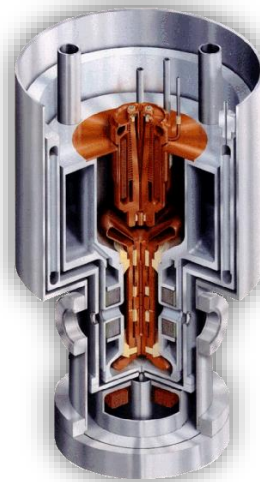
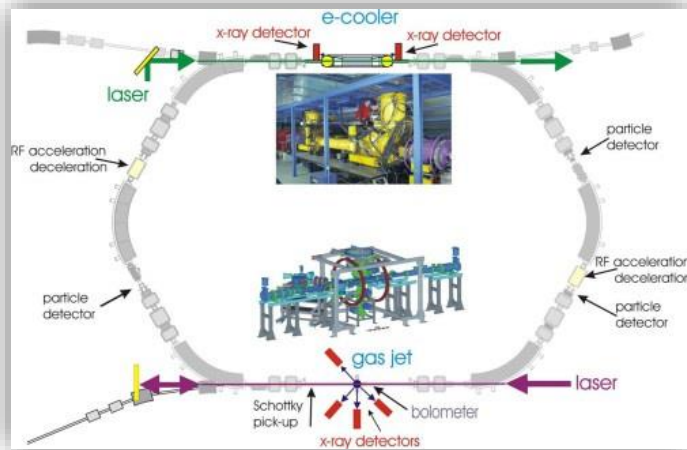
Almost “table-top” devices

In modern ion experiments both devices are used depending on particular needs.

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How we can “see” ions?

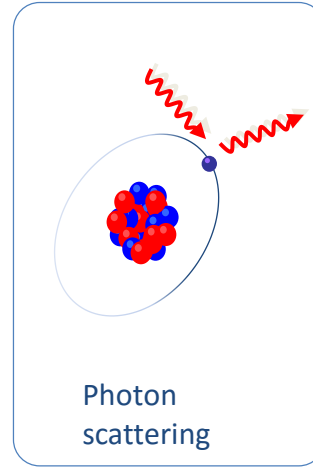
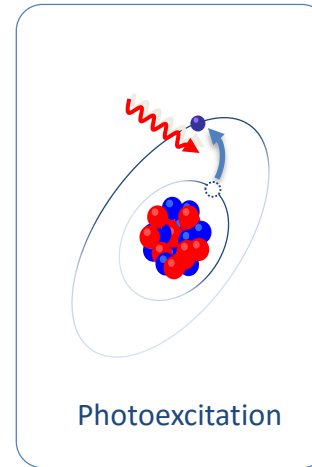
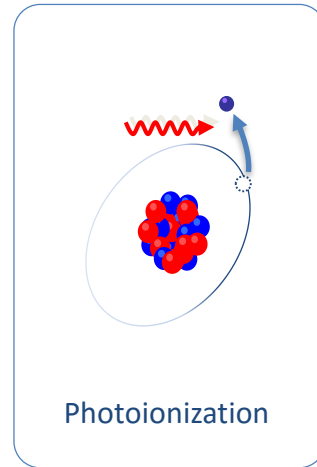
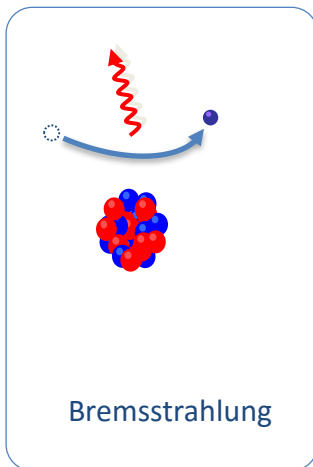
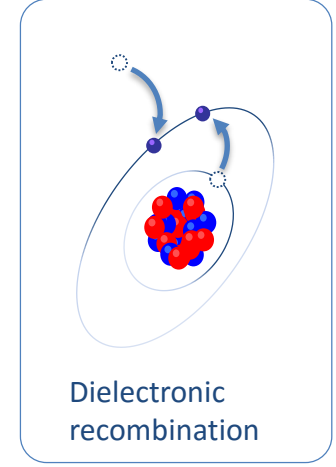
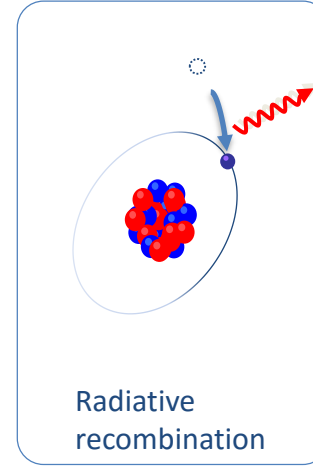
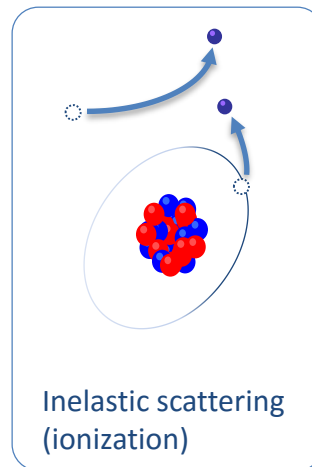
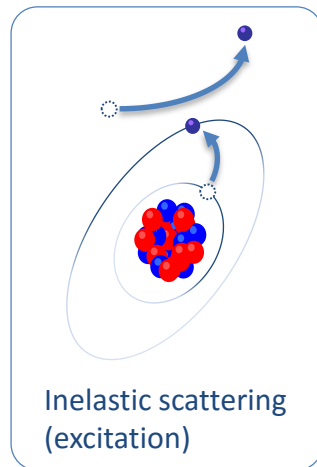
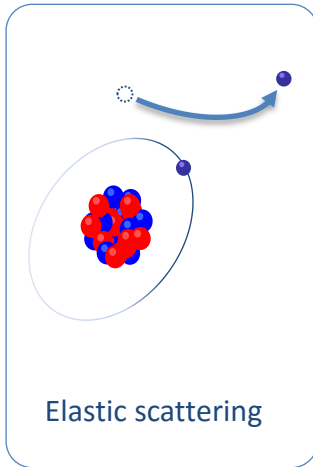


