Relativistic, quantum electrodynamic and nuclear effects in highly charged ions

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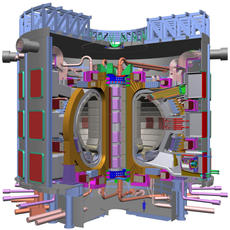
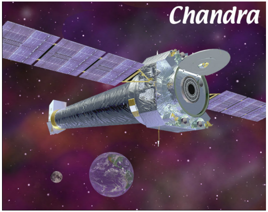
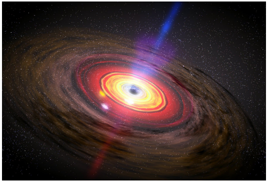
Motivation – Why to study HCI?







- Applications: magnetically confined fusion plasmas (tokamaks), astrophysical and technical plasmas
- sensitive tests of relativity, relativistic electron correlation
- tests of strong-field QED, nuclear effects (e.g. isotope shifts)

Outline

1. Dielectronic recombination with H-like U^{91+}
2. Higher-order resonant recombination processes
3. Two-center dielectronic recombination
4. X-ray resonant photoionization
5. Nuclear effects and isotope shifts
6. Summary

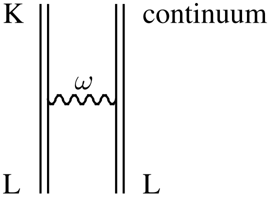
People

- **Theory, Max-Planck-Institut für Kernphysik:**
  Z. H., O. Postavaru, C. H. Keitel
  C. Müller, A. B. Voitkiv
- **Theory, St. Petersburg State University:**
  I. I. Tupitsyn
- **Theory, Uni Heidelberg:**
  A. N. Artemyev
- **ESR Experiment, GSI Darmstadt & Uni Giessen:**
  C. Brandau, D. Bernhardt, C. Kozhuharov, A. Müller,
  S. Schippers, E. W. Schmidt, A. Gumberidze, F. Bosch,
  H.-J. Kluge, Th. Stöhlker, *et al.*
- **EBIT Experiment, Max-Planck-Institut für Kernphysik**:
  M. C. Simon, C. Beilmann, M. Schwarz, S. W. Epp, V. Mäckel,
  K. Kubicek, P. H. Mokler, H. Tawara, J. R. Crespo
  López-Urrutia, J. Ullrich, *et al.*

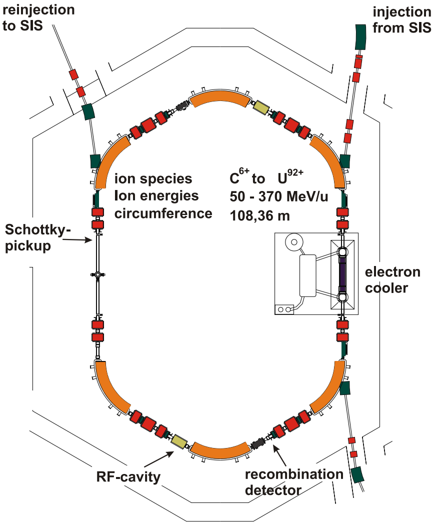
Hydrogenlike ions: highly stripped, only one electron left
ost simple system for studying electron interaction in a dynamic recombination process
The electron-electron interaction operator is given as the sum of the Coulomb and Breit terms:

- static Coulomb interaction
- magnetic (Gaunt) term (”Lorentz force“)
- scalar and transverse interaction retardation terms
- higher-order frequency-dependent retardation term

From: field theory, exchange of a virtual photon between the electrons

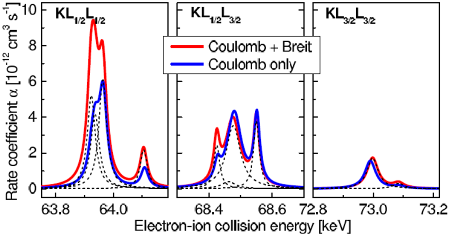


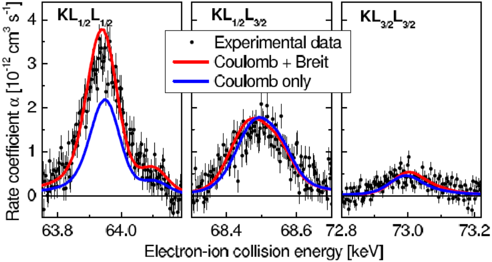
DR with H-like U^{91+} at the GSI ESR



- stochastically cooled ion beam
- electron cooler used as a target
- detection of recombined ions

