Atomic structure calculations

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Outline of the talk

- Introduction
- Lamb shifts in H-like ions
- Transition energies in Li-like ions
- Transition energies in He-like ions
- Binding energies in Be-like ions
- Conclusion

Introduction: QED theory of highly charged ions

Heavy few-electron ions:

$$N_e \ll Z$$

N_e is the number of electrons, Z is the nuclear charge number
To zeroth-order approximation:

$$\left[-i\vec{\alpha}\cdot\vec{\nabla} + m\beta + V_{\mathrm{C}}(r)\right]\psi(\vec{r}) = E\psi(\vec{r})$$

Interelectronic interaction and QED effects:

$$\frac{\text{Interelectronic interaction}}{\text{Binding energy}} \sim \frac{1}{Z} \qquad \frac{\text{QED}}{\text{Binding energy}} \sim \alpha(\alpha Z)^2$$

In contrast to light atoms, the parameter αZ is not small.
In uranium: $Z = 92$, $\alpha Z \approx 0.7$.

Introduction: QED theory of many-electron systems

Relativistic many-electron atoms and ions

The interelectronic interaction is not small and must be taken into account at the zero-order level:

$$V_{\mathrm{C}} \to V_{\mathrm{eff}} = V_{\mathrm{C}} + V_{\mathrm{scr}} \,,$$

where V_{scr} describes approximately the electron-electron interaction effects. Therefore, to zeroth order:

$$\left[-i\,\vec{\alpha}\cdot\vec{\nabla} + m\beta + V_{\mathrm{eff}}(r) \right]\,\psi\,(\vec{r}) = \,E\,\psi\,(\vec{r})$$

In higher orders, besides the interelectronic-interaction and QED effects, one must add the interaction with $-V_{\mathrm{scr}}$.

Introduction: Breit approximation

Middle and heavy neutral atoms

Calculations are mainly restricted to the Breit approximation:

$$H = \Lambda^{(+)} \Big[\sum_i h_i^{\rm D} + \sum_{i<j} (V_{ij}^{\rm C} + V_{ij}^{\rm B}) \Big] \Lambda^{(+)} \,,$$

where $\Lambda^{(+)}$ is the projector on the positive-energy states,

$$h_i^{\rm D} = \vec{\alpha}_i \cdot \vec{p}_i + m\beta_i + V_{\rm C}(r_i) \,, \qquad V_{\rm C}(r) = -\frac{\alpha Z}{r} \,,$$

$$V_{ij}^{\rm C} = \frac{\alpha}{r_{ij}} \,, \qquad V_{ij}^{\rm B} = -\alpha \Big[\frac{\vec{\alpha}_i \cdot \vec{\alpha}_j}{r_{ij}} + \frac{1}{2} (\vec{\nabla}_i \cdot \vec{\alpha}_i)(\vec{\nabla}_j \cdot \vec{\alpha}_j) r_{ij} \Big] \,.$$

$1s$ Lamb shift in H-like ions, in eV

Contribution	^{197}Au^{78+}	^{208}Pb^{81+}	^{238}U^{91+}
Furry picture QED	155.83(17)	177.14(21)	265.07(48)
Finite nuclear size	49.13(11)	67.18(5)	198.51(19)
Nuclear recoil	0.33(1)	0.35(1)	0.46(1)
Nuclear polarization	−0.05(5)	−0.03(2)	−0.20(10)
Total theory [1]	205.24(21)	244.64(22)	463.84(53)
Experiment	202(8) [2]	260(53) [3]	460.2(4.6) [4]

[1] V. A. Yerokhin and V. M. Shabaev, JPCRD, 2015.
[2] H. F. Beyer *et al.*, Z. Phys. D, 1995.
[3] S. Kraft-Bermuth *et al.*, JPB, 2017.
[4] A. Gumberidze *et al.*, PRL, 2005.

Few-electron Pb ions for the Gamma Factory project at CERN:
F.M. Kröger, G. Weber, V.P. Shevelko, S. Hirlaender, M.V. Krasny, and Th. Stöhlker, XRay Spectrometry, 2019.