OK, let us assume that in one or another way we did produce ions. Now the next questions come: How we can diagnose these ions? How we can study the properties of these ions?

We need to discuss what atomic processes may occur with ions in storage rings and traps.

Basic atomic processes

What may happen in electron-ion, photon-ion or photon-electron collisions?

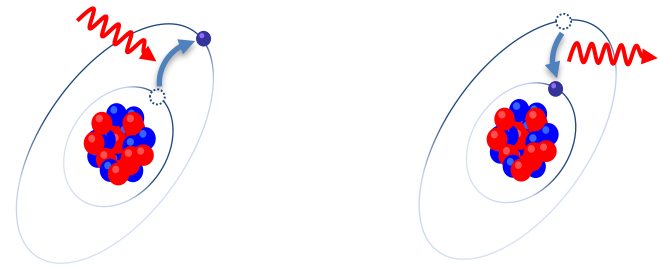
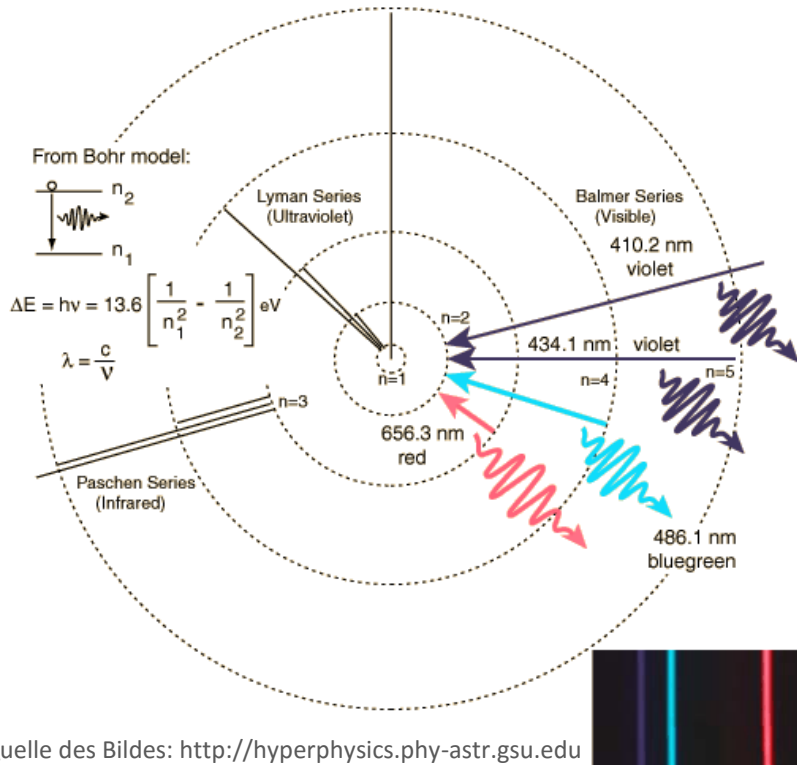


... and this is still
not a full list!