(More on ESR: Alexandre Gumberidze, talk tomorrow 11:30)





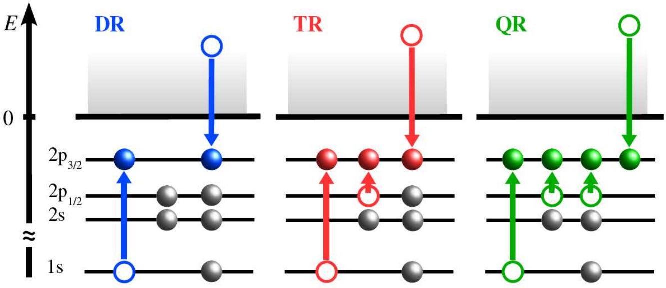
Agreement only if the Breit interaction is taken into account in the **dynamic** recombination process

D. Bernhardt, C. Brandau, Z. H., C. Kozhuharov, A. Müller, *et al.*, submitted (2010)

Higher-order resonant recombination processes

Dielectronic recombination (DR):

- Radiationless resonant capture of a continuum electron (inverse Auger effect)
- Radiative decay of the autoionizing state



3 electrons involved → trielectronic recombination (TR)
4 electrons involved → quadruelectronic recombination (QR)

Total cross section

T-matrix distorted wave formalism → total cross section of DR (/TR/QR/...):

$$\sigma_{idf}(\varepsilon) = \frac{2\pi^2}{p^2}\frac{A_r^{df}}{\Gamma_d}L_d(\varepsilon)\frac{2J_d+1}{2(2J_i+1)}A_a^{di} \quad \text{with}$$

$$L_d = \frac{\Gamma_d/(2\pi)}{(E_i+\varepsilon-E_d)^2+\Gamma_d^2/4}$$

The rates for autoionization and radiative decay are

$$A_a^{di} = \frac{2\pi}{2J_d+1}\sum_{M_i m_s M_d}\int d\Omega_p \left|\langle \Phi_i J_i M_i, \vec{p} m_s \left| V_C + V_B \right| \Phi_d J_d M_d\rangle\right|^2 \rho_i$$

$$A_r^{df} = \frac{2\pi}{2J_d+1}\sum_{M_d \lambda M_f}\int d\Omega_k \left|\left\langle \Phi_d J_d M_d \left| H_{er} \right| \Phi_f J_f M_f, \vec{k}\lambda \right\rangle\right|^2 \rho_f$$

How to treat the electronic many-body problem?

Non-relativistically

Hartree: *independent particles*

$$\Psi_{1,2} = \phi_1^S \phi_2^S$$

$\Downarrow$

Hartree-Fock: *Pauli principle*

$$\Psi_{1,2} = \frac{1}{\sqrt{2}} \left(\phi_1^S \phi_2^S - \phi_2^S \phi_1^S \right)$$

$\Downarrow$

Multiconfiguration Hartree-Fock:

$$\Psi_{1,2} = \frac{1}{\sqrt{2}} \sum_{ij} c_{ij} \left(\phi_i^S \phi_j^S - \phi_j^S \phi_i^S \right)$$

Relativistically

Dirac-Hartree:

$$\Psi_{1,2} = \phi_1^D \phi_2^D$$

$\Downarrow$

Dirac-(Hartree-)Fock:

$$\Psi(1,2) = \frac{1}{\sqrt{2}} \left(\phi_1^D \phi_2^D - \phi_2^D \phi_1^D \right)$$

$\Downarrow$

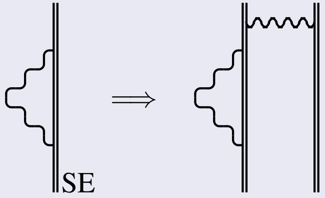
Multiconfiguration Dirac-Fock:

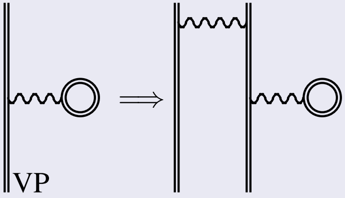
$$\Psi_{1,2} = \frac{1}{\sqrt{2}} \sum_{ij} c_{ij} \left(\phi_i^D \phi_j^D - \phi_j^D \phi_i^D \right)$$

