Theory of bound state QED at strong fields

Vladimir M. Shabaev

St. Petersburg State University

Outline of the talk

- Introduction
- Binding energy in heavy ions
- Hyperfine splitting in heavy ions
- Bound-electron g-factor
- PNC 6s-7s transition amplitude in neutral ^{133}Cs
- From strong to supercritical fields

Introduction

Heavy few-electron ions

$$N \ll Z\,,$$

where Z is the nuclear charge number and N is the number of electrons.

To zeroth-order approximation:

$$(-i\,\vec{\alpha}\,\vec{\nabla} + m\beta + V_{\mathrm{C}}(r)\,)\,\psi\,(\vec{r}) = \,E\,\psi\,(\vec{r})$$

Interelectronic-interaction and QED effects:

$$\frac{\text{Interelectronic interaction}}{\text{Binding energy}} \sim \frac{1}{Z}\,, \qquad \frac{\text{QED}}{\text{Binding energy}} \sim \alpha \approx \frac{1}{137}\,.$$

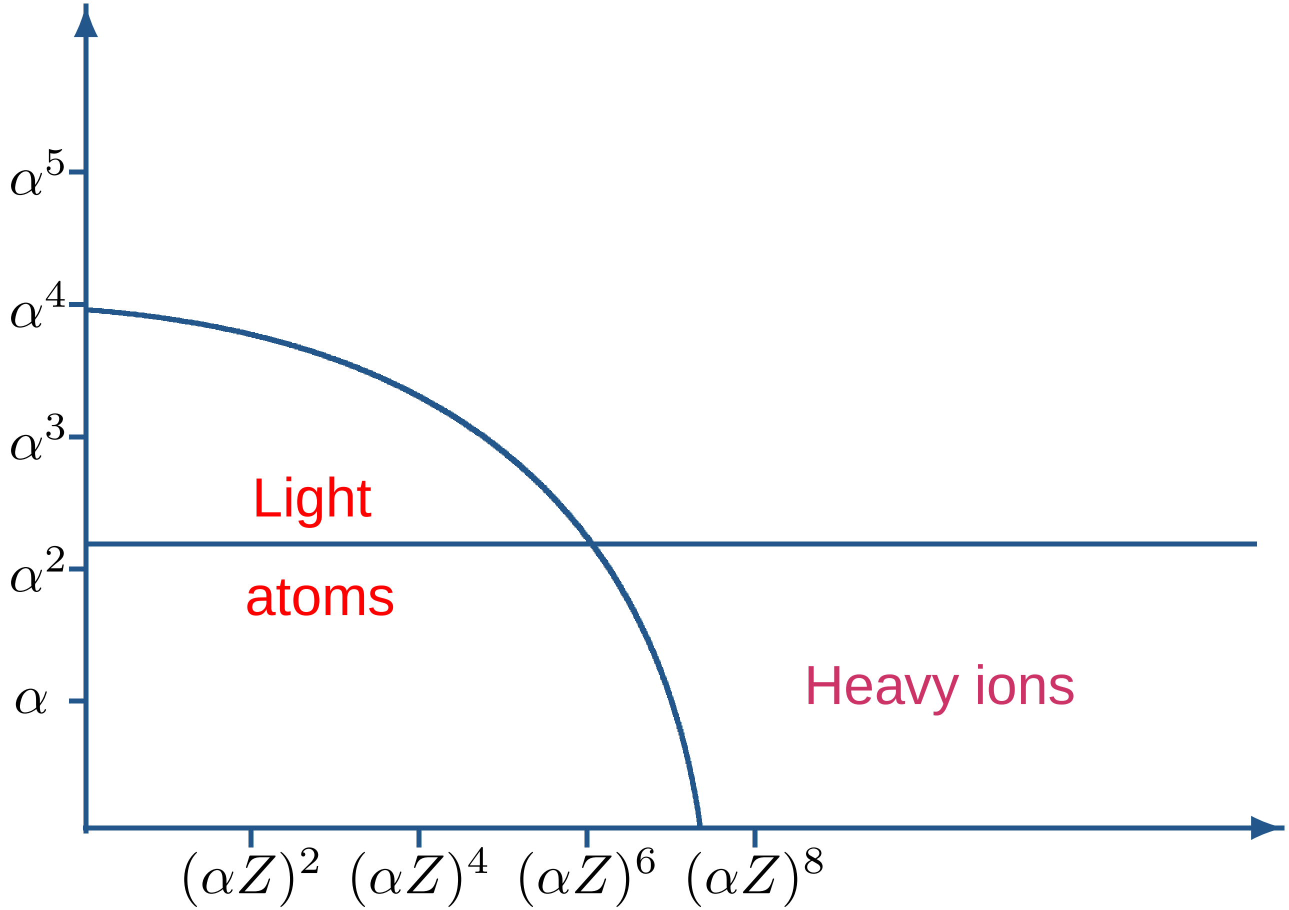
High-precision calculations are possible!

