Relativistic dynamics of (slow) highly-charged ions

Stephan Fritzsche GSI Darmstadt & Oulu University Eisenach, 28th June 2010



Thanks to: N.M. Kabachnik, A. Surzhykov, T. Stöhlker and GSI Atomic Physics Group

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Highly-charged ions provide a unique tool

-- for probing strong electro-magnetic fields



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electron-electron

Plan of this talk

- Electron capture: angular correlations & polarization
- Multipole mixing in strong fields
- Two-step processes: Capture vs. excitation
- Atomic PNC: Two-photon processes
 - Spectroscopy of (super-) heavy elements
 - Conclusions

<u>Thanks to:</u> N.M. Kaba

electron-photon

interaction

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Electron capture by bare ions

-- angular correlation and polarization studies

Electron capture into bare high-Z ions



So far...

angular distributions







 $\frac{d\,\sigma}{d\,\Omega}(\theta) \sim \sum_{polarization} |M|^2$

Electron capture into bare high-Z ions



Multipole mixing of the radiation field

-- in the capture and decay of highly-charged ions

Capture into the $2p_{3/2}$ excited states of initially bare ions



Capture into the $2p_{3/2}$ excited states of initially bare ions



Th. Stöhlker et al. PRL 79 (1997) 3270

J. Eichler et al. PRA 58 (1998) 2128

Effective anisotropy parameter: Multipole contributions



Effective anisotropy parameter: Multipole contributions





Effective anisotropy parameter: Multipole contributions



E1-M2 multipole mixing: Alignment of the $2p_{3/2}$ state



A. Surzhykov et al. PRL 88 (2002) 153001

Dynamical alignment studies enables one to explore magnetic interactions in the bound-bound transitions in H-like ions !

Two-photon coincidence studies



Two-photon coincidence studies



X-ray polarimetry for HCI

-- exploring a new `dimension' in the electron-photon interaction



K-shell capture or subsequent decay



Linear polarization of emitted x-ray photons

-- theoretical expectation



electric dipole approximation

Linear polarization is described in the plane, perpendicular to the photon momentum.



----- only 2 (Stokes) parameters are required ! $P_L = \sqrt{P_1^2 + P_2^2} \quad \cos(2\phi) = \frac{P_1}{P_1}$

Linear polarization of emitted x-ray photons

-- Statistical characteristics for photon ensembles



Stobbe, Ann. Phys. 5 (1930) 661

Photon angle (deg)

Linear polarization of emitted x-ray photons

-- Statistical characteristics for photon ensembles



- Proposal: to use REC linear polarization as a probe for ion spin polarization.
- Established theory from the "polarization transfer" in atomic photoionization.





U. Fano *et al.*, Phys. Rev. **116** (1959) 1147; R. Pratt *et al.*, Phys. Rev. **134** (1964) A916.

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• Calculations performed for the REC into (initially) hydrogen-like bismuth Bi^{82+} ions (I = 9/2) for the energy $T_n = 420$ MeV/u.



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A. Surzhykov et al., Phys. Rev. Lett. 94 (2005) 203202

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$$\tan 2\phi = \frac{P_2}{P_1} \sim \lambda_F \frac{I - 1/2}{I + 1/2}$$

S. Tashenov *et al.*, PRL **97** (2006) 223202; A. Surzhykov *et al.*, PRL **94** (2005) 203202.

- Rotation angle ϕ provides information on the <u>degree</u> of ion polarization !

Two-step processes: Capture vs. excitation -- Do we get more by following the dynamics of the ions ?



(initially) bare ion



(initially) H-like ion

Lyman- α vs. K- α emission from high-Z ions



Lyman- α vs. K- α emission from high-Z ions



-- angular distribution as "observed" in experiment

$$\begin{split} W(\theta)_{K\alpha_1} &\sim N_{J=1} W_{EI}(\theta) + N_{J=2} W_{M2}(\theta) & \text{A. Surzhykov et al., PRA 73 (2006) 032716.} \\ &= 1 + (N_{J=1} \frac{1}{\sqrt{2}} A_2(J=1) - N_{J=2} \sqrt{\frac{5}{14}} A_2(J=2)) P_2(\cos \theta) \end{split}$$

 $N_{J=1}$, $N_{J=2}$ relative populations of J=1, 2 states



-- for 220 MeV/u U⁹⁰⁺ ions following REC

$$\begin{split} W(\theta)_{K\alpha_1} &\sim N_{J=1} W_{EI}(\theta) + N_{J=2} W_{M2}(\theta) & \text{A. Surzhykov et al., PRA 73 (2006) 032716.} \\ &= 1 + (N_{J=1} \frac{1}{\sqrt{2}} A_2(J=1) - N_{J=2} \sqrt{\frac{5}{14}} A_2(J=2)) P_2(\cos \theta) \end{split}$$