Which processes are of greater importance?

Energy levels as *fingerprint* of atom

We can investigate the emission and absorption of light by atoms!



Electron, bound to the nucleus, can have only well-defined and quantized energies:

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

Due to the quantization of atomic energy levels, photons of some well-defined wave-lengths or frequencies can be absorbed by an atom.

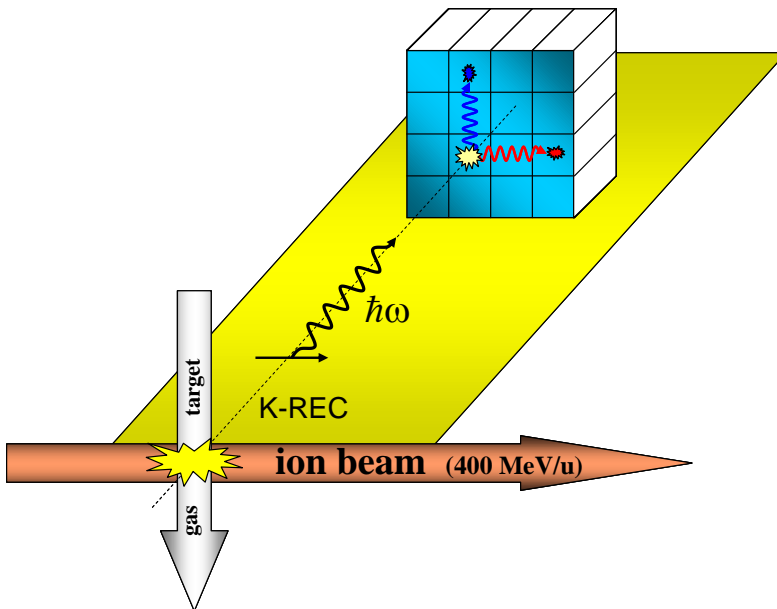
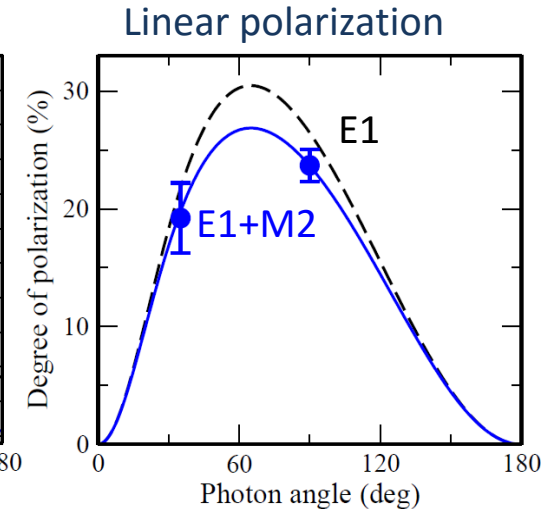
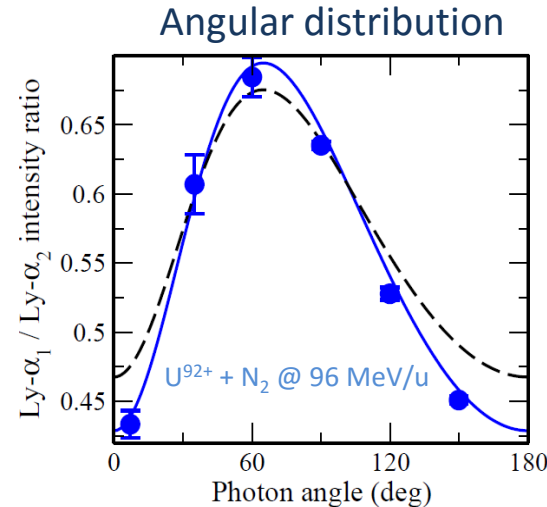
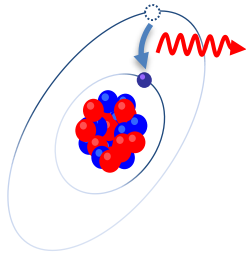
Structure of atom is “reflected” in the properties of emitted and absorbed light!