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

Introduction

Heavy few-electron ions

Tests of QED to lowest orders in α and to all orders in αZ



Theoretical problems:

a) technical

b) conceptual

c) physical

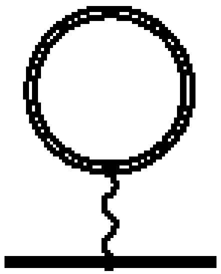
Binding energies in high-Z few-electron ions

a) Technical problems:

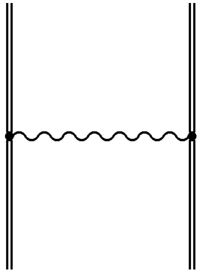
Calculations in the external field approximation ($M \to \infty$)

First-order QED corrections

P.J. Mohr, Ann. Phys., 1974

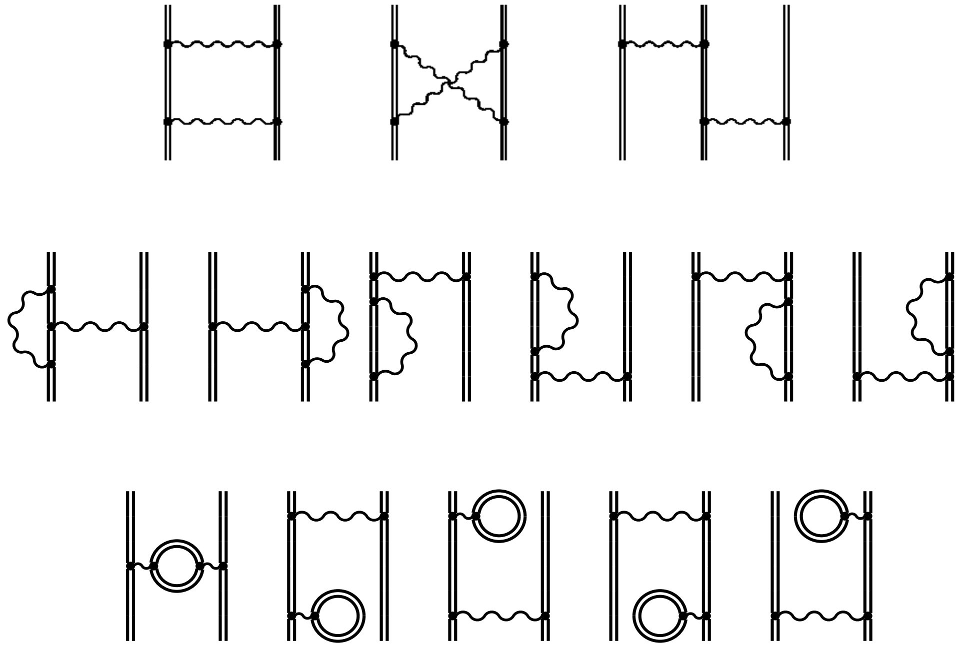


G. Soff and P.J. Mohr, PRA, 1988
N.L. Manakov et al., JETP, 1989



Binding energies in high-Z few-electron ions

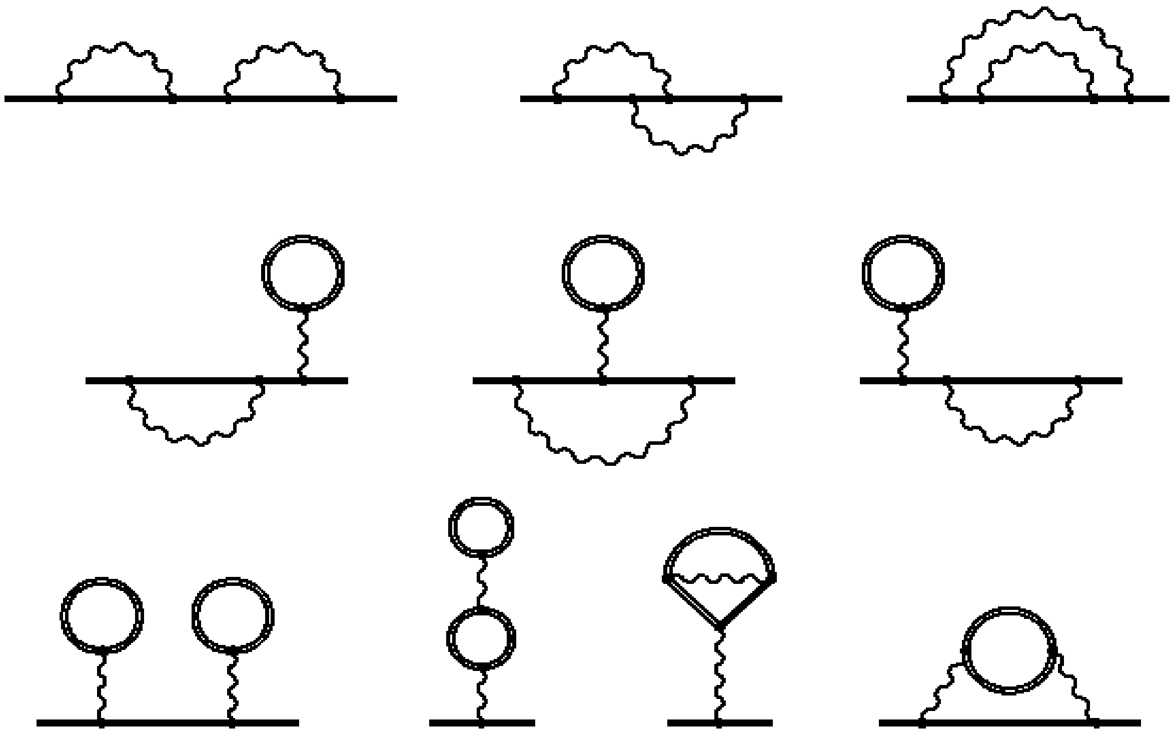
Two- and three-electron second-order QED corrections