QED corrections: self-energy and vacuum polarization

QED corrections: ≈ 10-30 eV in Kr

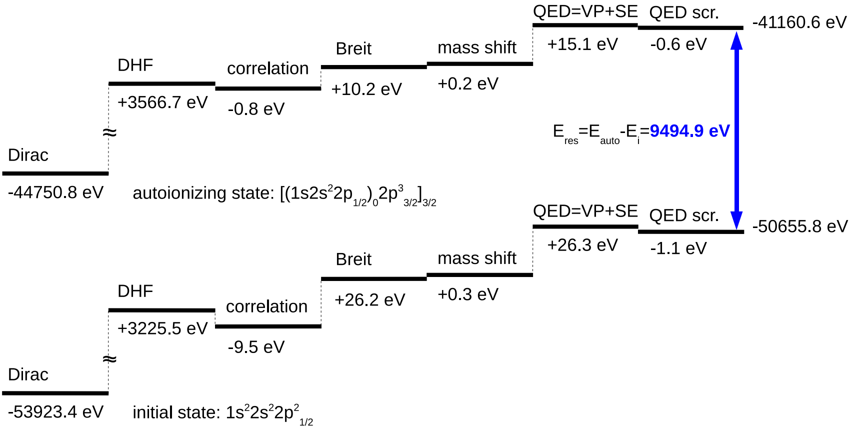
In many-body systems: interacting electrons, screening effects





Estimation of SE/VP screening by rescaling hydrogenic values

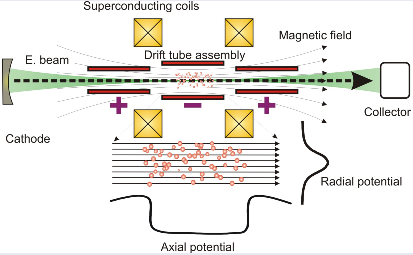
The bookkeeping part of theoretical physics: adding all the contributions to get one number



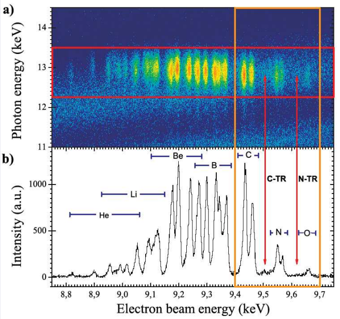
Line positions and cross sections are calculated

Experiments at the Heidelberg EBIT

Electron beam ion trap:

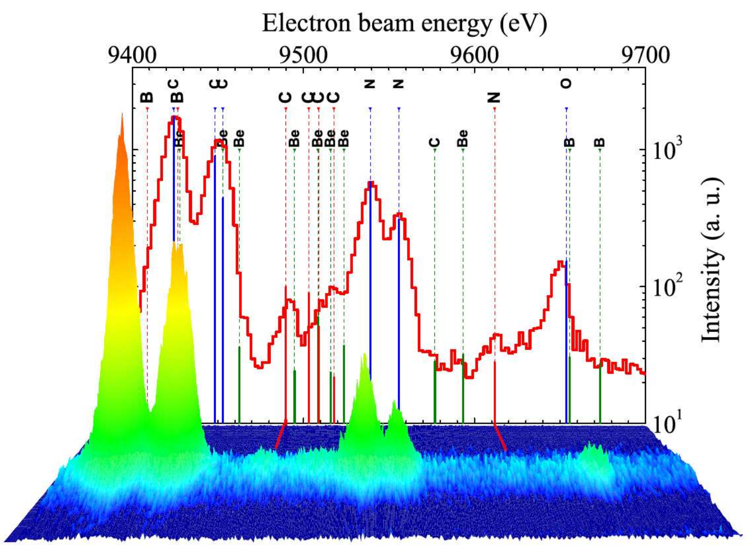


Resonances in Kr ions

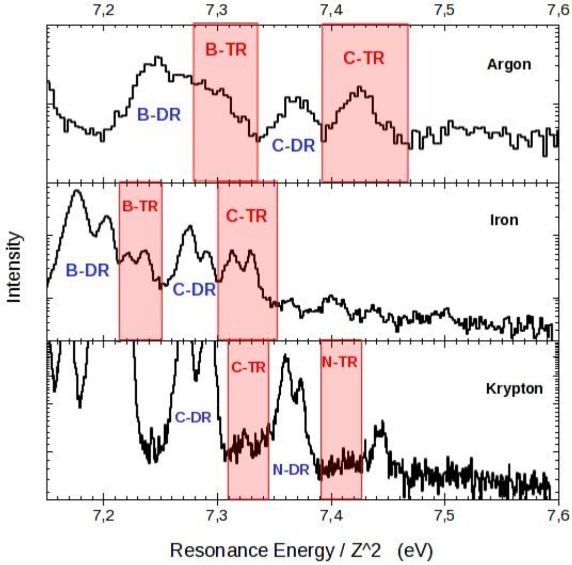


- C. Beilmann, O. Postavaru, L. H. Arntzen *et al.*, PRA **80**, 050702 (R) (2009)
- First observation of TR at the TSR of the MPIK: M. Schnell *et al.*, PRL, **91**, 043001 (2003)

