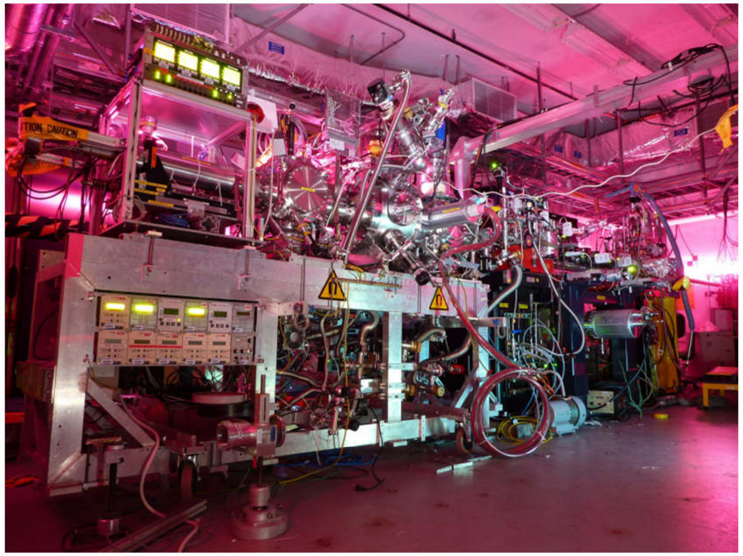
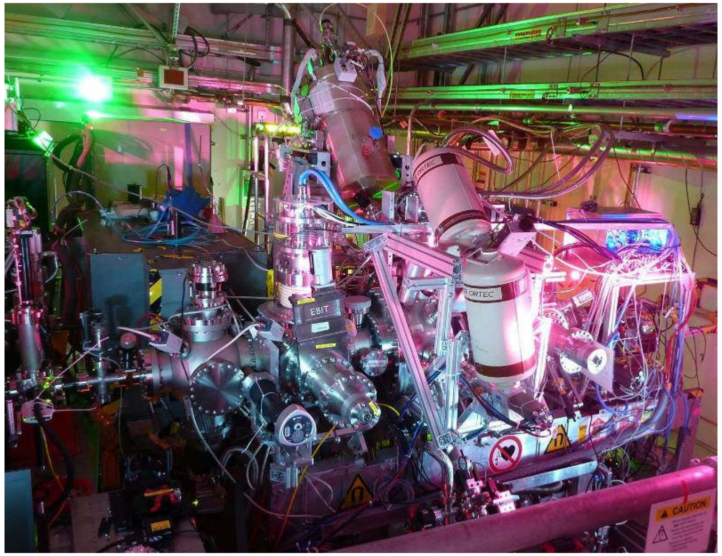
MAX-PLANCK-INSTITUT FÜR KERNPHYSIK

70-keV-hard bound-state quantum electrodynamics
&
Soft x-ray purely photo-ionized low-density plasmas at XFEL





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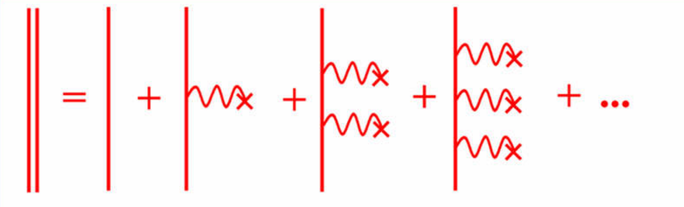
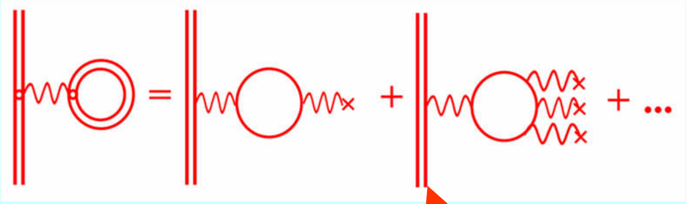
Bound-state quantum electrodynamics

- QED describes atomic, molecular and photonic interactions, and is the most accurate physical theory
- QED is the best understood quantum field theory, and serves as paradigm for all others
- In stable, bound systems, QED can be tested with ultimate precision
- For many-electron bound systems, QED calculations are essentially perturbative, and require approximations which still have to be benchmarked by experiments

Bound-state quantum electrodynamics

- Non-perturbative QED: coupling constant Zα ≈ 1





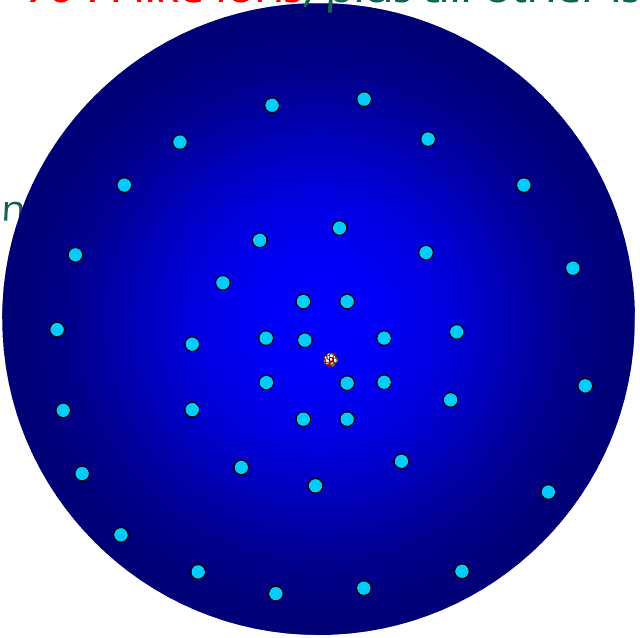
Bound electron expanded: sum of free electron propagators
Many virtual photons, each interaction Z times stronger than in H

- Few-particle QED unexplored
- Theory of (non-perturbative) QED still under construction
- General scaling law ~Z^4
- Large nuclear size effects ~ Z^3... Z^5
-

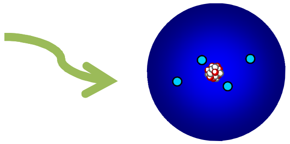
Highly charged ions (HCI)

- Study of hydrogen lead to quantum mechanics, relativistic fine structure and spin, hyperfine structure, QED…, proton size, antimatter asymmetry…
- HCI: Expanding to ~90 H-like ions, plus all other isoelectronic sequences

Atoms:
- size: 100 pm
- outer electrons weakly boun
- strong correlation effects



HCI:
- size: few pm
- few strongly bound electrons
- large electron-nucleus overlap



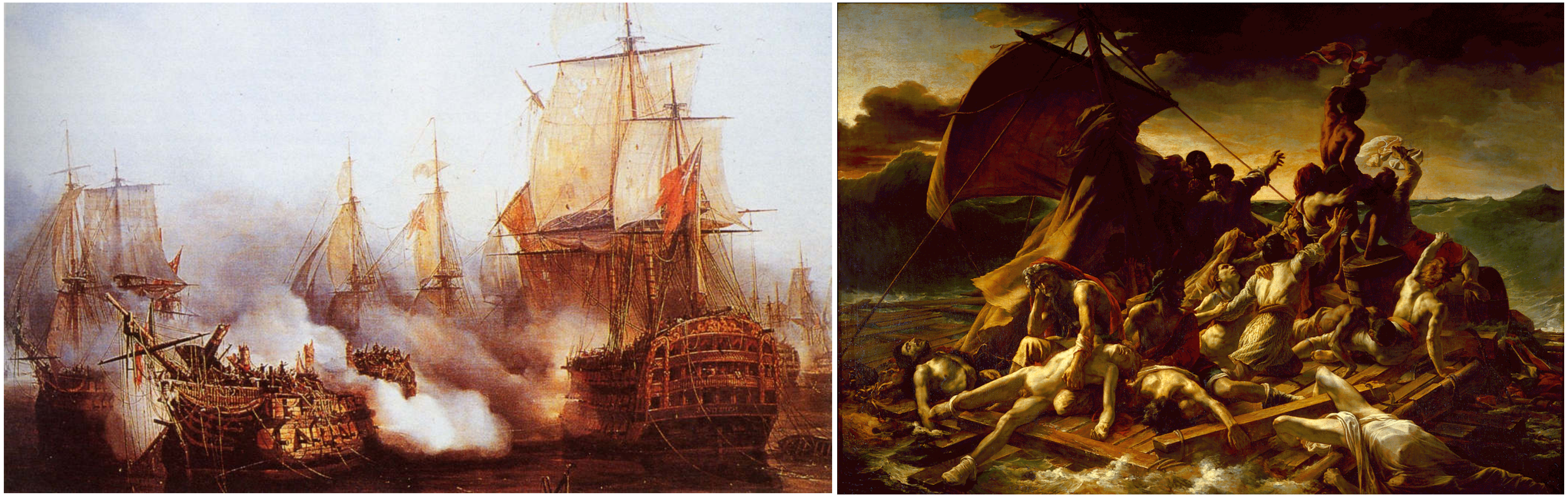
• Binding energy	~ Z^2
• Fine structure	~ Z^4
• QED effects	~ Z^4
• nuclear size effects	~ Z^6
• PNC contributions	~ Z^5
• Stark shifts, light shifts	~ $1/Z^6$

Bound-state quantum electrodynamics

- Understanding relativistic and QED effects is important to correctly model atoms (gold is yellow…) and molecules, and their interactions with X rays from first principles
- Every atom contains a core which can be investigated in detail using HCI
- Trapped HCI allow one to study QED and other interactions in a precise and controlled, steady-state fashion
- This stands in contrast to experiments using transient HCI sources with a very fast temporal evolution, strong spatial inhomogeneity, and density gradients
- In the XFEL world of ultra-high intensities, HCI become the natural survivors and can handle extremely powerful photon fluxes

Survivor core of atom

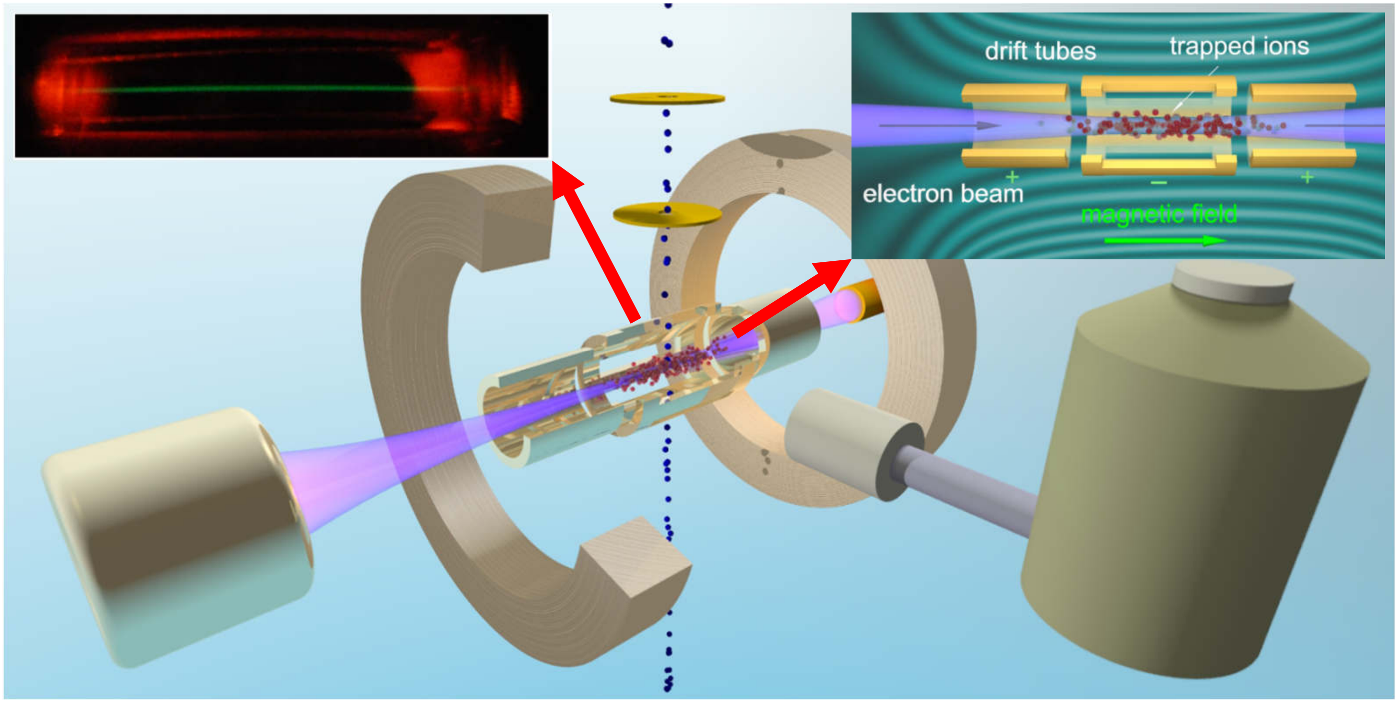
- XFEL exposure strips atoms and makes them HCI
- Exposing prepared HCI to XFEL makes stepwise analysis of dynamic processes easier to understand