This data is of fundamental interest for the analysis of relativistic, many-body and QED phenomena and, moreover, has a great impact for astrophysical studies.



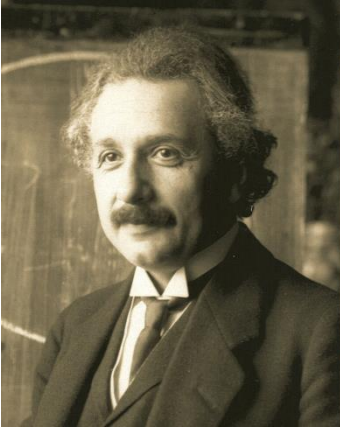
Characteristic emission from ions

We can measure not only energy spectra but also angular distribution and even polarization of characteristic photons!



One currently uses position-sensitive solid state detectors.

Photoionization and its reverse process



The Nobel Prize in Physics 1921

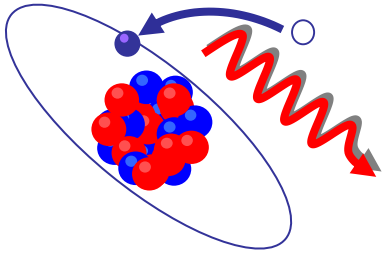
"for his services to Theoretical Physics, and especially for his discovery of the law of the photoelectric effect"



- Photoionization of hydrogen atom has been for many decades a “textbook” example in quantum mechanics.

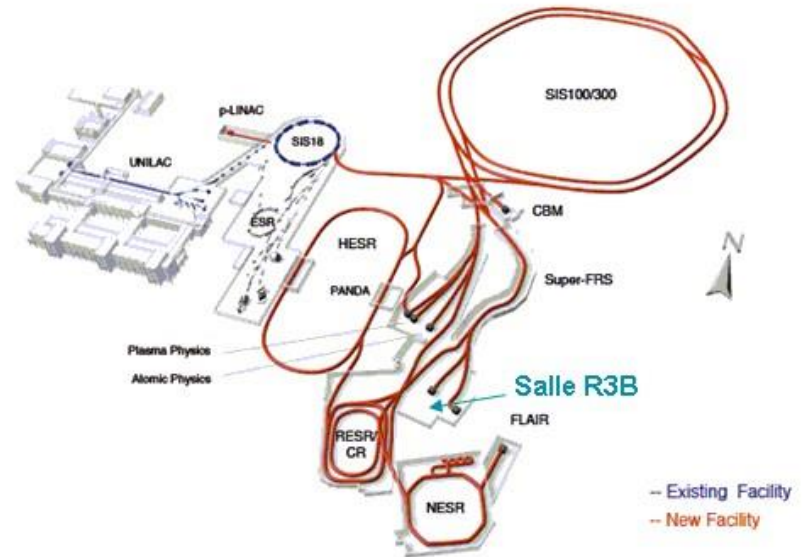
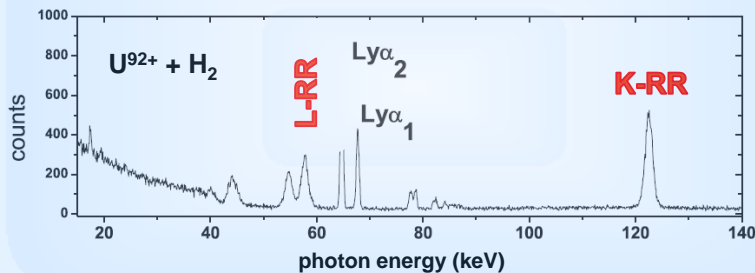
Radiative recombination

Radiative recombination



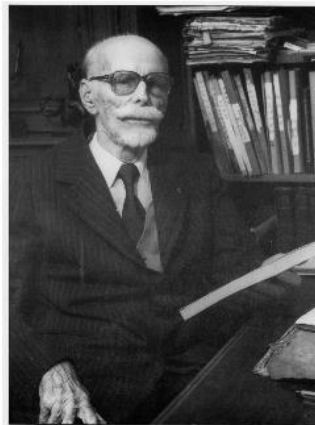
- A large number of experiments have been performed during last decades to study radiative recombination (RR).
- RR is the dominant process in ion-atom collisions.
- RR causes loss ions from the beam.
- RR allows to study photoionization at high energies.