DR, TR, and QR resonances in Kr ions

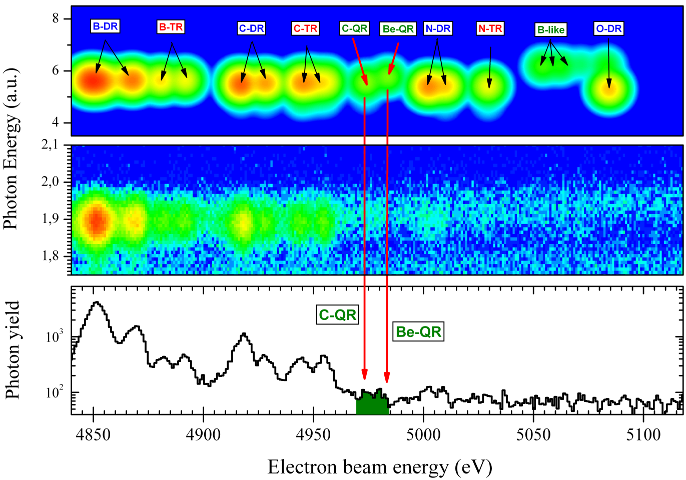


Experimental results for lighter elements



Quadruelectronic resonances in Fe ions

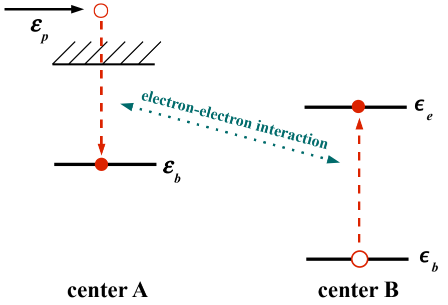
Fluorescence signal vs. electron energy **and** photon energy:



Environment-assisted recombination

Two-center dielectronic recombination (2CDR) process:

- electron recombination into center A; simultaneous resonant excitation in center B (time-reversed inter-atomic Auger process)
- radiative decay of the excited state in center B



"Center"=atom/ion/molecule

Energy transfer between the centers: exchange of a virtual photon with $\hbar\omega$

Competing process: radiative recombination (RR) with center A; 2CDR can exceed RR

Not observed yet (!)

Ratio of the 2CDR at resonance and RR (approx.):

$$\frac{\sigma_{2CDR}}{\sigma_{RR}^{(A)}} \sim \left(\frac{c}{R\omega}\right)^6$$

→ small distances R preferable ↔ large densities
→ low energies preferable: ≈ 1 eV, outer shells, low charge states

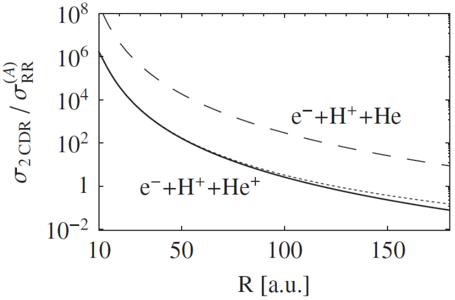
Examples and potential relevance:

$e^- + H^+ + He^+$ $(1s\text{–}2p)$

$e^- + H^+ + He$

- astrophysics - Sun?
- thermonuclear fusion plasmas
- warm dense matter in laser-solid interaction

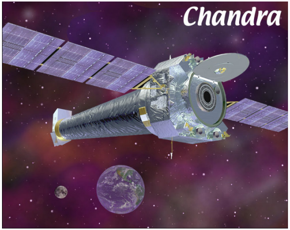
R=100 $a_0 \approx 5$ nm

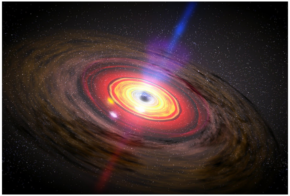


C. Müller, A. B. Voitkiv, J. R. Crespo López-Urrutia, Z. H., PRL **104**, 233202 (2010)

Photoionization of HCI in the x-ray regime

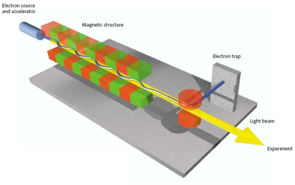
- Application: **astrophysical plasmas**
- half of the baryonic matter in the universe is in the form of HCIs comprised in the Warm-Hot Intergalactic Medium (WHIM); PI may be the dominant ionization process
- analysis of ionic absorption spectra (C, N, O, Ne, Ar, Fe ions) → temperature, density, mass and velocity