Bound-state quantum electrodynamics

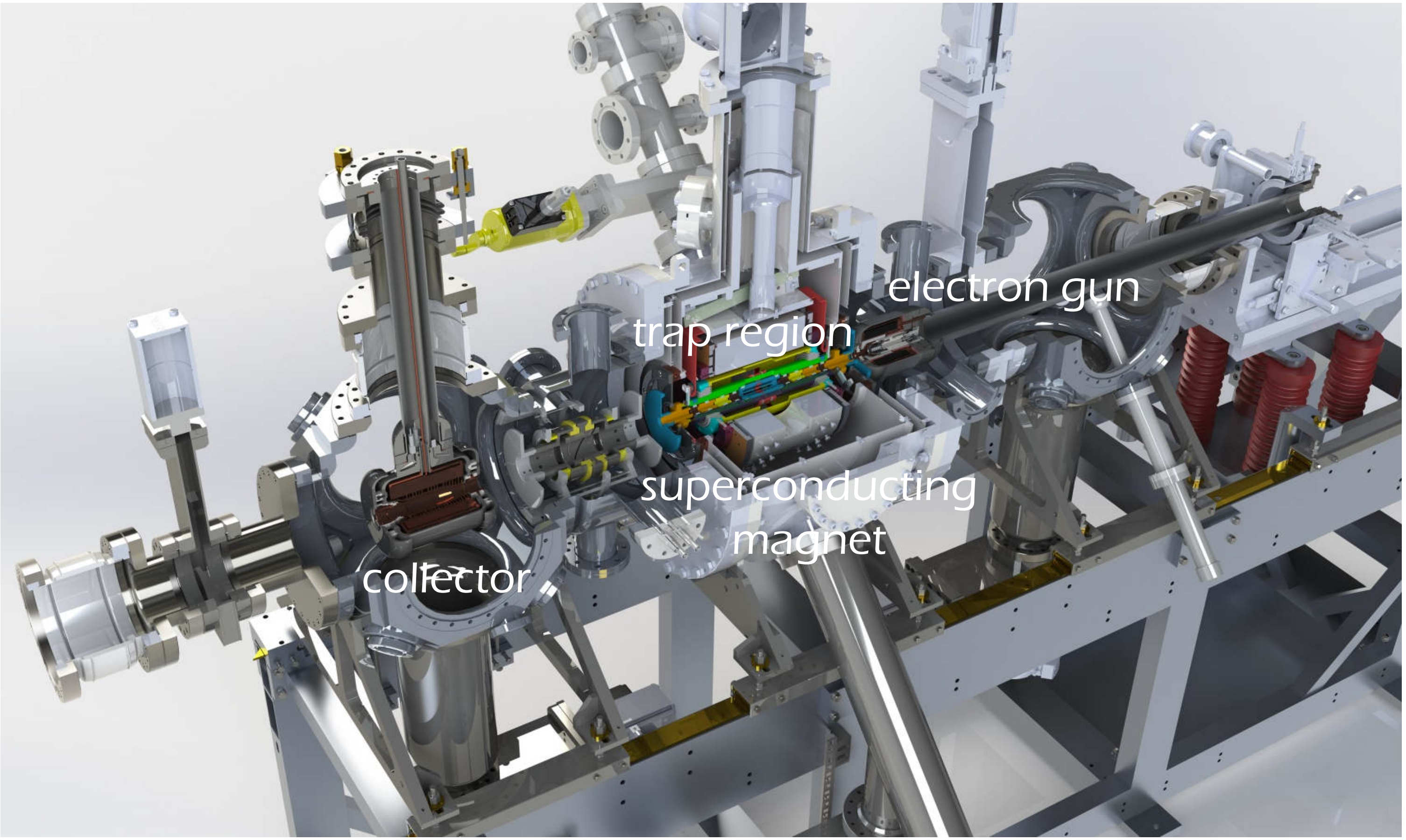
- Highly charged ions (HCI) are produced in accelerators and ions sources, and studied in storage rings and traps
- Electron beam ion traps (EBIT) are capable of producing and storing HCI in any charged state (from He^{+} to U^{92+})
- All x-ray spectroscopic measurements of HCI are limited by statistics and resolution, due to instrumental issues in both storage rings and EBITs
- At hard x-ray energies, photoexcitation cross sections (~10^{-18} cm^2) are many orders of magnitude higher than electron impact excitation cross sections (~10^{-24} cm^2)
- The combination of an XFEL and an EBIT provides enormous statistical and resolution advantages for bound-state QED studies

Electron beam ion trap (EBIT)

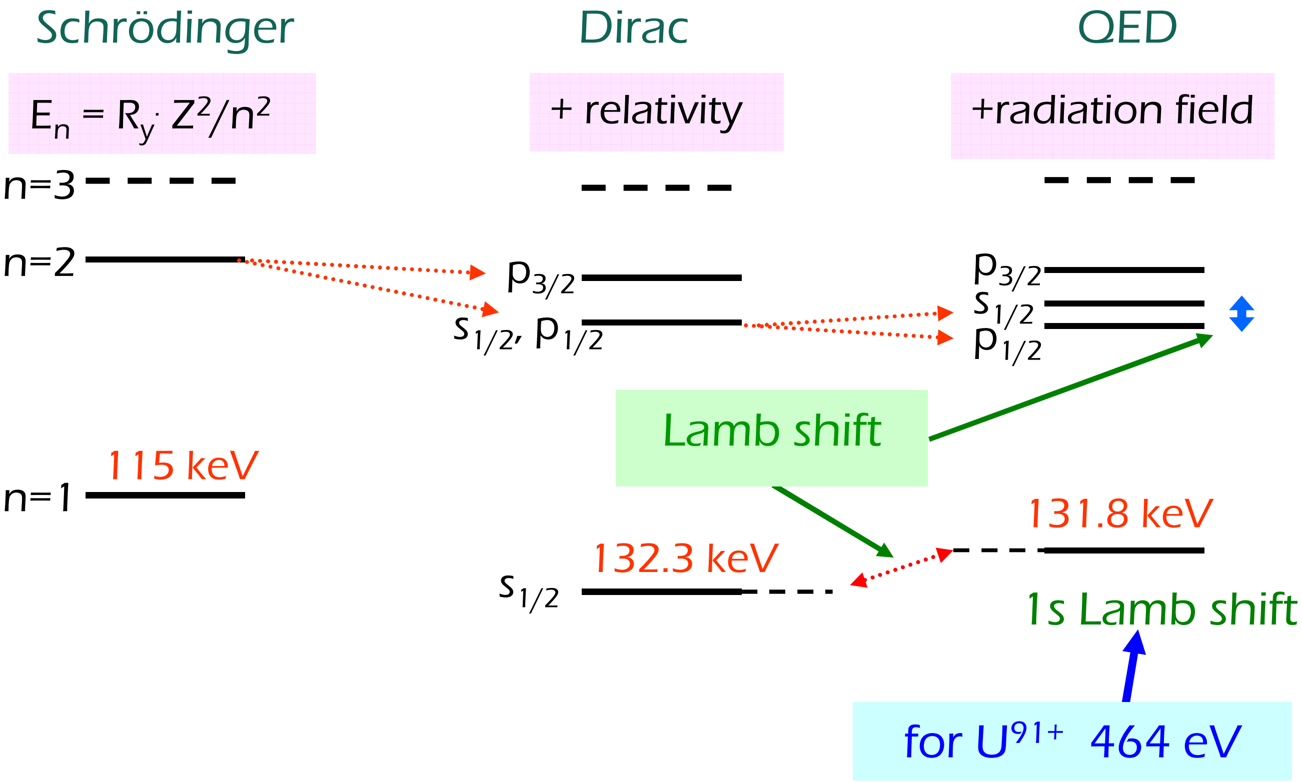


- *An electron beam produces, traps and excites HCI under well-defined, controlled conditions.*
- *Photon detectors, crystal and grating spectrometers, microcalorimeters, etc., are used for diagnostics from the optical to the hard x-ray range.*

Electron beam ion trap (EBIT)



Example: H-like uranium (U^{91+})



Schrödinger

$E_n = R_y \cdot Z^2/n^2$

n=3

n=2

n=1

115 keV

Dirac

+ relativity

$p_{3/2}$

$s_{1/2}, p_{1/2}$

$s_{1/2}$

132.3 keV

QED

+radiation field

$p_{3/2}$

$s_{1/2}$

$p_{1/2}$

Lamb shift

131.8 keV

1s Lamb shift

for U^{91+} 464 eV

Example: H-like uranium (U^{91+})

FWHM≈ 700 eV; total uncertainty ± 5 eV

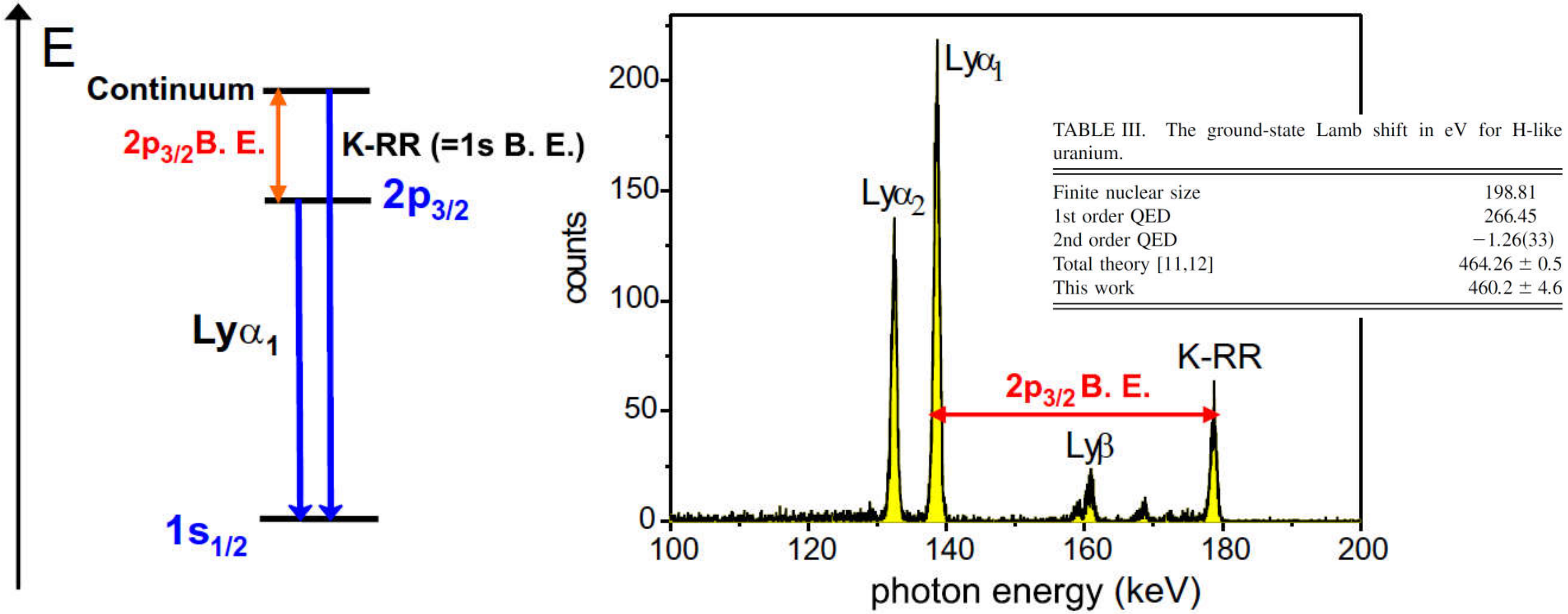
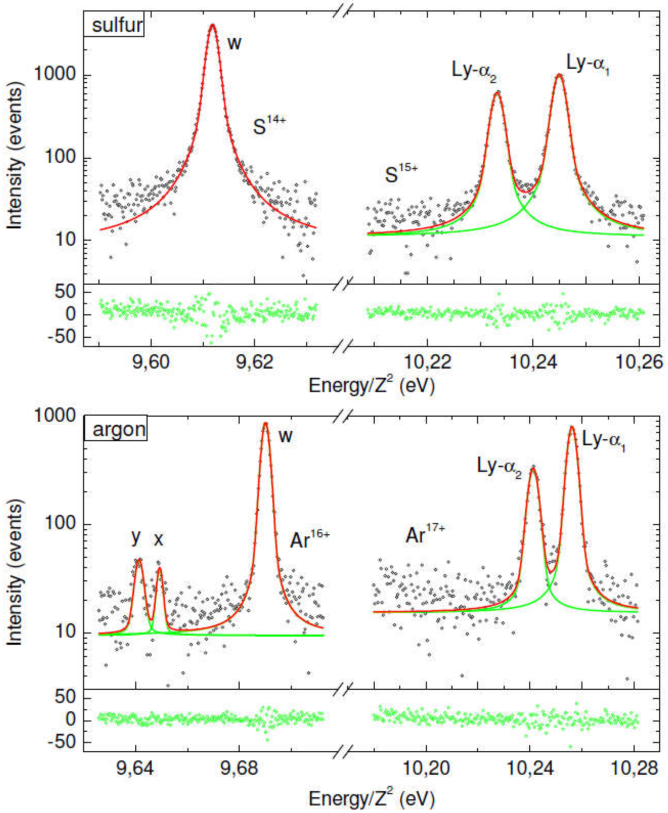