 Relative populations of the J = 1, 2 levels following REC (IPM model):

$$\frac{N_{J=1}}{N_{J=2}} = \frac{3}{5}$$

• By taking into account ${}^{3}P_{2} \rightarrow {}^{3}S_{1}$ channel:

$$\frac{\frac{N_{J=1}}{N_{J=2}} = \frac{6}{7}}{(\frac{N_{J=1} - N_{J=2}}{N_{J=1} + N_{J=2}})} \approx -0.08$$



-- following the Coulomb excitation of the projectiles

$$\begin{split} W(\theta)_{K\alpha_1} &\sim N_{J=1} W_{EI}(\theta) + N_{J=2} W_{M2}(\theta) & \text{A. Surzhykov et al., PRA 73 (2006) 032716.} \\ &= 1 + (N_{J=1} \frac{1}{\sqrt{2}} A_2(J=1) - N_{J=2} \sqrt{\frac{5}{14}} A_2(J=2)) P_2(\cos \theta) \end{split}$$





Excited states of He-like heavy ions can be produced also by the Coulomb excitation of the projectile in the field of target atoms.

Experiments were already performed at the GSI storage ring for He-like uranium ions U⁹⁰⁺.

• Strong anisotropy of the subsequent $K\alpha_1$ radiation has been observed!

-- following the Coulomb excitation of the projectiles

$$\begin{split} W(\theta)_{K\alpha_{1}} &\sim N_{J=1} W_{EI}(\theta) + N_{J=2} W_{M2}(\theta) \\ &= 1 + (N_{J=1} \frac{1}{\sqrt{2}} A_{2}(J=1) - N_{J=2} \sqrt{\frac{5}{14}} A(J=2)) P_{2}(\cos \theta) \end{split}$$

 $N_{J=1}$, $N_{J=2}$ relative populations of J=1, 2 states



 Angular distribution results dominantly from the decay of the J=1 level.

Role of electron-electron interactions still unexplored.



Atomic parity non-conservation processes -- Two-photon processes for HCI



nergy

S (+

D(-)

Exchange of Z-boson leads to the mixing of atomic levels with different parities.

$$\eta = \frac{\langle \Psi_s | G_F / 2\sqrt{2} (1 - 4\sin^2 \theta_w - N/Z) \rho_{el} \gamma_5 | \Psi_p \rangle}{E_s - E_p}$$

PNC studies with heavy, few-electron ions

-- enhancement of parity and time-reversal violating interactions

- Helium-like uranium U⁹⁰⁺ is a perfect candidate for PNC studies:
 - Simple system (only 2 electrons)
 - Large electron-nucleus overlap
 - Small $2^{1}S_{0}$ - $2^{3}P_{0}$ energy splitting





- Still many open questions:
 - How big is the $2^{1}S_{0}-2^{3}P_{0}$ energy splitting?
 - How strong laser fields do we need?
 - What is the role of e-e interactions?

There is a need for accurate many-electron calculations !

- Analysis and interpretation of optical and x-ray spectra (astro physics)
- Diagnostics of astro physical and laboratory plasmas
- Development of UV/EUV light sources and lithography
- Frequency standards and atomic clocks
- Spectroscopy on heavy and superheavy elements (actinides, transactinides)
- Isotope shifts and hyperfine structures
- Nonradiative (inner-shell) transitions and autoionization
- Ion recombination and photon emission
- Multi-photon processes

...

- "Complete experiments"
- Parity nonconservation (PNC)
- Search for electric dipole moments



"many but not so accurate"

Spectroscopy of heavy and super-heavy elements



Backe, Lauth, Sewtz (Mainz)

Theoretical challenges:

- strong relativistic and QED effects
- systems with open d- and f-shells
- many overlapping and nearly degenerate configurations
- large number of electron

M. Sewtz et al., Phys. Rev. Lett. 90 (2003) 163002

Optical spectroscopy of atomic Fermium (Z = 100)

First observation and classification of atomic levels



Theoretical request: Energies, lifetimes, transition rates





Breeding in High Flux Reactors N_{Fm} < 10¹²; ²⁵⁵Fm; t_{1/2}= 20.1 h

Experimental proposal: Optical spectroscopy of nobelium (Z=102)



S. Fritzsche, EJP D33, 15 (2005)

Zhou & Froese Fischer., Phys. Rev. Lett. 88 (2002) 183001.

Low-lying resonances of (super-) heavy elements ... for lutetium (Z=71) and lawrencium (Z=103)

TABLE I. The transition energies in cm⁻¹ of $nd^2 D_{3/2} - (n + 1)p^2 P_{1/2,3/2}^o$ and the size of CSF expansions for Lu (n = 5) and Lr (n = 6).

