Calculation of isotopic shifts of KLL dielectronic resonance peaks and x-ray lines in heavy few-electron ions

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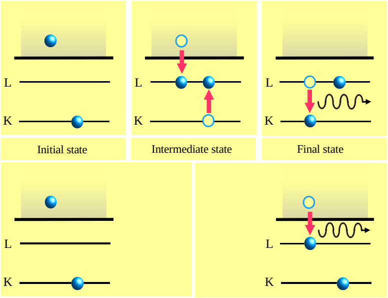
Outline

Introduction

- New approach: some nuclear properties are hard to measure by nuclear physics experiments
  precise atomic physics measurements + precise theory
- Laser spectroscopy: ^{6}He, ^{6,7}Li, ^{8,9} Li, ^{11}Li
  determination of nuclear root mean square charge radii $\sqrt{\langle r^2 \rangle}$
- Isotopic shifts in dielectronic recombination and x-ray spectra?
  EBITs and efficient crystal spectrometers

- Dielectronic recombination (DR):
  1. Radiationless resonant capture of a continuum electron
  2. Radiative decay of the autoionizing state

$$A^{q+}(i) + e^{-} \rightarrow [A^{(q-1)+}(d)]^{**} \rightarrow [A^{(q-1)+}(f)]^{*} + \omega$$



- Radiative recombination (RR): direct emission of a photon

$$A^{q+}(i) + e^{-} \rightarrow [A^{(q-1)+}(f)]^{*} + \omega'$$

Shift of DR resonances

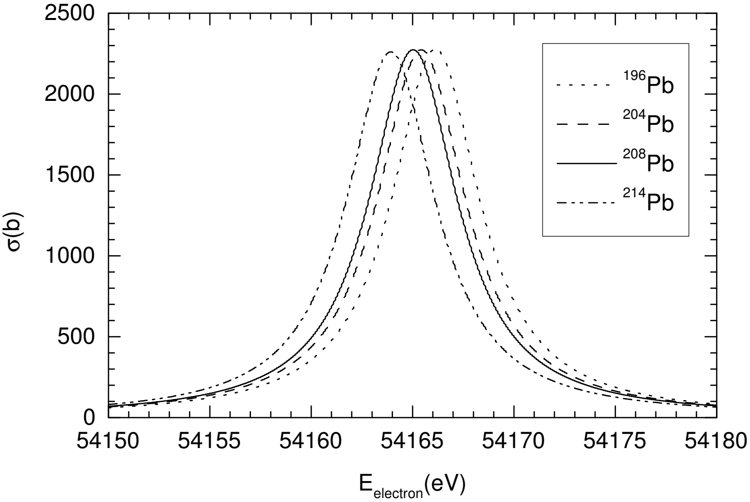
Total cross section of DR:

$$\sigma^{\mathrm{DR}}_{i\to d\to f}(\varepsilon) = \frac{2\pi^2}{p^2}\frac{A_r^{d\to f}}{\Gamma_d} L_d(\varepsilon) V_a^{i\to d} \,,$$

with the Lorentz profile

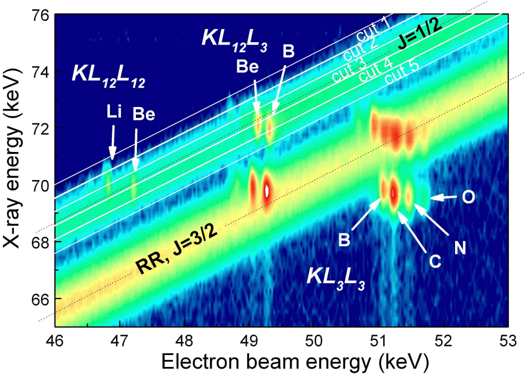
$$L_d(\varepsilon) = \frac{\Gamma_d/(2\pi)}{(E_i+\varepsilon-E_d)^2+\frac{\Gamma_d^2}{4}}$$

Shift of DR resonances



KLL DR measurement at the MPI Heidelberg EBIT

Antonio Javier González Martínez *et al.*
X-ray spectrum: the KLL recombination regime