TABLE III. The ground-state Lamb shift in eV for H-like uranium.

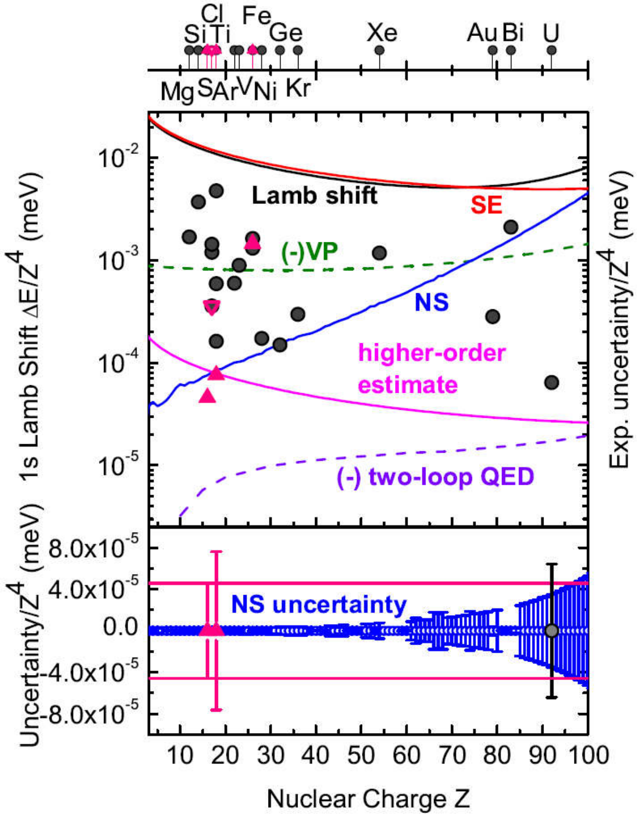
Finite nuclear size	198.81
1st order QED	266.45
2nd order QED	−1.26(33)
Total theory [11,12]	464.26 ± 0.5
This work	460.2 ± 4.6

X-ray spectrum (laboratory frame) following the radiative recombination of electrons with bare uranium ions. Left: Ly-α_1 and K-RR transitions in a hydrogenlike ion. Right: X-ray spectrum accumulated with a condition on the coincidence time. (From: Gumberidze et al., PRL 2005)

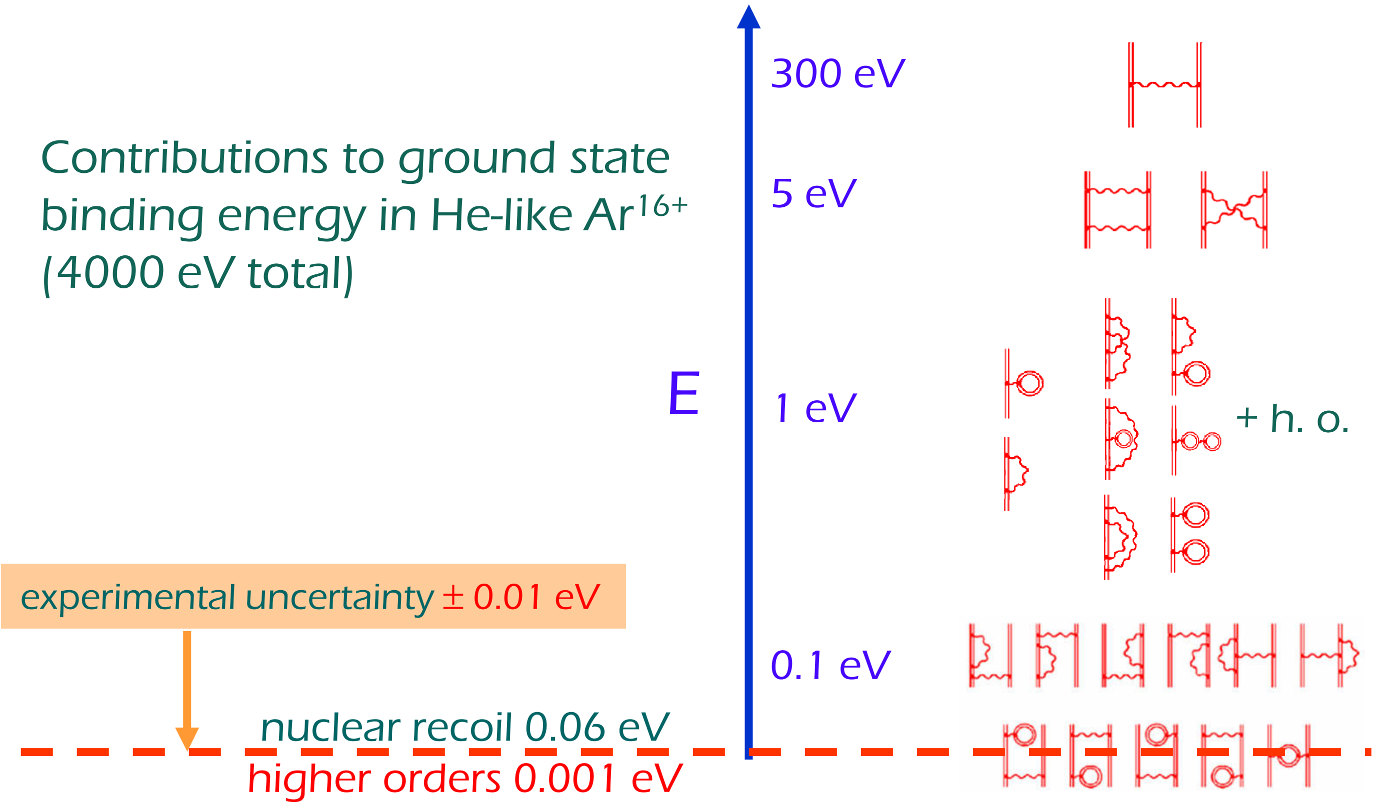
Bound-state quantum electrodynamics



- FWHM≈ 1 eV
- uncertainty ~ ± 0.01 eV



Two-electron QED Feynman diagrams



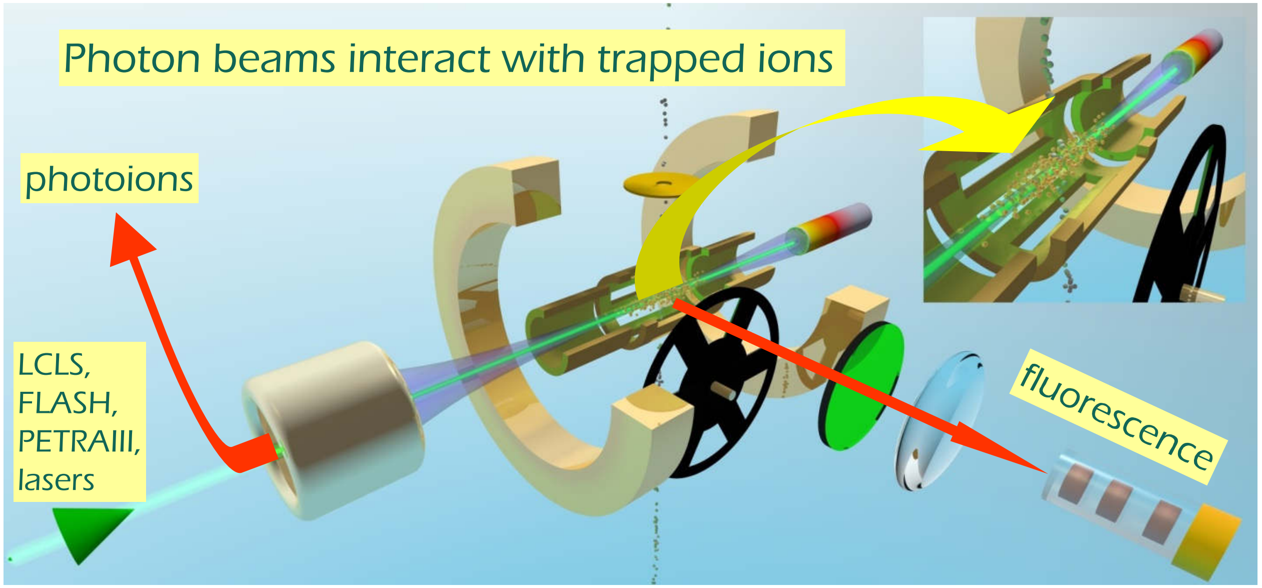
Contributions to ground state binding energy in He-like Ar^{16+} (4000 eV total)

experimental uncertainty ± 0.01 eV

nuclear recoil 0.06 eV

higher orders 0.001 eV

Resonantly photon-induced processes



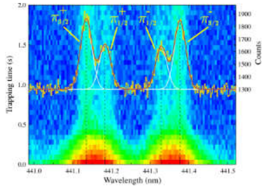
Photon beams interact with trapped ions

photoions

LCLS,
FLASH,
PETRAIII,
lasers

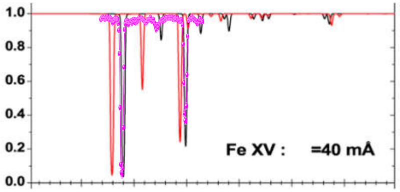
fluorescence

440 nm M1 Ar^{13+}



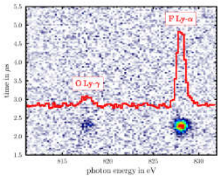
V. Mäckel et al.,
PRL **107** 143002 (2011)

800 eV photoionization Fe^{14+}



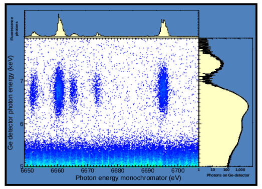
M. C. Simon et al.,
PRL **105** 183001 (2010)