Expansion	${}^{2}D_{3/2} - {}^{2}P_{1/2}^{o}$	${}^{2}D_{3/2} - {}^{2}P^{o}_{3/2}$	CSF $({}^{2}D_{3/2}/{}^{2}P_{1/2}^{o}/{}^{2}P_{3/2}^{o})$						
Lu									
$VV + CV(4f^{14})$	3989	7276	4354/2071/3813						
$VV + CV(5p^{6}4f^{14})$	8004	11 483	5600/2764/5073						
$VV + [(CV + CC)(5p^{6}4f^{14})]$	3857	7130	128 763/36 974/100 277						
$VV + [(CV + CC) (4d^{10}5s^25p^64f^{14})]$	4186	7462	305 717/87 241/236 554						
RCC [7]	3828	7140							
DFT [10]	3862								
Exp.	4136	7476							
DHF Breit Correction	87	53							
DHF Breit & QED Correction	76	43							
	Lr								
$VV + CV(5f^{14})$	-1298	9137	3659/1842/3338						
$VV + CV(6p^{6}5f^{14})$	1339	12 761	4708/2495/4495						
$VV + [(CV + CC)(6p^65f^{14})]$	-1953	6469	125 325/37 333/97 500						
$VV + [(CV + CC)(5d^{10}6s^26p^65f^{14})]$	-1127	7807	330 252/95 969/246 376						
RCC	-1388	6960							
RCC with Breit	-1263	7010							
DHF Breit Correction	97	4							
DHF Breit & QED Correction	59	-26							

RCC: Eliav et al., Phys. Rev. A52 (1995) 291; DFT: Vosko & Chevary, J. Phys. B26 (1993) 873

Low-lying resonances of (super-) heavy elements ... oscillator strengths in different gauges

		7	-1-;-1-			
	$^{2}D_{3/2} - ^{2}P_{1/2}^{o}$			$^{2}D_{3/2} - ^{2}P^{o}_{3/2}$		
Expansion	gf_L	gf_V	Scaled gf_L	gf_L	gf_V	Scaled gf_L
		Lu				
$VV + CV(4f^{14})$	0.0304	0.0582	0.0315	0.0111	0.0219	0.0114
$VV + CV(5p^{6}4f^{14})$	0.0511	0.1552	0.0264	0.0144	0.0467	0.0094
$VV + [(CV + CC)(5p^{6}4f^{14})]$	0.0908	0.3835	0.0974	0.0322	0.0856	0.0337
$VV + [(CV + CC)(4d^{10}5s^25p^64f^{14})]$	0.1043	0.3345	0.1031	0.0354	0.0742	0.0355
		Lr				
$VV + CV(5f^{14})$	-0.0162	-0.0076		0.0210	0.0313	
$VV + CV(6p^{6}5f^{14})$	0.0144	0.2359		0.0227	0.0839	
$VV + [(CV + CC)(6p^65f^{14})]$	-0.0624	-0.0002		0.0414	0.0867	
$VV + [(CV + CC)(5d^{10}6s^26p^65f^{14})]$	-0.0378	-0.0024		0.0519	0.0685	

TABLE II. The oscillator strengths of $nd^2D_{3/2} - (n + 1)p^2P_{1/2,3/2}^o$ for Lu (n = 5) and Lr (n = 6).

Good accuracy of the (atomic) energies is a necessary, but not a sufficient criterion !

S. Fritzsche, JESRP 114-116 (2001) 1155; Phys. Scr. T100 (2002) 46

RATIP Relativistic Atomic Transition and Ionization Properties (CPC library)

$$\boldsymbol{\psi}_{\boldsymbol{\alpha}}(PJM) = \sum_{r}^{n_{c}} c_{r}(\boldsymbol{\alpha}) \left| \boldsymbol{\gamma}_{r} PJM \right\rangle$$

Many-electron basis (wave function expansions)

- Construction and classification of N-particle Hilbert spaces
- Shell model: Systematically enlarged CSF basis

Interactions

- Dirac-Coulomb Hamiltonian
- Breit interactions + QED
- Electron continuum; scattering phases

• Coherence transfer and Rydberg dynamics



Relativistic CI wave functions including QED estimates and mass polarization

RELCI, CPC 148 (2002) 103

LSJ spectroscopic notation from jj-coupled computations

LSJ, CPC 157 (2003) 239

Auger rates, angular distributions and spin polarization; level widths

AUGER

Photoionization cross sections and (non-dipole) angular parameters

PHOTO

Radiative and dielectronic recombination; angle-angle correlations



AG A. Kellerbauer *et al.* MPIK Heidelberg

HFS & Isotope shift measurements for Os-



Typical spectrum ¹⁹²Os⁻:

