QED calculation of the ground-state energy of Be-like ions

A. V. Malyshev, A. V. Volotka, D. A. Glazov,

I. I. Tupitsyn, V. M. Shabaev, and G. Plunien

Department of Physics
Saint-Petersburg State University

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Outline:

- Introduction and Motivation
- Theoretical Description and Numerical Procedure
- Summary and Outlook

Motivation

- Test of QED at strong fields
  (along with investigations of H-, He-, Li-, and B-like ions)

Experiments:

H-like:	T. Stöhlker *et al.*,	PRL, 2000;
	A. Gumberidze *et al.*,	PRL, 2005;
He-like:	A. Gumberidze *et al.*,	PRL, 2004.
Li-like:	J. Schweppe *et al.*,	PRL, 1991;
	C. Brandau *et al.*,	PRL, 2003;
	P. Beiersdorfer *et al.*,	PRL, 2005.
Be-like:	P. Beiersdorfer *et al.*,	PRA, 1998;
	I. Draganić *et al.*,	PRL, 2003;
B-like:	I. Draganić *et al.*,	PRL, 2003;
	V. Mäckel *et al.*,	PRL, 2011;

- The ground-state energies of Be-like ions are of the great importance for mass spectrometry

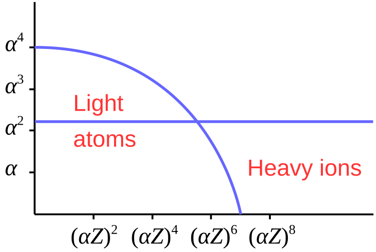
  J. Repp *et al.*, Appl. Phys. B, 2012;
  E. G. Myers, Int. J. Mass Spectrom., 2013.

QED in the Furry picture

<u>Highly-charged few-electron ions:</u>

$$N_e \ll Z$$

N_e is the number of electrons,
Z is the nuclear charge number



To zeroth-order approximation:

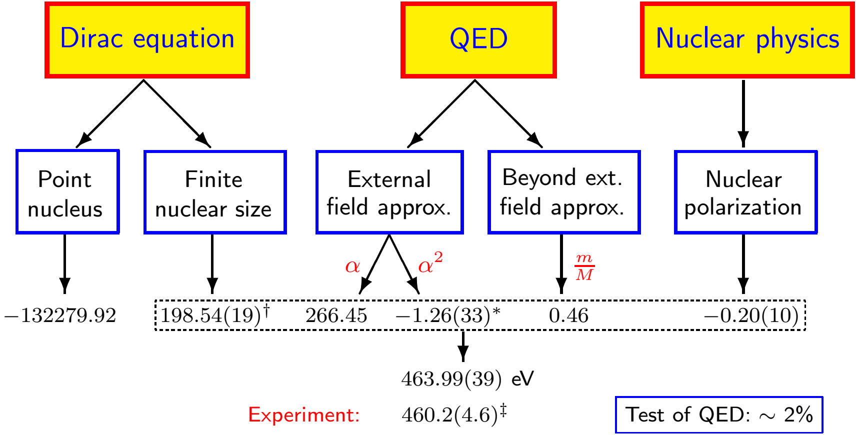
$$\left[-i\boldsymbol{\alpha}\cdot\nabla + \beta m + V_{\rm nuc}(\mathbf{r})\right]\psi_n(\mathbf{r}) = \varepsilon_n \psi_n(\mathbf{r})$$

Interelectronic interaction and QED effects:

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

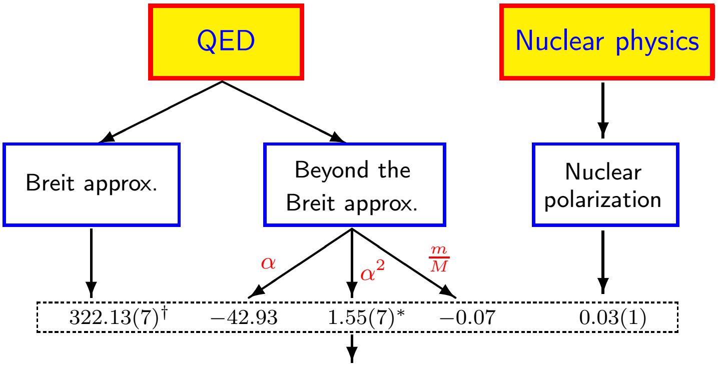
In uranium: $Z = 92$, $\alpha Z \approx 0.7$

Binding energy of H-like uranium, in eV



† Y. S. Kozhedub, O.V. Andreev, V.M. Shabaev *et al.*, PRA, 2008.
* V. A. Yerokhin, P. Indelicato, and V.M. Shabaev, PRL, 2006.
‡ A. Gumberidze, T. Stöhlker, D. Banaś *et al.*, PRL, 2005.

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



$280.71(10)$ eV

Experiment:	$280.59(10)$ eV	(J. Schweppe *et al.*, PRL, 1991)
	$280.52(10)$ eV	(C. Brandau *et al.*, PRL, 2003)
Test of QED: $\sim$ 0.2%	$280.645(15)$ eV	(P. Beiersdorfer *et al.*, PRL, 2005)

Test of many-electron QED effects!

† Y. S. Kozhedub, O. V. Andreev, V. M. Shabaev *et al.*, PRA, 2008.
* V. A. Yerokhin, P. Indelicato, and V. M. Shabaev, PRL, 2006.