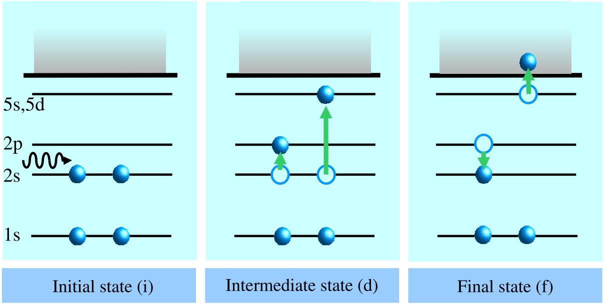


- PI data are important constituents of **astrophysical models**: reliable theories and measurements are called for
- interpretation of data from grating spectrometers on board of the Chandra and XMM Newton observatories

- **Photoionization of HCI:** novel light sources with high energies and brilliance (synchrotron radiation, XFEL lasers) → extending to higher ionic charge states
- high detection efficiency of the photoions: accurate measurements possible
- established methods: merged beam experiments, dual laser-produced plasmas, Penning traps
- new method: PI of HCI in an **electron beam ion trap (EBIT)**



Example: Be-like ions, excitation from the ground state $1s^2 2s^2$



Excitation: two-electron one-photon transition

Photoionization via 2p5s, 2p5d, 2p6s, 2p6d. . . states

Total cross section for a given photoionization channel
i (initial) $\rightarrow d$ (autoionizing) $\rightarrow f$ (final):

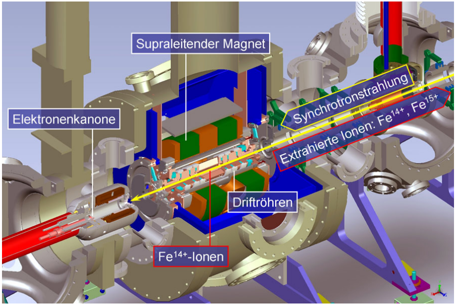
$$\sigma^{\mathrm{PI}}_{i\rightarrow d\rightarrow f}(\hbar\omega) = \frac{2\pi^2 c^2 \hbar^4}{(\hbar\omega)^2} \frac{A^{re}_{id} A^{a}_{df}}{\Gamma_d} L_d(\hbar\omega)$$

Lorentzian line shape function:

$$L_d(\hbar\omega) = \frac{\Gamma_d/(2\pi)}{(\hbar\omega + E_i - E_d)^2 + \Gamma_d^2/4}$$

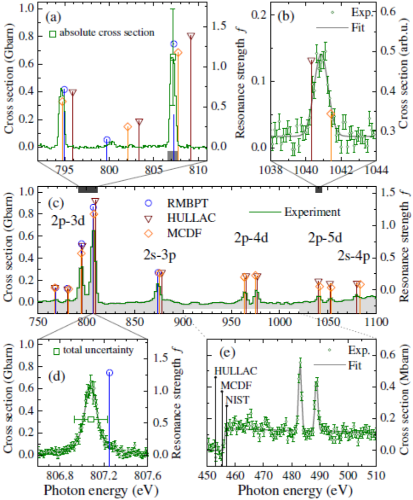
A^r_d, A^d_a: radiative and Auger decay rates;
A^{re}_{id}: radiative excitation rate

Experimental setup using synchrotron radiation and an EBIT equipped with ion extraction



HCI cloud area density: $\approx 10^{10}$ cm^{-2}

Experimental spectra for Mg-like Fe^{14+} ($E/\Delta E \approx 6500$); theory



- MCDF: this work
  10-20 eV dev.
- for the active galaxy NGC3783: velocity from Doppler shifts
- more brilliant x-ray beams from synchrotrons (e.g. Petra III) and x-ray free electron lasers (e.g. XFEL, LCLS) in the near future: multi-keV regime, multiphoton excitations