Signal: Neutral atoms as function of laser frequency

⇒
$$v = 257.831190(30)$$
 THz
 $\lambda = 1162.74706(14)$ nm

U. Warring et al., Phys. Rev. Lett. 102 (2009) 043001

HFS & Isotope shift measurements for Os-



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U. Warring et al., Phys. Rev. Lett. 102 (2009) 043001

$$M_{\rm NMS} = v_0 \frac{m_e}{1 \rm u} = 0.14 \text{ THz u}$$

Experiment:
$$M_{\rm SMS} = 2(11) \text{ THz u}$$
$$F = 16(9) \text{ GHz fm}^{-2}$$

Theory:
$$M_{\rm SMS} = 4.9 \text{ THz u}$$
$$F = 12.4 \text{ GHz fm}^{-2}$$

Transition for all stable isotopes:



A. Fischer et al., Phys. Rev. Lett. 104 (2010) 073004

Atomic and heavy-ion theory @ SPARC collaboration

-- Recent developments and progress

Key topics of this collaboration:



GS

• Test of quantum electrodynamics in strong fields for light and high-Z ions

... two-times Green's functions; 2-photon, 3-photon (??) diagrams; differences with experiment

especially for the HFS; systematic QED approach in the MBPT framework

- Collision & capture dynamics in strong fields at relativistic energies
 - ... U28+ electron loss; few-body dynamics; polarization effects; multi-electron processes
- Atomic physics techniques applied to nuclear physics
- Multi-photon processes
- Antiproton physics
- Test of fundamental interactions and symmetries beside of QED
- Interaction of ions with intensive (laser) light

... dynamics in strong fields, high-harmonics generation

Atomic and heavy-ion theory @ SPARC collaboration

-- Recent developments and progress

of QED

Key topics of this collaboration:

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- Collision & capture dynamics in strong fields at relativistic energies
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- Atomic physics techniques applied to nuclear physics

nsiv

ih-ha

- Multi-photon processes
- Antiproton physics
- Test of fundamental
- Interaction of ions with i

... dynamics in strong fields

Time-independent density matrix theory $\hat{S} - \text{ scattering operator}$ $\hat{f}_{f} = \hat{S} \hat{\rho}_{i} \hat{S}^{+}$ $\langle \eta_{1} ... \eta_{m} | \hat{\rho}_{f} | \eta'_{1} ... \eta'_{m} \rangle = \sum_{\xi_{1}, \xi_{2}...} \langle \xi_{1} ... \xi_{n} | \hat{\rho}_{i} | \xi'_{1} ... \xi'_{n} \rangle \langle \eta_{1} ... \eta_{n} | \hat{R} | \xi_{1} ... \xi_{n} \rangle \langle \eta'_{1} ... \eta'_{n} | \hat{R} | \xi'_{1} ... \xi'_{n} \rangle^{+}$

Measurement of physical properties:

- 'detector operator' describes the experimental setup:
- probability to get a 'click' at the detectors:

$$W = Tr\left(\hat{P}\,\hat{\rho}_{f}\right) = \sum_{\eta_{1}...\eta_{m}} \langle \eta_{1}...\eta_{m} | \hat{P}\,\hat{\rho}_{f} | \eta_{1}...\eta_{m} \rangle$$

$$\hat{P} = |\epsilon > < \epsilon|$$

Time-independent density matrix theory



of the interaction which may lead to the emission of photons, electrons, ...



Studying fundamental constants (time variations, ...)



Supercritical fields in ion-atom collisions





Mokler & Liesen (1982)

Processes during the collision:

- excitation into higher shells
- ionization (δ -electrons)
- MO radiation
- characteristic x-rays

Laser spectroscopy of Os-

@ MPI-K in Heidelberg (A. Kellerbauer et al.)

2.00 1.50 6**D**0 1.00 e J = 3/2J = 5/24**⊢**e 0.50 J = 7/2Os- $J_{a} = 9/2$ (eV) 0



Measurement principle:

- Laser frequency is scanned around transition frequency
- Excited state is detached by electric field

Neutrals detected on forward MCP

SPARC-Collaboration @ FAIR

Stored and Cooled

- Highly-Charged Ions and Exotic Nuclei from Rest to Relativistic Energies
- Intense Beams of Radioactive Isotopes
- Virtual Photon Sources at X- and γ-Ray Energies
- XUV Energies via Lorentz Boost of optical wavelengths





... with Novel Instrumentation

- Ultracold Electron-Beam Target
- High Resolution X-Ray and Electron Spectrometers
- In-Ring Recoil Momentum Microscope
- Highly Intense Laser Beams
- Traps

Polarization of the K-shell REC photons

position sensitive detector