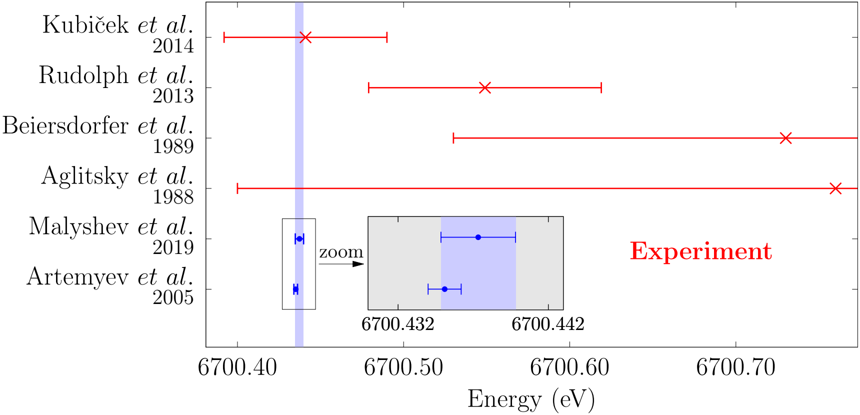
$2p_{1/2} - 2s$ transition energy in Li-like ions, in eV

Ion	Energy [eV]	Reference
^{208}Pb^{79+}	230.82(5)	[1,2] (Theory)
	230.76(4)	[3] (Theory)
^{238}U^{89+}	280.71(10)	[1,4] (Theory)
	280.65(8)	[3] (Theory)
	280.645(15)	[5] (Experiment)

[1] V.A. Yerokhin, P. Indelicato, and V.M. Shabaev, PRL, 2006.
[2] V.A. Yerokhin and A. Surzhykov, JPCRD, 2018.
[3] J. Sapirstein and K.T. Cheng, PRA, 2011.
[4] Y.S. Kozhedub, O.V. Andreev, V.M. Shabaev *et al.*, PRA, 2008.
[5] P. Beiersdorfer, H. Chen, D.B. Thorn, and E. Träbert, PRL, 2005.

The w-line transition energy in He-like Fe^{24+}

The $w(2^1P_1 - 1^1S_0)$-line transition energy, in eV



Comparison of the **theoretical** prediction for the w-line in Fe^{24+} with available **experimental** values

Transition energies in He-like ions, in eV

Z	$1s2p\,^1P_1 \to 1s^2\,^1S_0$	$1s2p\,^3P_2 \to 1s^2\,^1S_0$	$1s2p\,^3P_1 \to 1s^2\,^1S_0$	$1s2s\,^3S_1 \to 1s^2\,^1S_0$	$1s2p\,^3P_2 \to 1s2s\,^3S_1$	Ref.
54	30 630.059(27)	30 594.369(27)	30 206.273(27)	30 129.157(27)	465.2119(96)	[1]
	30 630.053(18)	30 594.365(18)	30 206.267(18)	30 129.143(36)	465.222(33)	[2]
92	100 610.68(54)	100 536.95(54)	96 169.43(54)	96 027.07(54)	4509.88(11)	[1]
	100 611.21(65)	100 537.50(65)	96 169.94(65)	96 027.41(68)	4510.09(26)	[2]
					4509.71(99)	[3]

Transition energies in heliumlike **Xe** and **U**, in eV

[1] Y. S. Kozhedub, A. V. Malyshev, D. A. Glazov *et al.*, PRA, 2019.

[2] A. N. Artemyev, V. M. Shabaev, V. A. Yerokhin *et al.*, PRA, 2005.

[3] M. Trassinelli *et al.*, Eur. Phys. Lett., 2009.

Be-like ions: overview

Highly charged Be-like ions severely challenge atomic-structure calculations within bound-state QED.

Reason: strong interplay of electron correlation and QED effects.

Quasi-degenerate levels:

$$1s^2(2s2s)_0 \qquad 1s^2(2p_{1/2}2p_{1/2})_0 \qquad 1s^2(2p_{3/2}2p_{3/2})_0$$

Correlation effects within the Breit appox. can be treated to all order in $1/Z$ by means of the CI approach.