The extended Furry picture

$V_{\rm scr}$ describes approximately the electron-electron interaction effects

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

To zeroth-order approximation:

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

The extended Furry picture is used to accelerate the convergence of the perturbation series

Screening potentials

- Local Dirac-Fock potential (LDF)

  V. M. Shabaev, I. I. Tupitsyn, K. Pachucki *et al.*, PRA, 2005.

- Kohn-Sham potential (KS)

  W. Kohn and L. J. Sham, PRA, 1965.

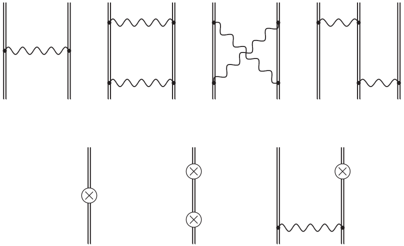
- Perdew-Zunger potential (PZ)

  J. P. Perdew and A. Zunger, PRB, 1981.

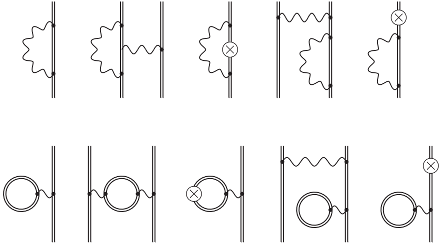
The screening potential partly accounts for the interelectronic interaction in the zeroth-order Hamiltonian

Contributions

- The interelectronic interaction diagrams



- First- and second-order QED diagrams



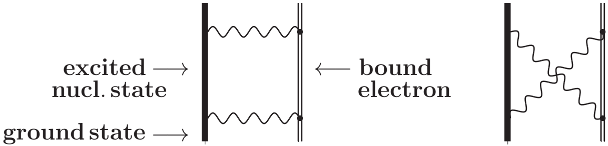
- Third- and higher-order electron-correlation contributions within the Breit approx. (the large-scale configuration-interaction Dirac-Fock-Sturm method)

- One-electron two-loop diagrams

Contributions

Beyond external field approximation:

- Nuclear recoil $\left(\text{finite nuclear mass, } \sim \frac{m}{M}\right)$
    - Breit approx. (all orders in $1/Z$)
    - QED recoil effect in zeroth order
- Nuclear polarization (internal degrees of freedom)



Uranium ($Z = 92$): individual contributions, in eV

Contribution	LDF	KS	PZ
$E^{(0)}_{\mathrm{Dirac}}$	-320572.56	-320871.02	-321276.02
$E^{(1)}_{\mathrm{int}}$	-6637.37	-6338.62	-5933.84
$E^{(2)}_{\mathrm{int,Breit}}$	-20.87	-20.45	-23.97
$E^{(2)}_{\mathrm{int,QED}}$	2.04	1.96	2.05
$E^{(\geqslant 3)}_{\mathrm{int,Breit}}$	3.03	2.39	6.05
$E_{\mathrm{int,total}}$	-327225.74	-327225.74	-327225.74
$E^{(1)}_{\mathrm{QED}}$	618.61	620.18	618.97
$E^{(2)}_{\mathrm{ScrQED}}$	0.73	-0.86	0.36
$E^{(2l)}_{\mathrm{QED}}$	-2.92	-2.92	-2.92
$E_{\mathrm{QED,total}}$	616.41	616.40	616.41
$E_{\mathrm{Rec,Breit}}$	0.60	0.60	0.60
$E_{\mathrm{Rec,QED}}$	0.56	0.56	0.56
$E_{\mathrm{Nucl.Pol.}}$	-0.45	-0.45	-0.45
E_{total}	-326608.62	-326608.63	-326608.63

Individual contributions to the binding energy of Be-like U (in eV)

Binding energies of Be-like ions, in eV

Nucl.	This work	Other theory	NIST
$^{56}_{26}$Fe	$-22102.960(45)$	-22103.37[a]	$-22102.1(1.8)$
		-22103.299[b]	
		$-22102.98(8)$[c]	
$^{132}_{54}$Xe	$-100972.921(85)$	-100973.7[a]	$-100963(4)$
		-100973.75[b]	
$^{184}_{74}$W	$-198983.71(32)$	-198984.71[b]	$-198987(3)$
$^{238}_{92}$U	$-326608.6(1.2)$	-326608.5[b]	$-326600(300)$

This work: A. V. Malyshev *et al.*, arXiv:1410.1961 [physics.atom-ph]

[a] M. F. Gu, At. Data Nucl. Data Tables, 2005.
[b] M. H. Chen and K. T. Cheng, PRA, 1997.
[c] V. A. Yerokhin, A. Surzhykov, and S. Fritzsche, PRA, 2014.

Summary

- The calculations of the ground-state binding energies of Be-like ions are performed in the range: $18 \leqslant Z \leqslant 96$.
- The accuracy was significantly improved and the most precise theoretical predictions for the ground-state binding energies in Be-like ions have been obtained.
- Achieved accuracy allows tests of bound-state QED with Be-like ions on the level $\sim 0.2\%$, provided the corresponding experiments are performed to the required precision (FAIR facilities).

Outlook

High-precision QED calculations of

- Ionization potentials for the ground states of Be-like ions
- Ionization potentials for the valence electrons in the $1s^2 2s^2 2p_{1/2}$ and $1s^2 2s^2 2p_{3/2}$ states of B-like ions
- Binding energies of excited states in Be-like ions

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Thank You for Your attention!

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