800 eV Fe^{16+}



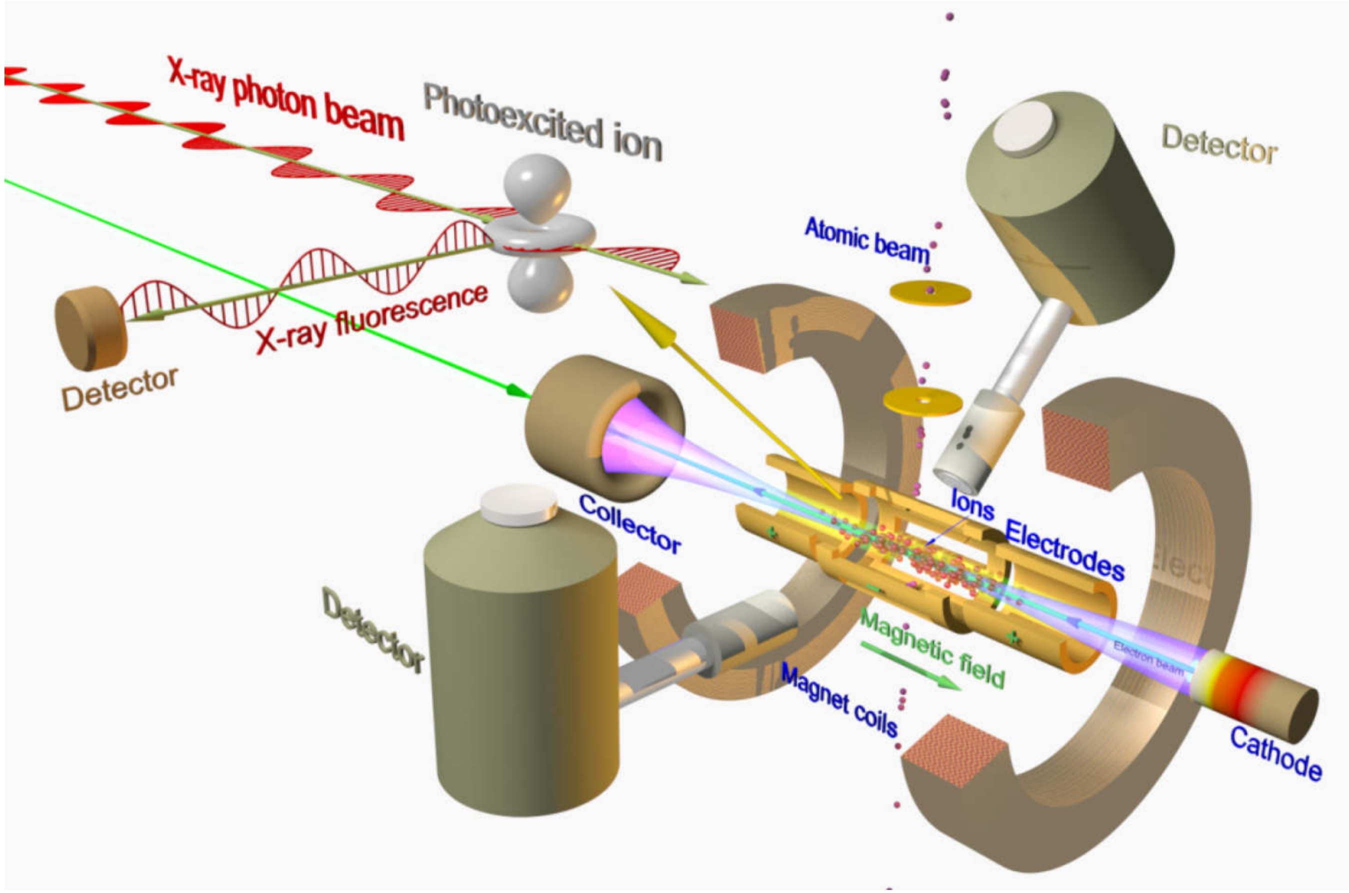
S. Bernitt et al.,
Nature **492**, 225 (2012)

6 keV Fe^{24+}, 13 keV Kr^{34+}

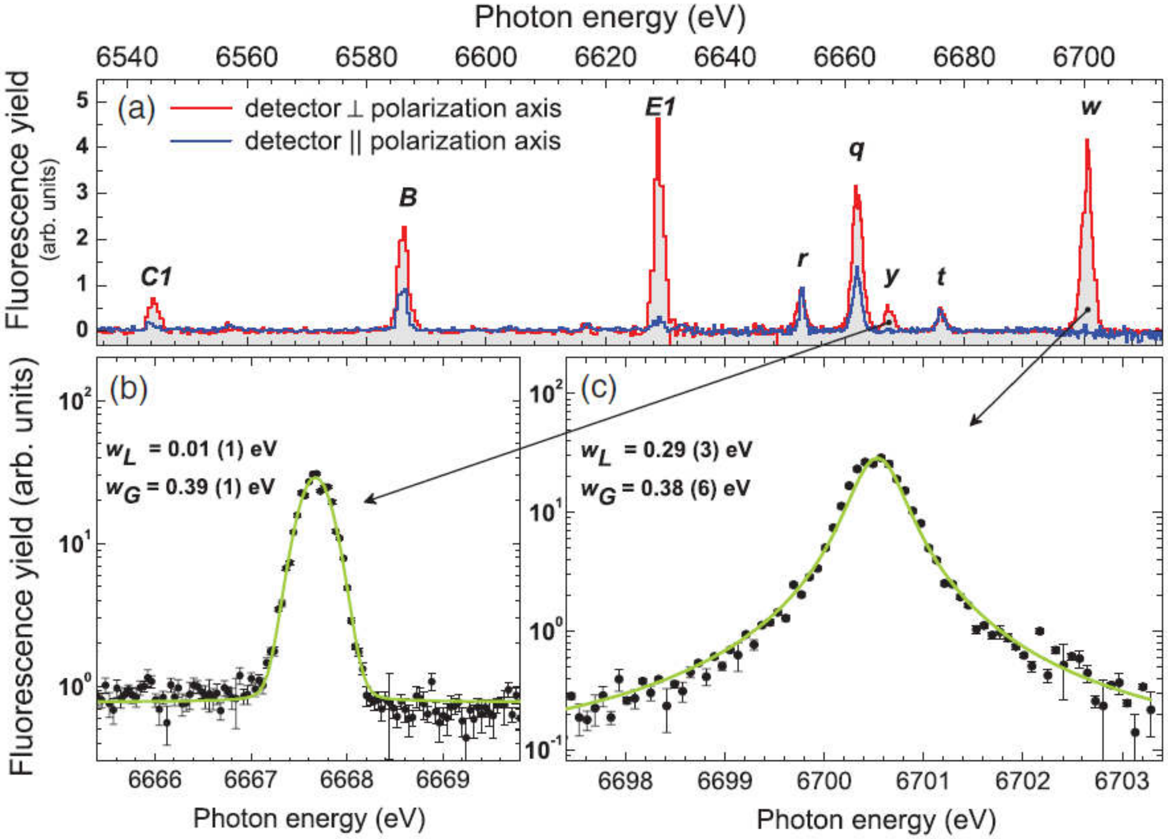


J. Rudolph et al.,
PRL **111**, 103002 (2013)

EBIT at XFEL


X-ray photon beam
Photoexcited ion
Detector
Atomic beam
X-ray fluorescence
Detector
Collector
Ions
Electrodes
Detector
Magnetic field
Electron beam
Magnet coils
Cathode

Bound-state quantum electrodynamics

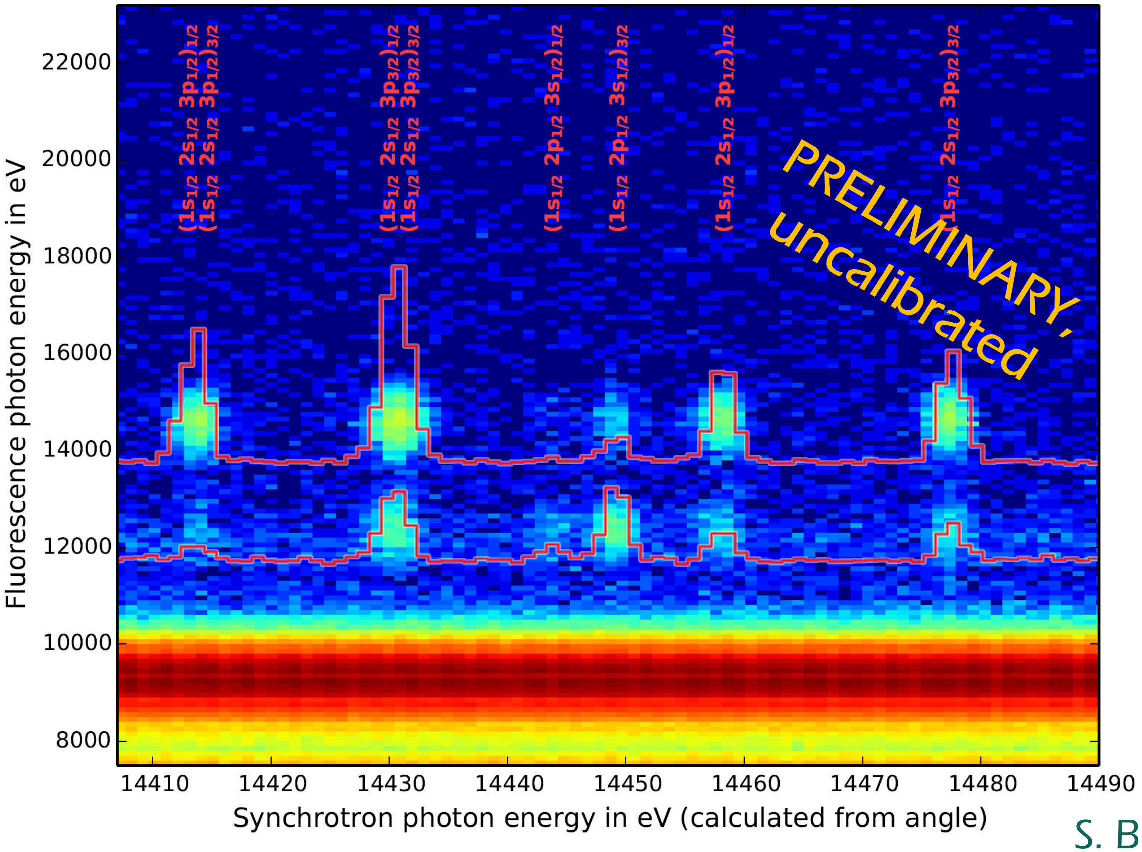


- Fe^{24+} and friends Kα lines
- At P01: FWHM≈ 0.4 eV
- Uncertainty ± 0.01 eV
- Four-crystal spectrometers would improve resolution
- XFEL needed for H-like HCI to suppress background
- Next step: cold ions

In EBIT currently 10^5 K; with our RF traps currently 10^{-4} K achieved, nine orders of magnitude drop)

J. K. Rudolph et al., PRL 111, 103002 (2013)

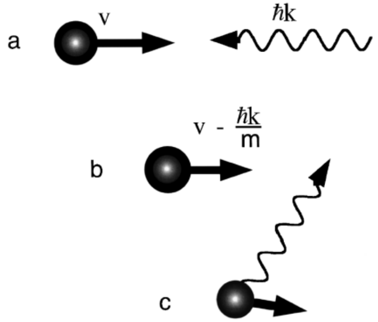
Going to higher energies: background suppression at XFEL



S. Bernitt, MPIK (2016)

The HCI attosecond transitions

- The $n=1 \rightarrow 2$ transition in He-like and H-like ions have very high transition rates on the order of $A_{ik} \approx 5 \cdot 10^{16}/s$, and excited states have lifetimes $\tau \approx 20$ as
- Within a 10 fs XFEL pulse, a single HCI can absorb and emit ~500 X-ray photons
- Even at recoiling velocity of 100 km/s, it keeps absorbing if bandwidth $\Delta E/E > 10^{-5}$
- Stimulated Raman transitions also possible, two-color techniques
- Ejection of recoiling HCI from trap and subsequent TOF detection
- Opportunities for atomic (ionic) interferometry, mass and photon energy comparison