M. C. Simon, J. R. Crespo López-Urrutia, C. Beilmann, M. Schwarz, Z. H., *et al.*, PRL **105**, 183001 (2010)

M. C. Simon, M. Schwarz, S. W. Epp, C. Beilmann, B. L. Schmitt, et al., JPB. **43**, 065003 (2010)

Nuclear effects and isotope shifts

Nuclear property		Effect on electronic structure
charge $+Ze$	$\rightarrow$	binding energy
size or radius $r_{\text{RMS}} = \sqrt{\langle r^2 \rangle}$	$\rightarrow$	field shift (FS)
mass $M < \infty$, nuclear recoil	$\rightarrow$	normal and specific mass shift (MS)
polarizability	$\rightarrow$	nuclear polarization (NP) shift
spin and magnetic moment	$\rightarrow$	magnetic hyperfine splitting (HFS)
quadrupole moment	$\rightarrow$	quadrupole hyperfine splitting
weak interaction	$\rightarrow$	parity non-conservation (PNC)

These are usually small corrections to level and transition energies

Best studied by comparing two different isotopes, i.e. by measuring isotope shifts

E.g. two-photon laser spectroscopy: $2s \rightarrow 3s$ transitions with short-lived Li isotopes $\rightarrow \delta r_{\text{RMS}}$ for ^{8,9}Li, ^{9,11}Li

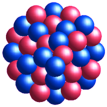
G. Ewald, W. Nörtershäuser, A. Dax, *et al.*, PRL (2004);

R. Sánchez, W. Nörtershäuser, G. Ewald, *et al.*, PRL (2006)

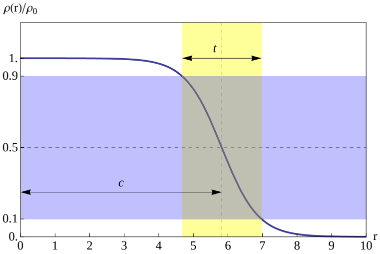
Nuclear charge distribution

Fermi two-parameter distribution for describing the charge distribution of the considered nuclei:

$$\rho_{\text{nuc}}(r) = \frac{\rho_0}{1 + e^{(r-c)/a}}, \qquad a = t\,4\ln 3$$

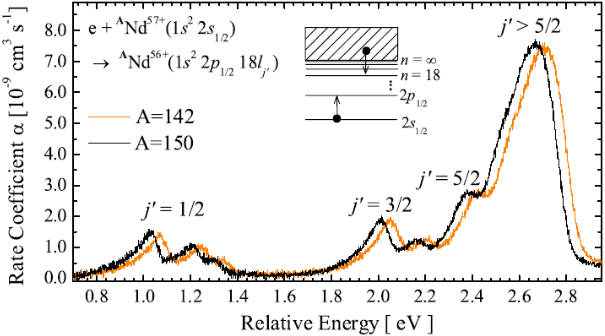


$\Longrightarrow$



- Numerical integration of the many-electron Dirac equations with V_{nuc}
- Nuclear size dependence of SE and VP terms: analytically calculated formulae
- Mass shifts taken into account

DR isotope shift measurement at the ESR with Nd $^{57+}$



High accuracy for low-lying resonances

$\delta E_{\rm res}$=40.2(3)(6) meV $\rightarrow$
$\delta\langle r^2\rangle$=-1.36(1)(3) fm^2

A new method to gain information on the nuclear size

C. Brandau, C. Kozhuharov, Z. H., A. Müller, S. Schippers *et al.*, PRL 100, 073201 (2008)

Similar measurements are planned with nuclei of non-zero spin: hyperfine splitting, nuclear moments

Summary

- Dielectronic recombination with U^{91+}: relativistic electron interaction
- Theoretical and experimental K-LL DR and KL-LLL TR spectra for Be-, B-, C-, and N-like Kr (Z=36), Fe (Z=26), Ar (Z=18) Trielectronic and quadruelectronic recombination: nonlinear electron-electron interaction
- Two-center dielectronic recombination: new process in warm-dense matter and in chemical environments
- Photoionization of HCI: extending to higher charge states (14+) and photon energies ($\approx$ 1 keV) identification and analysis of structures in astrophysical spectra
- Isotope shifts in HCI spectra: determination of nuclear properties
- Work in progress: QED and nuclear effects on the bound electron g factor

Grazie per l'attenzione!

Köszönöm a figyelmet!

Merci à tous pour votre attention!

Muchas gracias por su atención!

Mulţumesc pentru atenţie!

Obrigado pela atenção!

Spasibo za vnimanie!

Thank you for your attention!

Vielen Dank für Ihre Aufmerksamkeit!