The multiconfiguration Dirac-Fock method

Dirac-Coulomb Hamiltonian:

$$H^{\mathrm{DC}} = \sum_{i=1}^{N} h_i + \sum_{i<j}^{N} \frac{1}{r_{ij}}$$

with the one-particle operators

$$h_i = c\vec{\alpha}_i\vec{p}_i + (\beta_i - 1)c^2 + V_{nuc}(r_i)$$

Atomic state function (ASF) ansatz:

$$|\Gamma PJM\rangle = \sum_{i=1}^{n_c} c_i |\gamma_i PJM\rangle$$

The CSFs are constructed as *jj*-coupled *N*-particle Slater determinants
One-particle Dirac orbitals:

$$\psi_{n\kappa\mu}(\vec{r}) = \frac{1}{r} \begin{pmatrix} P_{n\kappa}(r)\Omega_{\kappa\mu}(\hat{r}) \\ iQ_{n\kappa}(r)\Omega_{-\kappa\mu}(\hat{r}) \end{pmatrix}$$

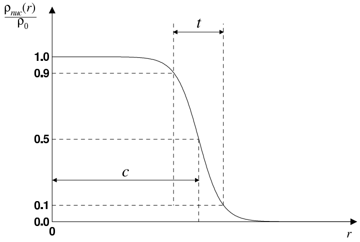
From variation of the c_i in the energy functional (defined as the expectation value of H^{DC}):

$$\sum_{j=1}^{n_c} (\langle \gamma_i PJM | H^{\mathrm{DC}} | \gamma_j PJM \rangle - E_\Gamma^{DC} \delta_{ij}) c_j = 0$$

$\longrightarrow$ configuration interaction method (CI)
If the variation of the orbital wave functions is also allowed
$\longrightarrow$ multiconfiguration Dirac-Fock equations

- Nuclear finite-size effects: Fermi two-parameter distribution

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



Numerical integration of the Dirac equations with $V_{nuc}(\rho_{nuc}(r))$

- Nuclear finite-mass effects:
  1. The reduced mass correction

$$m_e \to \frac{m_e m_{\mathrm{nuc}}(A)}{m_e + m_{\mathrm{nuc}}(A)}$$

  2. The correction due to the correlated motions of the electrons: specific mass shift (SMS) described by the non-relativistic operator

$$H_{\mathrm{SMS}} = \frac{1}{m_{\mathrm{nuc}}(A)} \sum_{i<j}^{N} \vec{p}_i \cdot \vec{p}_j$$

- Nuclear polarization: virtual excitation of collective nuclear degrees of freedom by shell electrons (Coulomb excitation and current-current interaction) $\rightarrow$ *not included*

- The self-energy in hydrogenlike systems

$$E_{n\kappa}^{\mathrm{SE}} = \frac{Z^4}{\pi c^3 n^3} F_{n\kappa}(Z\alpha)$$

  Estimation of the self-energy screening
- Vacuum polarization correction: Uehling potential approximation + screening
- Breit interaction:

$$V_0^B = \frac{1}{r_{12}} \left(-\frac{1}{2}\vec{\alpha}_1\vec{\alpha}_2 - \frac{(\vec{\alpha}_1\vec{r}_{12})(\vec{\alpha}_2\vec{r}_{12})}{2r_{12}^2} \right)$$

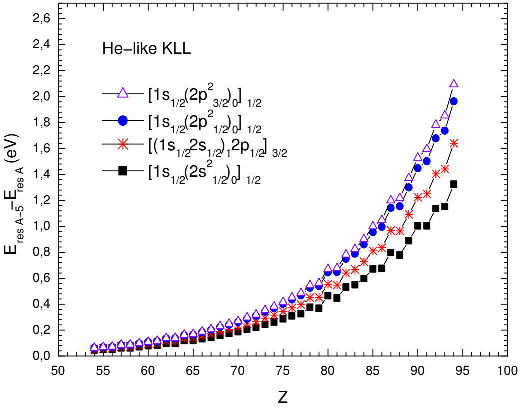
Numerical implementation: GRASP (General-Purpose Relativistic Atomic Structure Program) of Grant, Dyall et al. (versions: GRASP 1.0, GRASP92)