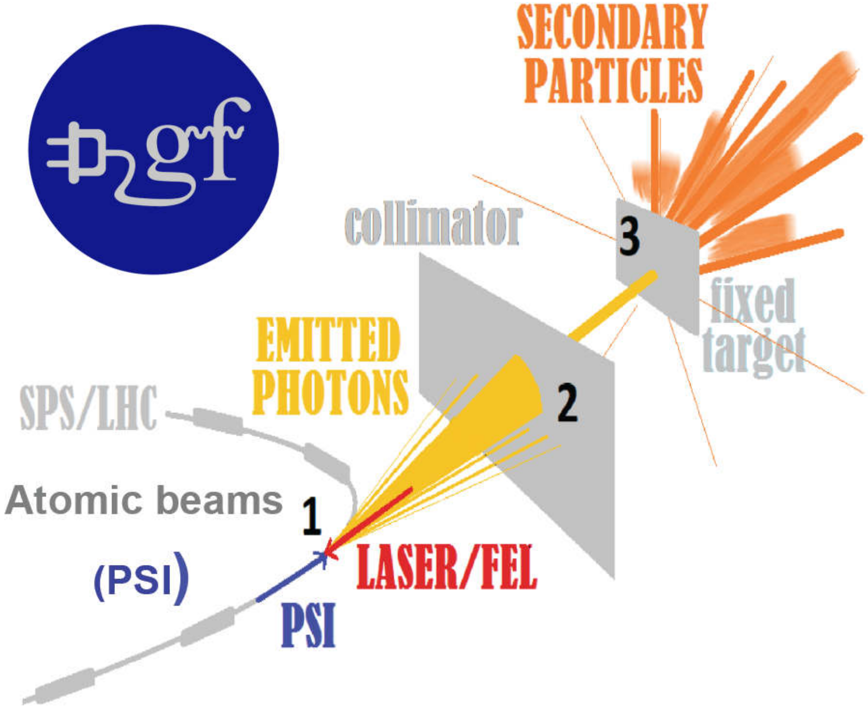
Bound-state quantum electrodynamics

- Isoelectronic sequences of few-electron ions are the ideal testing ground for QED, providing a controlled scaling of QED strength and electron-correlation effects
- Analogously, nuclear-size effects also scale with high powers of Z and become important for an accurate description of the system
- A proposed CERN extension, Gamma Factory [1], would use few-electron HCI to generate the most powerful γ beams, and use them for producing secundary particle beams, investigate QED and particle physics.

[1] From: Krasny, arXiv:1511.07794 [hep-ex]

Gamma Factory in a nutshell

- Produce, accelerate and store high energy atomic beams of Partially Stripped Ions (PSI) (remark: a.k.a. as HCI) and excite their atomic degrees of freedom, by laser photons to form high intensity primary beams of gamma rays and, in turn, secondary beams of polarised leptons, neutrinos, vector mesons, neutrons and radioactive ions.
- Provide a new, efficient scheme of transforming the accelerator RF power (selectively) to the above primary and secondary beams trying to achieve a leap, by several orders of magnitude, in their intensity and/or brightness, with respect to all the existing facilities.
- Use the primary and the secondary beams as principal tools of the Gamma Factory broad research programme.



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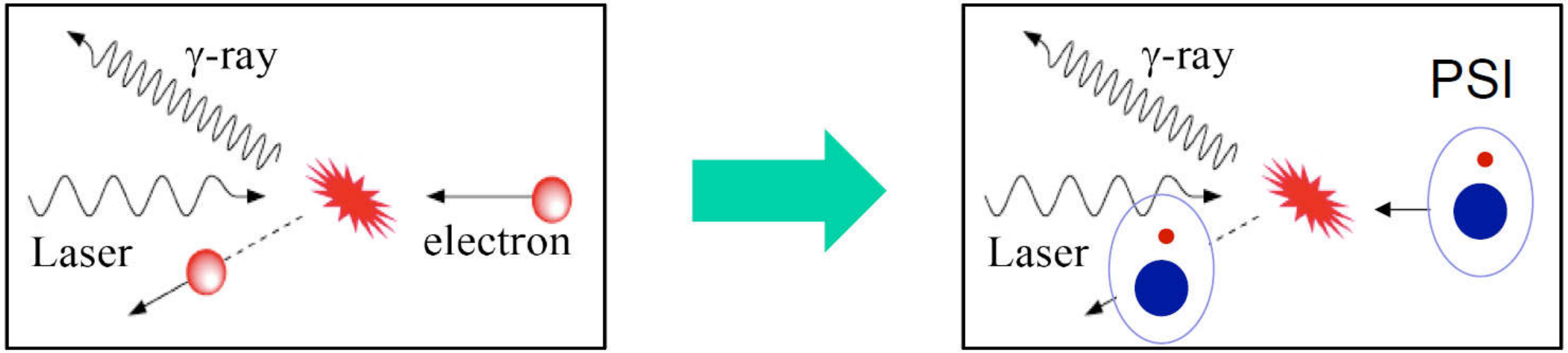
Gamma Factory in a nutshell



- Beam energy, isoelectronic sequence and choice of laser type yield γ-ray energies in the range 40 keV – 400 MeV
- Presently, strong interest in interest Pb^{79+} to Pb^{81+}

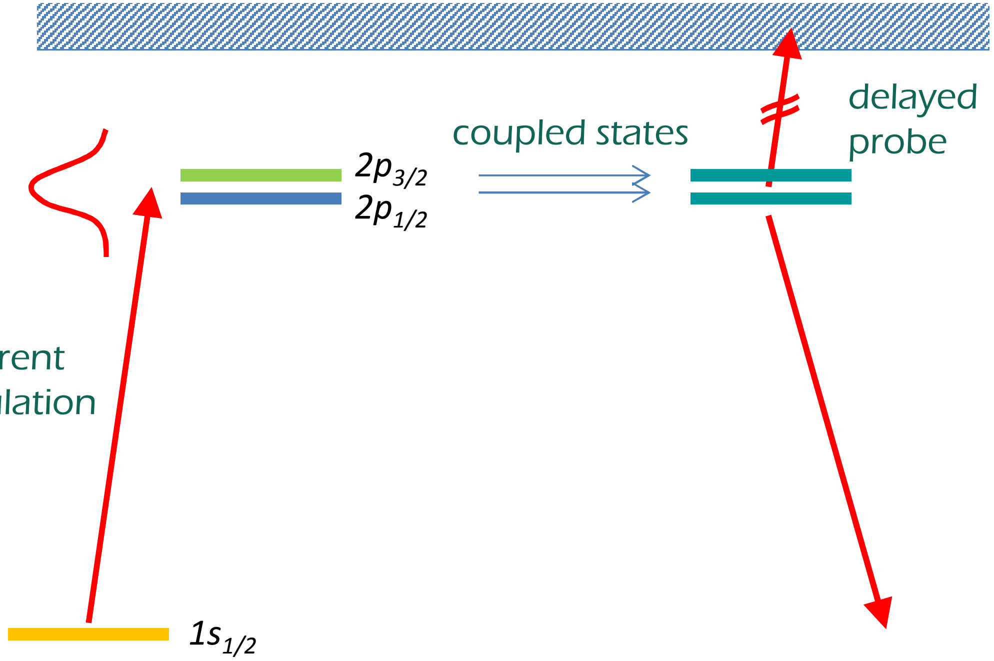
From talk by Mieczyslaw Witold Krasny, CERN at Trento ECT 2018

Electron excitation dynamics in the attosecond scale

- Electronic wave packages (e. g., coupled spin states) can be prepared in systems which are impervious to Auger decay within the experimental time
- Multi-photon (sequential) absorption is possible in the 80 keV range
- Pump-probe experiments can track the dynamic evolution of the spin system recording both fluorescence and/or photoions (quantum beats, Ramsey-type methods)
- Such experiments could, e. g., allow to better understand the role of the Breit interaction (spin-spin) in strongly bound, relativistic electrons by exaggerating those effects in a well-defined way

Generic pump-probe experiments

- Fine structure and hyperfine/isotopic energy differences in the meV…eV range result in fs-scale beatings that can be used to analyze energy differences and spontaneous transition rates



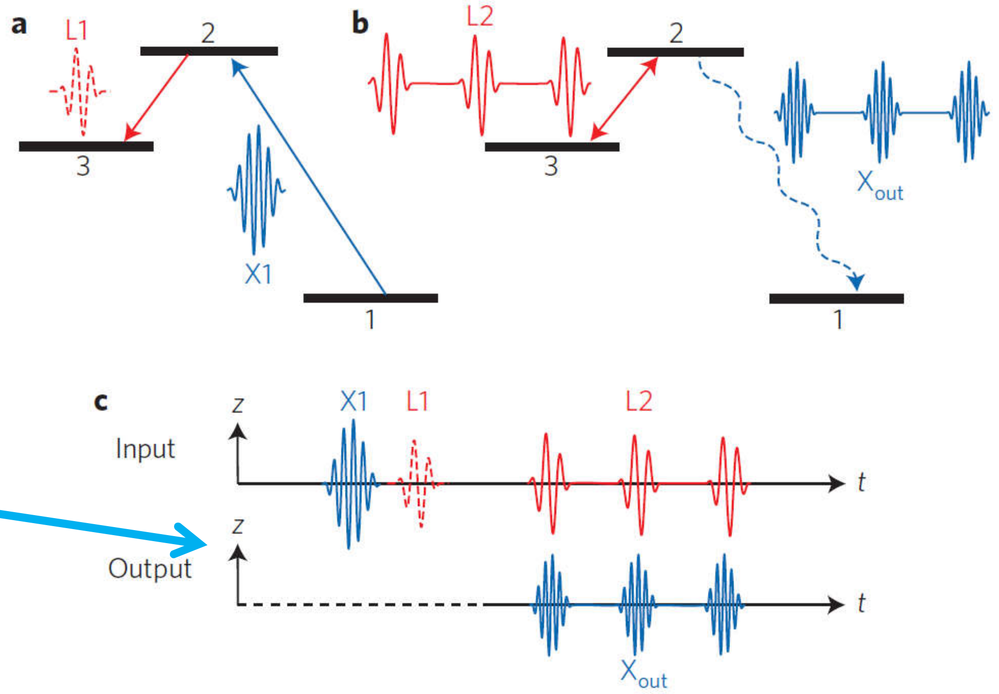
Frequency comb generation

Coherent superpositions of states in hard X-ray driven systems can be modulated by optical or VUV frequency combs for the generation of X-ray frequency combs

a) An ion ensemble is driven by an ultrashort, broadband X-ray pulse (X1) exciting from 1 the fast-decaying level 2, which an optical pulse (L1) couples to the metastable state 3. This generates a superposition of 1 and 3.

b) An optical frequency comb (L2) drives 2↔3. The emitted X-rays (X_{out}) amplify or attenuate X1 as it propagates through the medium, and constitute an X-ray comb.

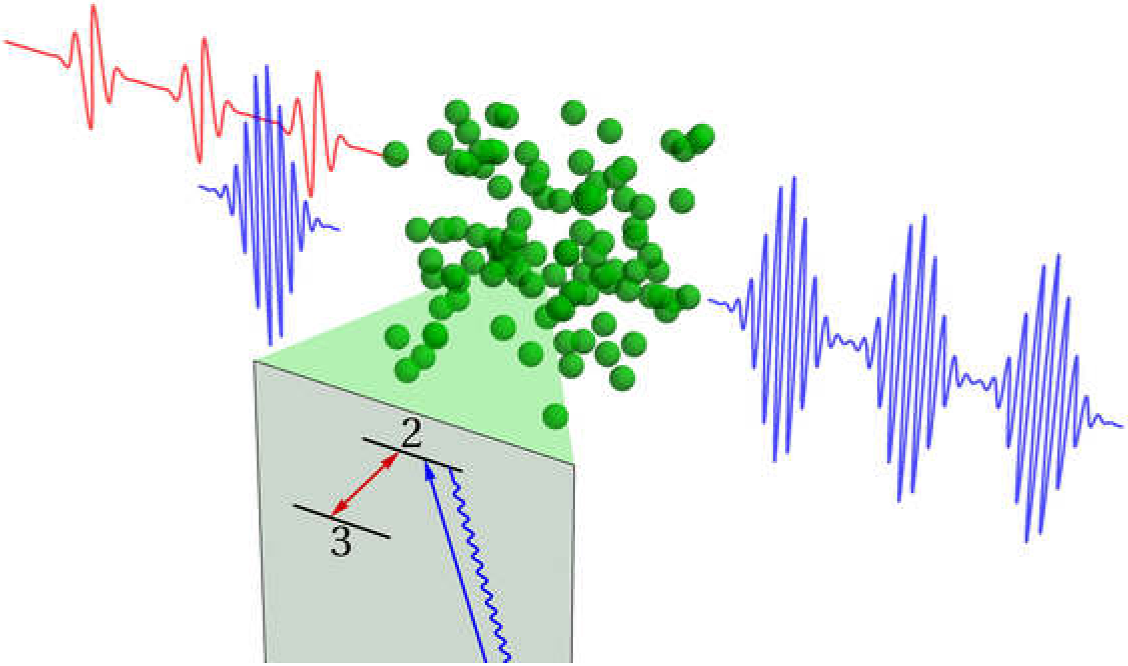
c) All pulses from a) and b) are polarized and co-propagating.