Example: energy spectrum of x-rays in ion-atom collisions



Auger decay

- What if we have atom or ion in doubly-excited state?
- Two possibilities arise:
 - Excited states may decay via a photon emission.
 - Doubly-excited state can decay via a radiationless transition: autoionization or Auger decay.



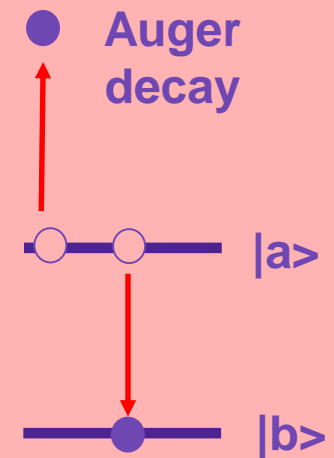
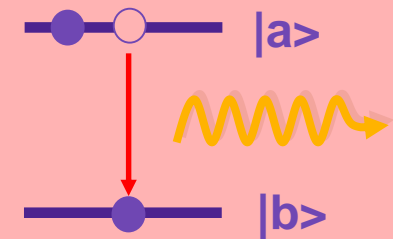
Pierre Auger



Lise Meitner

spontaneous emission

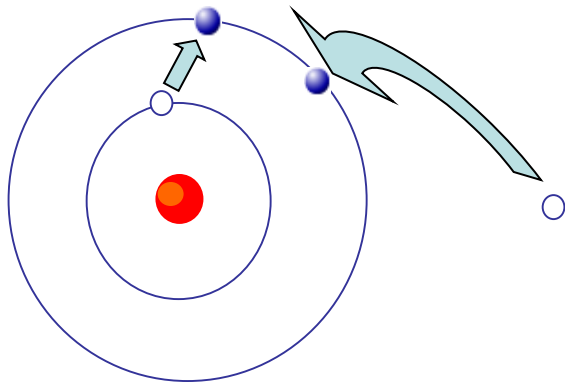
$$E_b = E_a - \hbar\omega$$



Dielectronic recombinations

- One may consider process reversed to Auger decay: dielectronic recombination

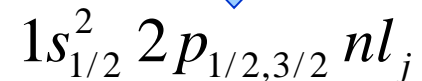
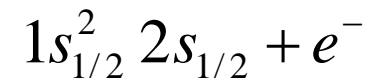
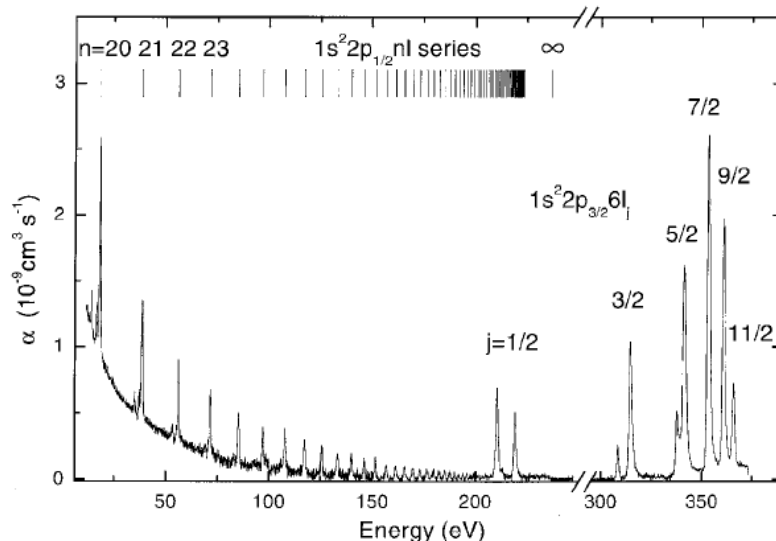
Very important for spectroscopic purposes: dielectronic recombination is resonant capture process!



$$T_{kin} + E_b = E^{**}$$

One can vary kinetic energy of electrons (or ion beam) and to study DR cross sections (rates).

- Example: DR of initially lithium-like bismuth ions Bi^{80+}



Plan of the lecture

- Organization questions: how the lecture will be structured
- Motivation: what you will learn at the lecture?
- Heavy multiply-charged ions: what is so special with them?
- Production and storage of multiply-charged ions
 - Accelerator and storage ring facilities
 - Ion trap devices
- Experimental “observation” of ions
 - Basic atomic processes
 - Detectors

Lectures in the web: www.ptb.de/fpm
(password: Uranium\$92)