State-of-the-art QED calculations are limited by the second-order contributions.

Be-like ions: perturbation theory

Types of perturbation theory to evaluate
the ground-state binding energy in Be-like Xe^{50+}

Size	Ω
1×1	$(2s2s)_0$
2×2	$(2s2s)_0$, $(2p_{1/2}2p_{1/2})_0$
3×3	$(2s2s)_0$, $(2p_{1/2}2p_{1/2})_0$, $(2p_{3/2}2p_{3/2})_0$

Ω is the model space of the quasi-degenerate levels.

The extended Furry picture:

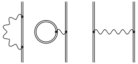
$$\left[-i\boldsymbol{\alpha}\cdot\nabla + \beta m + V_{\rm eff}(\mathbf{r})\right]\psi_n(\mathbf{r}) = \varepsilon_n \psi_n(\mathbf{r})$$

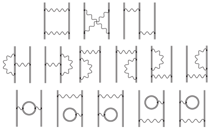
$$V_{\rm nuc}(\mathbf{r}) \longrightarrow V_{\rm eff}(\mathbf{r}) = V_{\rm nuc}(\mathbf{r}) + V_{\rm scr}(\mathbf{r})$$

Binding energy of the ground state in Xe^{50+}, in eV [A.V. Malyshev *et al.*, arXiv:2009.01222]

Ω	$V_{\rm eff}$	**A**	**B**	**C**	**D**	
1×1	Coul	101 071.884	100 970.193	100 973.026	—	$(2s2s)_0$
	CH	101 071.948	100 973.924	100 972.977	100 973.569	
	LDF	101 071.928	100 973.451	100 972.981	100 973.400	
2×2	Coul	101 071.884	100 970.443	100 973.244	100 973.263	$(2s2s)_0$
	CH	101 071.948	100 974.157	100 973.194	100 973.246	$(2p_{1/2}2p_{1/2})_0$
	LDF	101 071.928	100 973.682	100 973.198	100 973.237	
3×3	Coul	101 071.884	100 970.487	100 973.278	100 973.240	$(2s2s)_0$
	CH	101 071.948	100 974.199	100 973.229	100 973.241	$(2p_{1/2}2p_{1/2})_0$
	LDF	101 071.928	100 973.724	100 973.233	100 973.236	$(2p_{3/2}2p_{3/2})_0$

A: Breit approx.

B:  + nucl. recoil

C:  + 2loop

D: Estimation of the $1/Z^2$ screening QED effects via the model Lamb-shift operator

Excitation energies in Xe^{50+}, in eV

$2s2p\,^3P_0$	$2s2p\,^3P_1$	$2s2p\,^3P_2$	$2s2p\,^1P_1$	Reference
		Theory		
104.531(9)	127.300(9)	469.484(7)	532.802(7)	Malyshev *et al.*, arXiv:2009.01222
104.5(25)	127.3(25)	469.6(25)	532.9(25)	Kaygorodov *et al.*, PRA, 2019
104.475	127.282	469.449	532.877	Cheng *et al.*, PRA, 2008
104.663	127.475	470.004	533.401	Gu, ADNDT, 2005
	127.168	469.25	532.62	Safronova, Mol.Phys., 2000
	127.301		532.854	Chen & Cheng, PRA, 1997
104.482	127.267	469.386	532.759	Safronova *et al.*, PRA, 1996
		Experiment		
	127.269(46)	469.474(81)	532.801(16)	Bernhardt *et al.*, JPB, 2015
	127.260(26)			Feili *et al.*, Phys.Scr., 2005
	127.255(12)			Träbert *et al.*, PRA, 2003

Excitation energies for the $2s2p\,^{2S+1}P_J$ states in Be-like Xe, in eV

Summary

Main results:

- The binding energies in He- and Be-like ions are evaluated employing the most advanced methods which are available to date.
- Our results for He-like ions are consistent with our old calculations (A.N. Artemyev *et al.*, PRA, 2005) and with most recent experiments.
- Our results for Be-like ions are in perfect agreement with the recent experiment by D. Bernhardt *et al.*, JPB, 2015.