KLL DR resonance peaks

Intermediate state $\lvert d \rangle$	$E_{res}(238)$	228	230	232	233	234	235	236	S_d
$[1s2s^2]_{1/2}$	63058	-2.20	-1.75	-1.29	-1.06	-0.83	-0.61	-0.45	3.70e+4
$[(1s2s)_1 2p_{1/2})]_{3/2}$	63104	-2.73	-2.17	-1.61	-1.32	-1.05	-0.77	-0.56	2.02e+3
$[(1s2s)_1 2p_{1/2})]_{1/2}$	63138	-2.74	-2.17	-1.61	-1.32	-1.05	-0.77	-0.56	1.76e+4
$[(1s2s)_0 2p_{1/2})]_{1/2}$	63392	-2.75	-2.19	-1.62	-1.33	-1.05	-0.77	-0.56	5.54e+4
$[1s2p^2_{1/2}]_{1/2}$	63445	-3.28	-2.61	-1.94	-1.59	-1.26	-0.93	-0.66	2.19e+1
$[(1s2s)_1 2p_{3/2}]_{5/2}$	67373	-2.81	-2.23	-1.66	-1.36	-1.07	-0.79	-0.57	1.97e+2
$[(1s2s)_1 2p_{3/2}]_{3/2}$	67493	-2.81	-2.23	-1.66	-1.36	-1.07	-0.79	-0.57	3.66e+2
$[(1s2s)_1 2p_{3/2}]_{1/2}$	67570	-2.81	-2.23	-1.66	-1.36	-1.07	-0.79	-0.57	2.48e+2
$[(1s2p_{1/2})_1 2p_{3/2}]_{5/2}$	67643	-3.41	-2.71	-2.02	-1.66	-1.31	-0.97	-0.69	2.30e+4
$[(1s2p_{1/2})_0 2p_{3/2}]_{3/2}$	67662	-3.41	-2.71	-2.02	-1.66	-1.31	-0.97	-0.69	7.83e+3
$[(1s2p_{1/2})_1 2p_{3/2}]_{1/2}$	67700	-3.41	-2.71	-2.02	-1.66	-1.31	-0.97	-0.69	1.19e+3
$[(1s2s)_0 2p_{3/2}]_{3/2}$	67702	-2.83	-2.25	-1.67	-1.37	-1.08	-0.80	-0.57	2.64e+4
$[(1s2p_{1/2})_1 2p_{3/2}]_{3/2}$	67791	-3.41	-2.71	-2.02	-1.66	-1.31	-0.97	-0.69	1.07e+4
$[1s(2p^2_{3/2})_2]_{5/2}$	71977	-3.49	-2.77	-2.06	-1.70	-1.34	-0.99	-0.70	1.33e+4
$[1s(2p^2_{3/2})_2]_{3/2}$	72069	-3.48	-2.77	-2.06	-1.69	-1.34	-0.99	-0.70	1.33e+3
$[1s(2p^2_{3/2})_0]_{1/2}$	72108	-3.48	-2.77	-2.06	-1.70	-1.34	-0.99	-0.70	2.58e+3

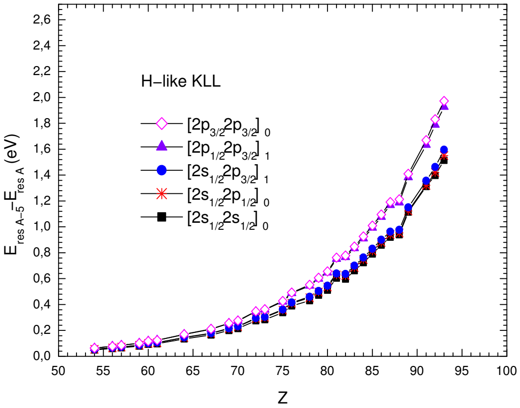
Table: KLL-DR Resonance energies E_{res} for initially He-like ^{238}U ions in eV. The resonance strenghts S_d are given in barn·eV

Z-scaling of resonance shifts: He-like



From: R. Şchiopu, Z. Harman, W. Scheid and N. Grün, Eur. Phys. J. D **31**, 21 (2004)

Z-scaling of resonance shifts: H-like



From: R. Şchiopu, Z. Harman, W. Scheid and N. Grün, Eur. Phys. J. D **31**, 21 (2004)