Broadband high-resolution X-ray frequency combs, S. M. Cavaletto et al., Nature Photonics 8, 520 (2014)

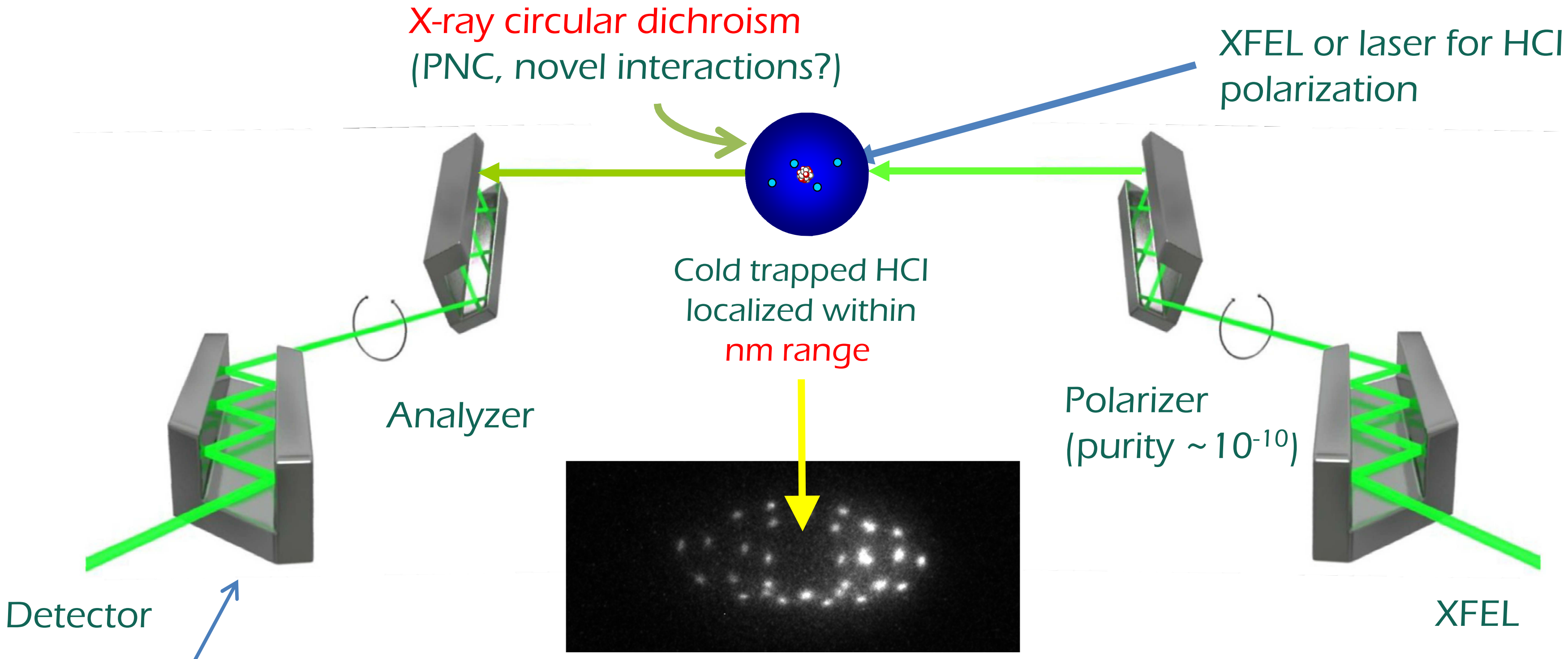
X-ray frequency comb generation

Coherent superpositions of states in hard X-ray driven systems can be modulated by optical or VUV frequency combs for the generation of X-ray frequency combs



Broadband high-resolution X-ray frequency combs, S. M. Cavaletto et al., Nature Photonics 8, 520 (2014)

X-ray precision polarimetry with HCI



X-ray circular dichroism
(PNC, novel interactions?)

XFEL or laser for HCI polarization

Cold trapped HCI localized within nm range

Analyzer

Polarizer (purity ~10^{-10})

Detector

XFEL

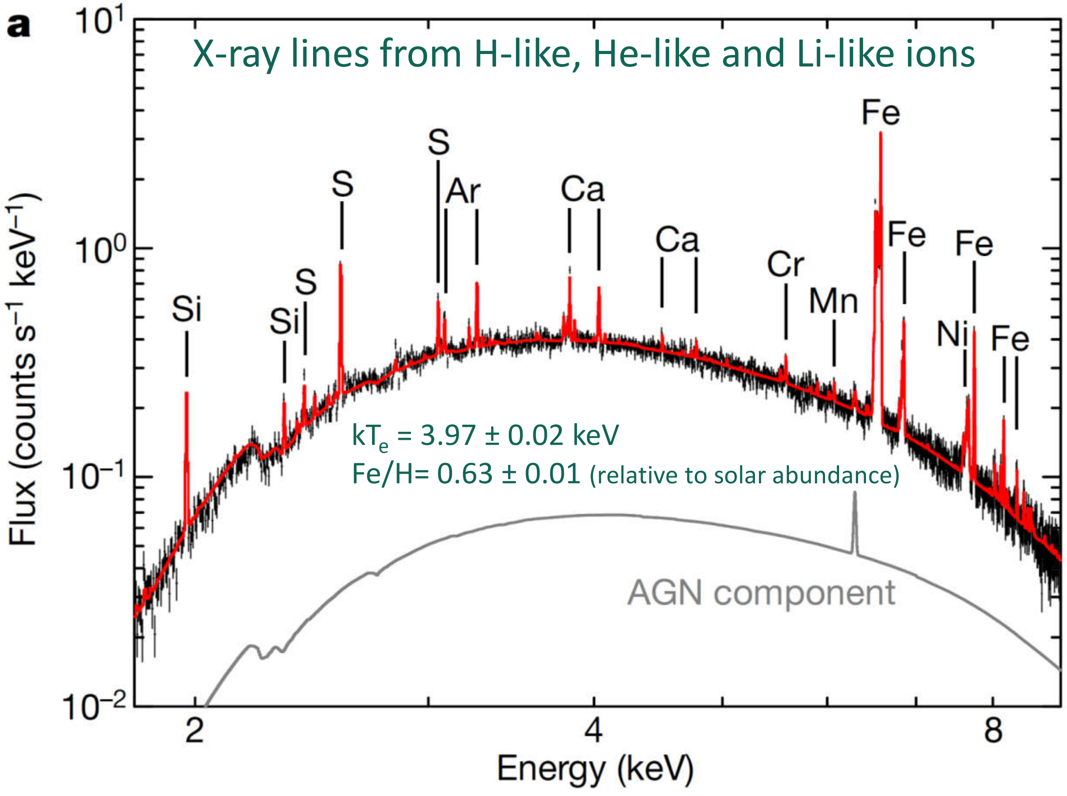
L. Schmöger et al., Science **347**, 1233 (2015)

B. Marx, et al., High-precision x-ray polarimetry, PRL **110**, 254801 (2013)
H. Bernhardt, et al., High purity x-ray polarimetry with single-crystal diamonds, APL **109**, 121106 (2016)

X-ray astrophysics observatories

- Most of the baryonic matter is highly ionized; the strongest X-ray emitters at stellar, galactic, and intergalactic scales are HCI
- The first high-resolution X-ray microcalorimeter mission, *Hitomi*, has shaken many theories in only a few days of test operation before its untimely demise
- Several space missions equipped with microcalorimeters (Athena, XRISM Resolve, Arcus…) will be launched in the next decade for studying the ‘violent universe’
- Observational high-resolution X-ray data require laboratory astrophysics for testing atomic structure and dynamics in order to understand astrophysical plasmas

Hitomi SXS spectra of the Perseus cluster of galaxies



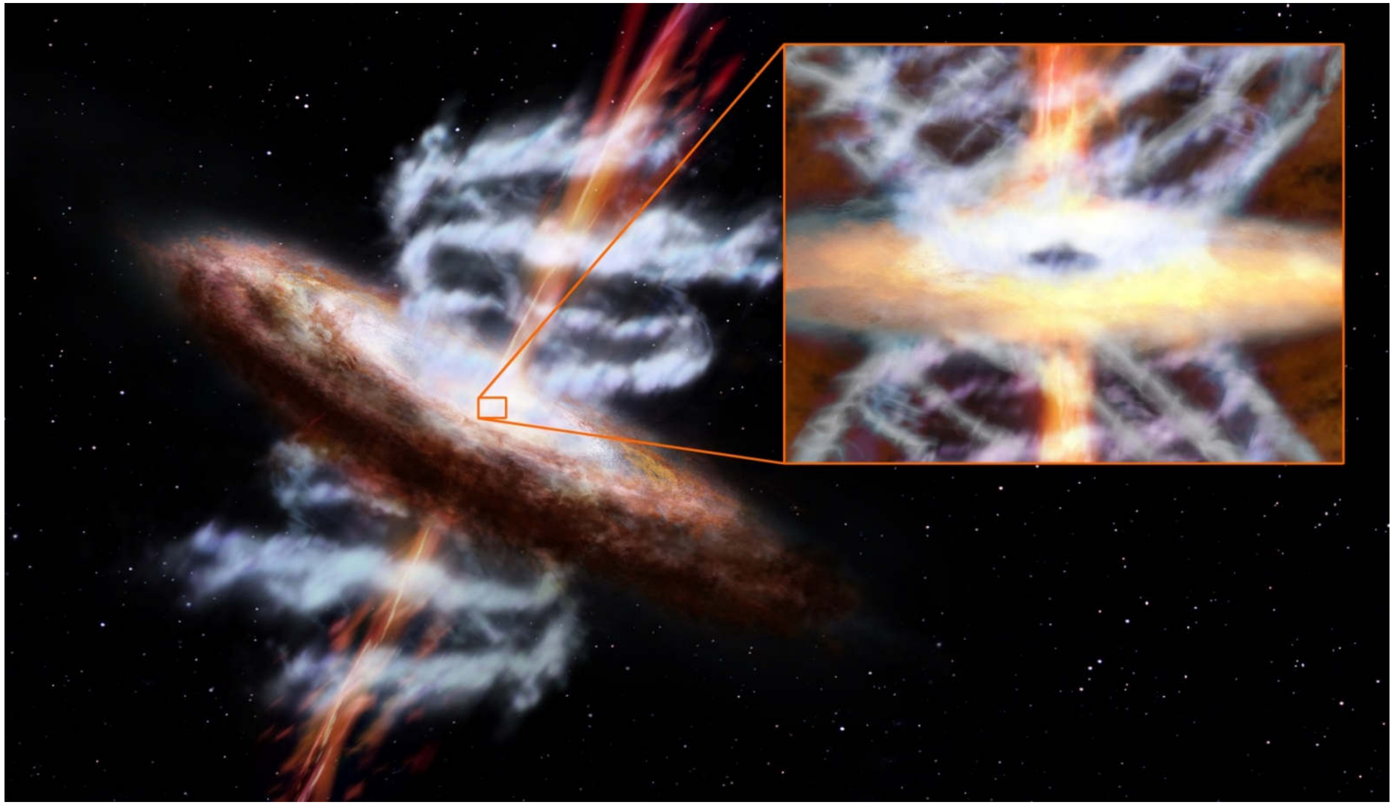
X-ray lines from H-like, He-like and Li-like ions

kT_e = 3.97 ± 0.02 keV

Fe/H= 0.63 ± 0.01 (relative to solar abundance)