Recent progress: Evaluation of all these diagrams for excited states in He-like ions *(A.N. Artemyev et. al., PRA, 2005)* and for B-like Ar *(A.N. Artemyev et al., PRL, 2007)*.

Binding energies in high-Z few-electron ions

One-electron second-order QED corrections



Recent progress: Evaluation of the two-loop self-energy diagrams
(V.A. Yerokhin, P. Indelicato, and V.M. Shabaev, PRL, 2006).

Binding energies in high-Z few-electron ions

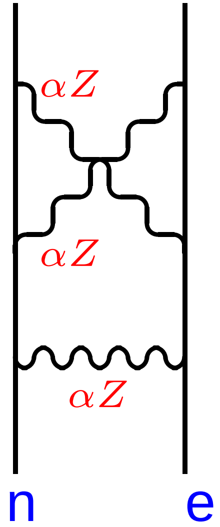
b) Conceptual problems

Nuclear recoil effect

Nonrelativistic theory: $m \to \mu = mM/(m+M)$.

Recoil effect in the full relativistic theory

A typical diagram:



Does a closed formula for the recoil correction to all orders in αZ exist?

Binding energies in high-Z few-electron ions

Formula for the nuclear recoil effect to first order in m/M and to all orders in αZ *(V.M. Shabaev, Theor. Math. Phys., 1985)*:

$$\Delta E = \Delta E_{\rm L} + \Delta E_{\rm H}$$

$$\Delta E_{\rm L} = \frac{1}{2M}\langle a|[\vec{p}^2 - (\vec{D}(0)\cdot\vec{p} + \vec{p}\cdot\vec{D}(0))]|a\rangle\,,$$

$$\Delta E_{\rm H} = \frac{i}{2\pi M}\int_{-\infty}^{\infty} d\omega\,\langle a|\Big(\vec{D}(\omega) - \frac{[\vec{p},V_{\rm C}]}{\omega+i0}\Big)G(\omega+E_a)\Big(\vec{D}(\omega) + \frac{[\vec{p},V_{\rm C}]}{\omega+i0}\Big)|a\rangle\,.$$

Here $\vec{p}$ is the momentum operator, $G(\omega)$ is the Coulomb Green function, $D_m(\omega) = -4\pi\alpha Z\alpha_l D_{lm}(\omega)$, and $D_{ik}(\omega,r)$ is the transverse part of the photon propagator in the Coulomb gauge.

Extention to many-electron atoms: *V.M. Shabaev, Sov. J. Nucl. Phys., 1988.*

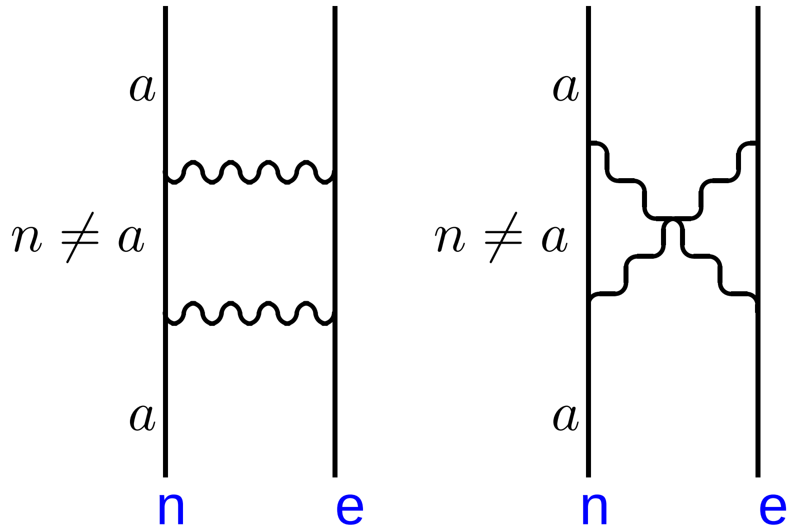
Numerical evaluation: *A.N. Artemyev, V.M. Shabaev, V.A. Yerokhin, PRA, 1995.*