Kα x-rays following KLL DR

Intermediate state $\|d\rangle$	Final state $\|f\rangle$	E_x (238)	228	230	232	233	234	A_r
$[1s2s^2]_{1/2}$	$[1s^2 2s]_{1/2}$	95897	-2.93	-2.34	-1.75	-1.45	-1.16	1.68e+14
	$[1s^2 2p_{1/2}]_{1/2}$	95614	-2.34	-1.87	-1.40	-1.16	-0.93	2.42e+15
$[(1s2s)_1 2p_{1/2})]_{3/2}$	$[1s^2 2s]_{1/2}$	95943	-3.46	-2.76	-2.07	-1.71	-1.37	3.11e+16
	$[1s^2 2p_{1/2}]_{1/2}$	95660	-2.87	-2.29	-1.72	-1.42	-1.14	1.17e+14
$[(1s2s)_1 2p_{1/2})]_{1/2}$	$[1s^2 2s]_{1/2}$	95977	-3.46	-2.76	-2.07	-1.71	-1.37	1.55e+16
	$[1s^2 2p_{1/2}]_{1/2}$	95694	-2.87	-2.29	-1.72	-1.42	-1.14	1.09e+14
$[(1s2s)_0 2p_{1/2})]_{1/2}$	$[1s^2 2s]_{1/2}$	96231	-3.48	-2.78	-2.08	-1.72	-1.38	1.67e+16
$[1s2p^2_{1/2}]_{1/2}$	$[1s^2 2p_{1/2}]_{1/2}$	96001	-3.41	-2.72	-2.04	-1.69	-1.35	4.48e+16
$[(1s2s)_1 2p_{3/2}]_{5/2}$	$[1s^2 2s]_{1/2}$	100212	-3.53	-2.82	-2.12	-1.75	-1.40	2.03e+14
	$[1s^2 2p_{3/2}]_{3/2}$	95751	-2.87	-2.29	-1.72	-1.42	-1.14	1.18e+14
$[(1s2s)_1 2p_{3/2}]_{3/2}$	$[1s^2 2s]_{1/2}$	100332	-3.53	-2.82	-2.12	-1.75	-1.40	3.21e+16
	$[1s^2 2p_{3/2}]_{3/2}$	95871	-2.87	-2.29	-1.72	-1.42	-1.14	1.16e+14
$[(1s2s)_1 2p_{3/2}]_{1/2}$	$[1s^2 2s]_{1/2}$	100409	-3.53	-2.82	-2.12	-1.75	-1.40	4.20e+16
	$[1s^2 2p_{3/2}]_{3/2}$	95948	-2.87	-2.30	-1.72	-1.42	-1.14	1.18e+14
$[(1s2p_{1/2})_1 2p_{3/2}]_{5/2}$	$[1s^2 2p_{1/2}]_{1/2}$	100199	-3.54	-2.83	-2.12	-1.76	-1.40	2.03e+14
	$[1s^2 2p_{3/2}]_{3/2}$	96021	-3.47	-2.78	-2.08	-1.72	-1.38	3.14e+16
$[(1s2p_{1/2})_0 2p_{3/2}]_{3/2}$	$[1s^2 2p_{1/2}]_{1/2}$	100218	-3.54	-2.83	-2.12	-1.76	-1.40	1.13e+16
	$[1s^2 2p_{3/2}]_{3/2}$	96040	-3.47	-2.78	-2.08	-1.72	-1.38	2.74e+16

KLL DR resonance peaks and Kα x-rays:
Large isotope shifts
but high absolute energies