Solar abundance ratios of the iron-peak elements in the Perseus cluster, Hitomi Collaboration, Nature (2017)

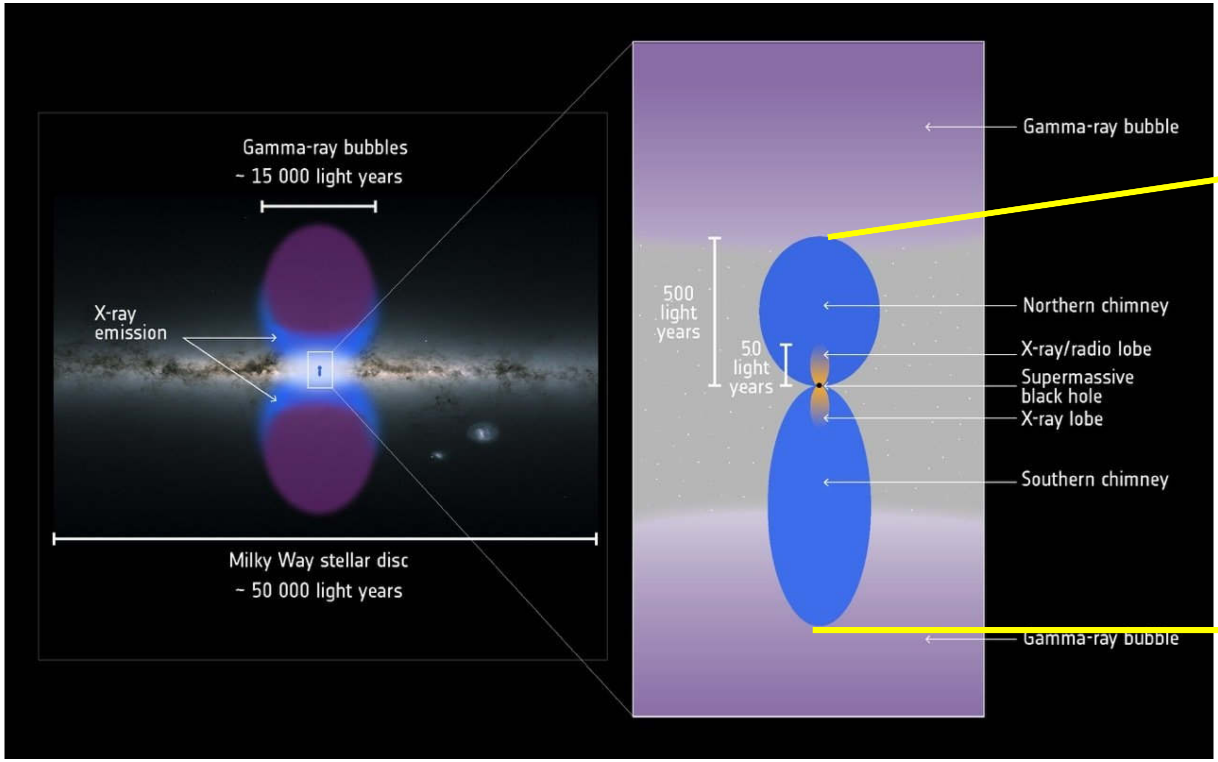
Ultra-fast outflows



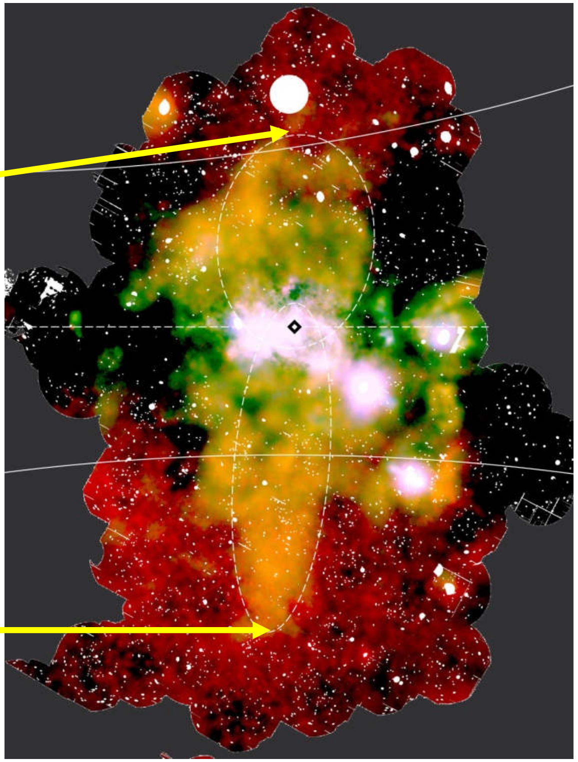
Supermassive black holes produce narrow particle jets (orange) and wider streams of gas (blue-gray) which can regulate both gallactic star formation and the growth of the black hole

F. Tombesi et al., ApJ, MNRAS 2010,2011,2012

Gamma bubbles and X-ray chimneys



Scheme of size relationship between new-found chimneys and the already known "Fermi Bubbles" and X-ray lobes at the centre (orange, in the panel to the right).
ESA/XMM-Newton/G. Ponti et al. 2019; ESA/Gaia/DPAC (Milky Way map); CC BY-SA 3.0 IGO



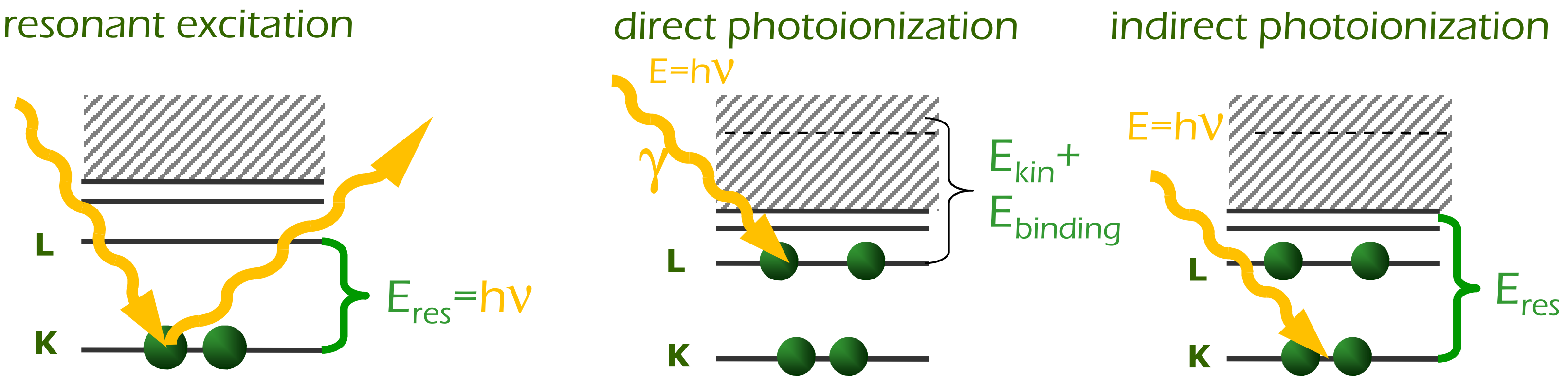
False colour image of X-rays from central Milky Way.
MPE/ESA/XMM-Newton/G. Ponti et al. 2019, Nature

Photoionized plasmas in astrophysics and HCI traps

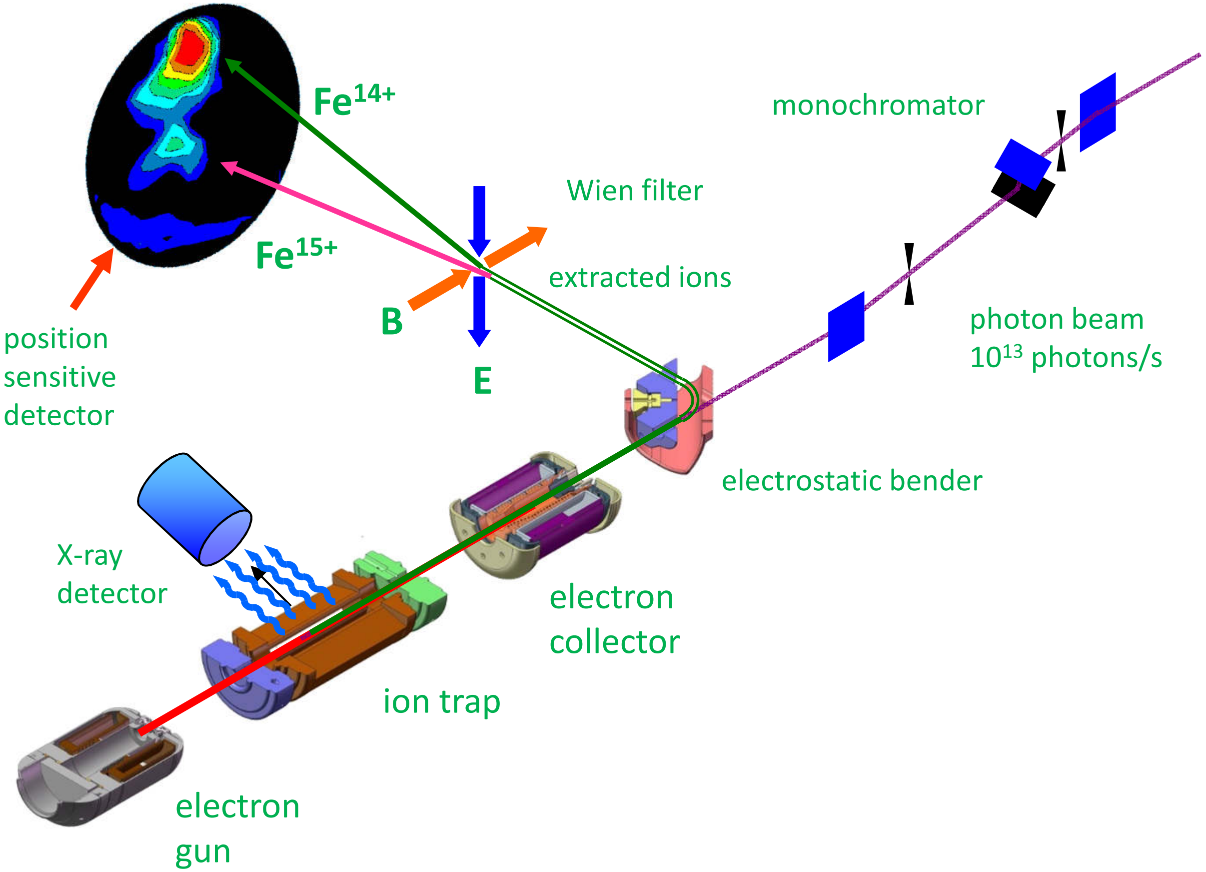
- In particular, photoionized plasmas produced by active galactic nuclei (AGN)are very interesting, since they can yield information about the most energetic processes driving galaxy formation
- XFELs are currently the only tools capable of generating photon-dominated plasmas
- Inside a trap (magnetic trapping mode EBIT, Penning or RF traps) the 'educt' HCI can be prepared, and the interaction products can be analyzed in great detail both in terms of structure and dynamics
- Photon-beam ion source (PhoBIS) is an old concept that XFELs could enable

What is needed for X-ray laser spectroscopy?

1. Two bound states separated by x-ray energies
   - Atoms are unsuitable at energies beyond their ionization potential
   - Nuclei require much higher photon energies
2. Many photons of the right energy
   - Intensity, collimation and frequency control are much better with lasers than in other sources.



Photoionization studies



Redistribution of energy by radiation

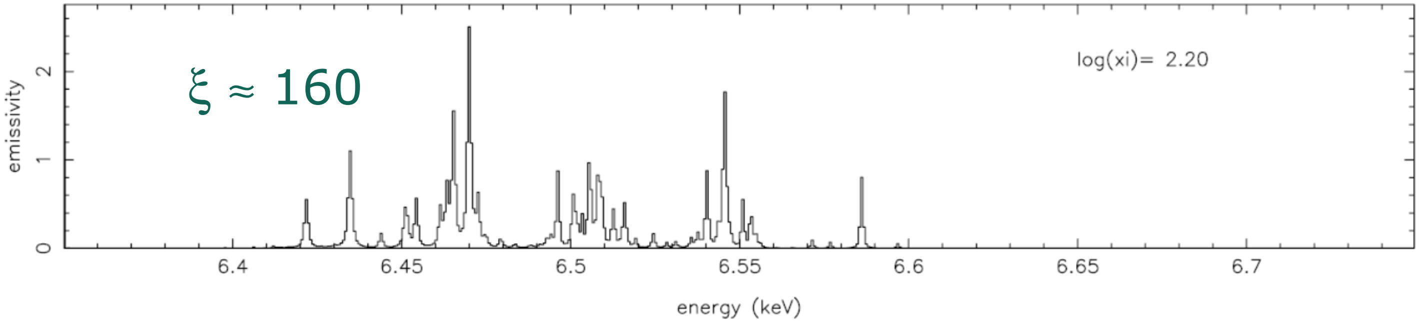
- Light is faster than shocks, even than relativistic jets
- X rays transport more energy than visible light
- In astrophysics, ξ is the ratio of photon flux (ergs/cm^{2}s) over electron density N

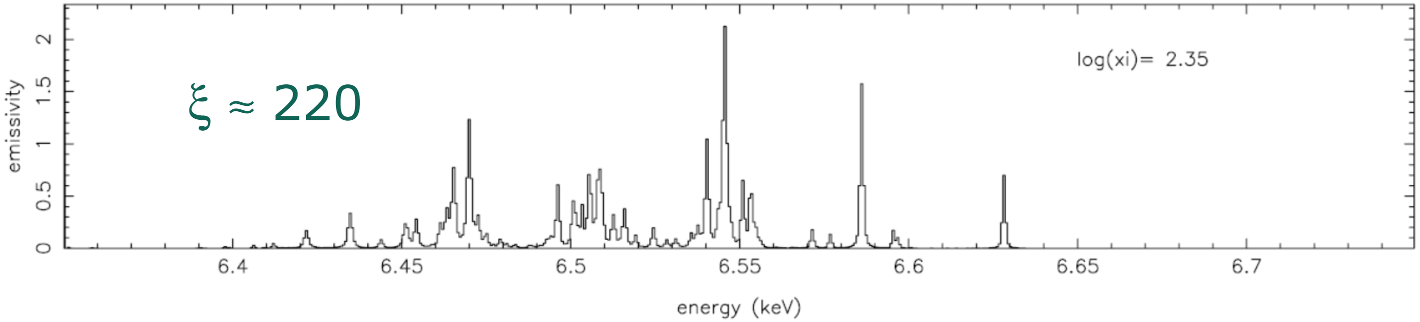
$$\xi = 4\pi I/N$$

- Used to describe the dominance of photoionization over collisional ionization
- In photoionized astrophysical plasmas, typical values are $10 < \xi < 10000$
- In laboratory plasmas: up to $\xi < 10$ (lasers, Z pinches)

- Also: X-ray opacity issues...

Emission line profiles at high ξ





- *Photoionization parameter $\xi \approx 200$: dominant*
- *Emission line profiles for $N_{column} \approx 10^{17}$ cm^2 slabs*
- *Density $\approx 10^{12}$ cm^3*

Purely photoionized plasma

Example:

- Fe atom photoionization cross section at 800 eV

$$\sigma_{PI\ 2p} \approx 1\ \text{Mbarn} \approx 10^{-18}\ \text{cm}^2$$

Exposed to one 5 mJ pulse of $4{\cdot}10^{13}$ photons, 10^{-4} cm^2 focus (100 μm)

→ Probability for photoionization per pulse ≈ 0.4

- *2p* vacancies cause autoionizing decays, and eventually complete removal of the outer shells
- Metastable states can also contribute
- Photoions remain trapped, and highest charge states that are produced can be investigated
- With 2 μm focus, multiphoton regime becomes accessible

Laser cooling and heating with X-rays

- At high XFEL intensities it is possible to produce a purely photoionized plasma without electronic collisions
- The translational temperature can be controlled when the XFEL is red or blue detuned within the natural line width of strongly absorbing transitions
- A resolution of $\Delta E/E \approx 10^{-4}$ would allow for photon heating and cooling
- The coupling regime of this non-neutral plasma could be controlled through its temperature
- Beyond the spectroscopic accuracy, this new regime could be used to simulate certain strongly coupled plasmas

Further science possibilities

- Highly polarized ion (beams) by X-ray optical pumping in combination with polarized XFEL photon beams:
  - Studies of parity non-conservation & Lorentz invariance with deeply bound electrons
  - Probing ‘long range’ (fm to pm) hypothetical Yukawa interactions
  - Providing accurate electronic binding energies for neutrino mass determinations physics
  - Pump-probe (soft and hard) X-ray studies of lifetimes, mixings between different multipole matrix elements in few-electron systems
- Ultra-cold ions in RF traps: Momentum transfer as a tool for atom interferometry with non-negligible relativistic component
- Absolute energy determinations in X-ray in direct comparison with Mössbauer transitions, transfer of frequency stability from Mössbauer to XFELO…
- Combination with VUV frequency combs for X-ray comb modulation

MPIK

S. Bernitt, C. Shah, S. Kühn, S. Dobrodey, M. Blessenohl, R. Steinbrügge, J. Rudolph, C. Beilmann, S. W. Epp, S. Eberle, M. C. Simon, K. Kubicek, V. Mäckel, P. Mokler, JRCLU, J. Ullrich, T. Pfeifer

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HI-LIGHT Collab.

G. V. Brown, LLNL
E. Behar, Technion
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E. Träbert, Bochum
A. Graf, SLAC
M. Leutenegger, NASA
A. Rassmussen, SLAC
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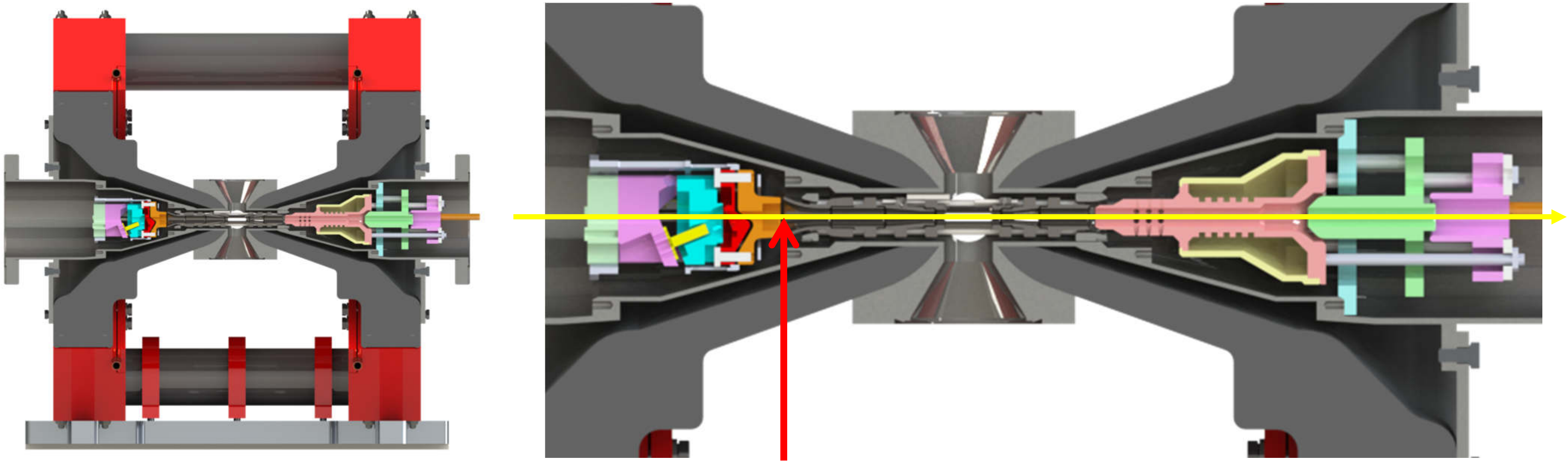
MAX PLANCK GESELLSCHAFT

SLAC NATIONAL ACCELERATOR LABORATORY

U.S. DEPARTMENT OF ENERGY Office of Science

Lawrence Livermore National Laboratory

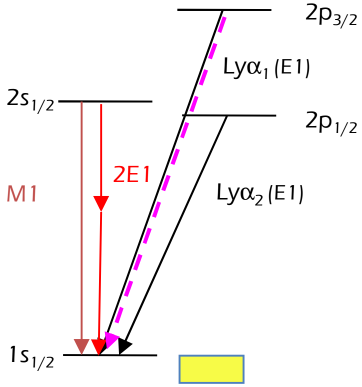
Off-axis electron gun



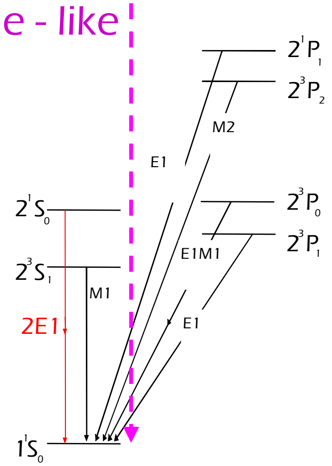
Photon beam

QED in few-electron systems: H-, He- and Li-like ions

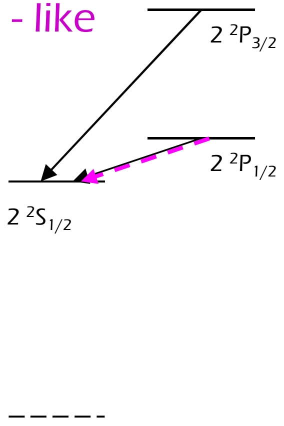
H - like

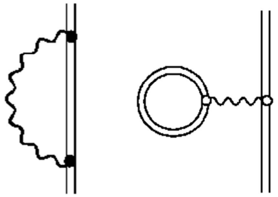


He - like



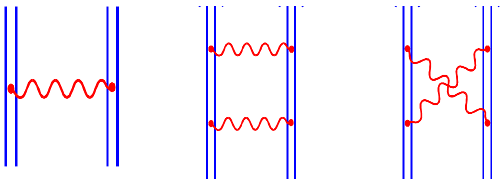
Li - like



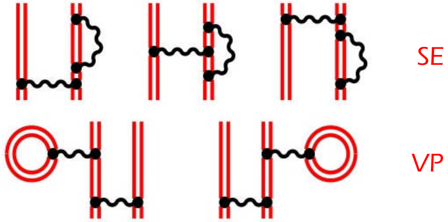


SE

VP



(HO)-screening
(non rad. QED)



screened QED

J. Berengut, D. Budker, C. Delaunay, V. V. Flambaum, C. Frugiuele, E. Fuchs, Ch. Grojean, R. Harnik, R. Ozeri, G. Perez, and Y. Soreq, *Probing New Long-Range Interactions by Isotope Shift Spectroscopy,* PRL 120, 091801 (2018)

Possibilities using EU-XFEL

The time structure of FELs allows one to

- Measure femtosecond lifetimes by pump-probe techniques
- Investigate fundamental properties of “survivor atomic core” through resonance scattering

With the XFEL photon flux, the photon-hungry

- VUV photoemission after x-ray excitation
- Sequential excitation processes
- Purely photoionized (trapped) plasmas
- Nuclear excitation studies

Electrons:

Atomic cross section typically : $\pi\cdot a_0^2 = \pi\cdot(0.511 \cdot 10^{-8}\,\text{cm})^2 = 8 \cdot 10^{-17}\,\text{cm}^2$

For H-like U^{91+}, a factor of 10^{-8} applies for the electron impact excitation cross section

$$\sigma_{EIE} = 2.6 \cdot 10^{-25}\,\text{cm}^2$$

Photons at 100 keV:
$(10^{-9}\,\text{cm})^2 = 10^{-18}\,\text{cm}^2$

Say, 5 orders of magnitude less for electrons than for photons…

10^9 photons per pulse, 27000 pulses/s = 3e13 photons/s, equivalent to $3 \cdot 10^{19}$ electrons/ s≈ 5 A
Photon beam density of X-rays 20 times higher

Assuming same geometric cross section, excitation rates would be similar