$2p_{3/2} \longrightarrow 2s$ x-rays following KLL DR

Intermediate state $\|d\rangle$	Final state $\|f\rangle$	E_x (238)	228	230	232	233	234	235
$[(1s2s)_1 2p_{3/2}]_{3/2}$	$[1s(2s^2)_0]_{1/2}$	4433	-0.60	-0.48	-0.36	-0.30	-0.24	-0.18
$[(1s2s)_1 2p_{3/2}]_{1/2}$	$[1s(2s^2)_0]_{1/2}$	4509	-0.61	-0.48	-0.36	-0.30	-0.24	-0.18
$[(1s2s)_0 2p_{3/2}]_{3/2}$	$[1s(2s^2)_0]_{1/2}$	4646	-0.62	-0.50	-0.37	-0.31	-0.25	-0.19
$[(1s2p_{1/2})_1 2p_{3/2}]_{5/2}$	$[(1s2s)_1 2p_{1/2}]_{3/2}$	4540	-0.68	-0.54	-0.41	-0.34	-0.27	-0.20
$[(1s2p_{1/2})_0 2p_{3/2}]_{3/2}$	$[(1s2s)_1 2p_{1/2}]_{3/2}$	4558	-0.68	-0.54	-0.41	-0.34	-0.27	-0.20
$[(1s2p_{1/2})_0 2p_{3/2}]_{3/2}$	$[(1s2s)_1 2p_{1/2}]_{1/2}$	4524	-0.67	-0.54	-0.40	-0.33	-0.27	-0.20
$[(1s2p_{1/2})_1 2p_{3/2}]_{3/2}$	$[(1s2s)_0 2p_{1/2}]_{1/2}$	4395	-0.66	-0.53	-0.39	-0.33	-0.26	-0.20
$[1s(2p^2_{3/2})_2]_{5/2}$	$[(1s2s)_1 2p_{3/2}]_{5/2}$	4604	-0.68	-0.54	-0.41	-0.34	-0.27	-0.20
$[1s(2p^2_{3/2})_2]_{5/2}$	$[(1s2s)_1 2p_{3/2}]_{3/2}$	4484	-0.68	-0.54	-0.41	-0.34	-0.27	-0.20
$[1s(2p^2_{3/2})_2]_{3/2}$	$[(1s2s)_1 2p_{3/2}]_{3/2}$	4575	-0.68	-0.54	-0.40	-0.33	-0.27	-0.20
$[1s(2p^2_{3/2})_0]_{1/2}$	$[(1s2s)_1 2p_{3/2}]_{3/2}$	4614	-0.68	-0.54	-0.41	-0.34	-0.27	-0.20
$[1s(2p^2_{3/2})_2]_{3/2}$	$[(1s2s)_1 2p_{3/2}]_{1/2}$	4499	-0.67	-0.54	-0.40	-0.33	-0.27	-0.20
$[1s(2p^2_{3/2})_0]_{1/2}$	$[(1s2s)_1 2p_{3/2}]_{1/2}$	4538	-0.68	-0.54	-0.41	-0.34	-0.27	-0.20
$[1s(2p^2_{3/2})_2]_{5/2}$	$[(1s2s)_0 2p_{3/2}]_{3/2}$	4271	-0.66	-0.53	-0.39	-0.33	-0.26	-0.20
$[1s(2p^2_{3/2})_2]_{3/2}$	$[(1s2s)_0 2p_{3/2}]_{3/2}$	4362	-0.66	-0.52	-0.39	-0.32	-0.26	-0.19
$[1s(2p^2_{3/2})_0]_{1/2}$	$[(1s2s)_0 2p_{3/2}]_{3/2}$	4401	-0.66	-0.53	-0.39	-0.33	-0.26	-0.20

$2p_{3/2} \longrightarrow 2s$ x-rays:
Only slightly smaller isotope shifts
and much lower transition energies $\longrightarrow$ preferable for experimental observation

$2p_{3/2} \rightarrow 2s$ x-rays to the Li-like ground state

Transition		E_x(238)	228	230	232	233	A_r
$1s^2 2p_{3/2} \rightarrow 1s^2 2s$	This work	4461	0.66	0.53	0.39	0.33	1.39e+13
	Experiment	4459.37±0.35				0.256± 0.118	

Experiment:
S. R. Elliott, P. Beiersdorfer and M. H. Chen (LLNL SEBIT)
Trapped-Ion Technique for Measuring the Nuclear Charge Radii of Highly Charged Radioactive Isotopes
PRL **76**, 1031 (1996)

Summary

Provide a guideline for TITAN isotope shift measurements:
Theoretical absolute energies and isotope shifts for

- KLL DR resonance peaks Kα x-rays
- Kα x-rays following DR
- $2p_{3/2} \rightarrow 2s$ x-ray lines $\rightarrow$ most likely to be measurable

Outlook

- Pick an element and isotopes
- Make the experiment
- Extract $\delta\langle r^2\rangle$

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