Binding energies in high-Z few-electron ions

c) Physical problems

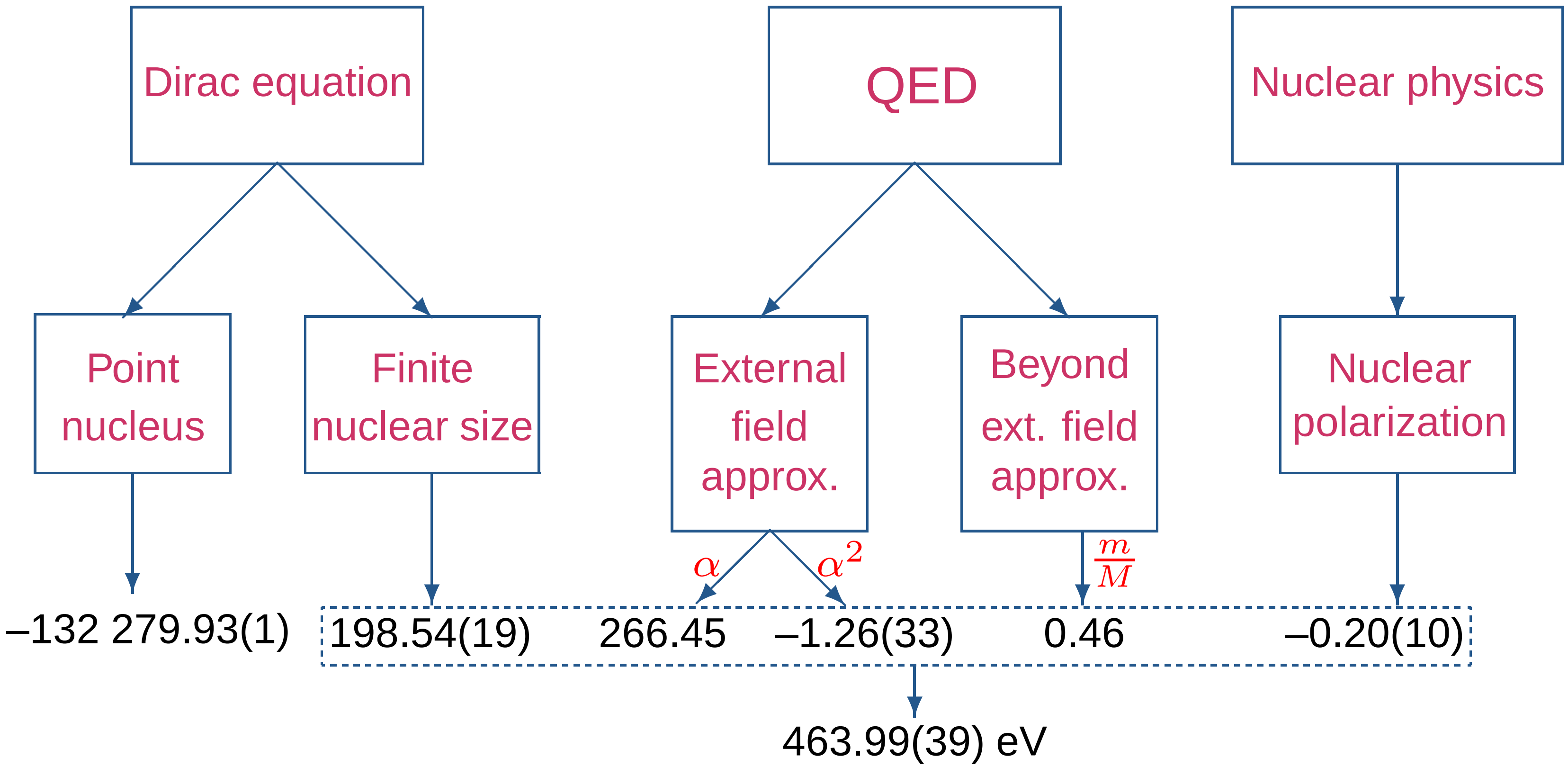
Nuclear polarization effect

The interaction between the electron and the nucleons causes the nucleus to make virtual transitions to excited states.



Evaluation: *G. Plunien and G. Soff, PRA, 1995;*
A.V. Nefiodov, L.N. Labzowsky, G. Plunien, and G. Soff, PLA, 1996.

1s Lamb shift in H-like uranium, in eV

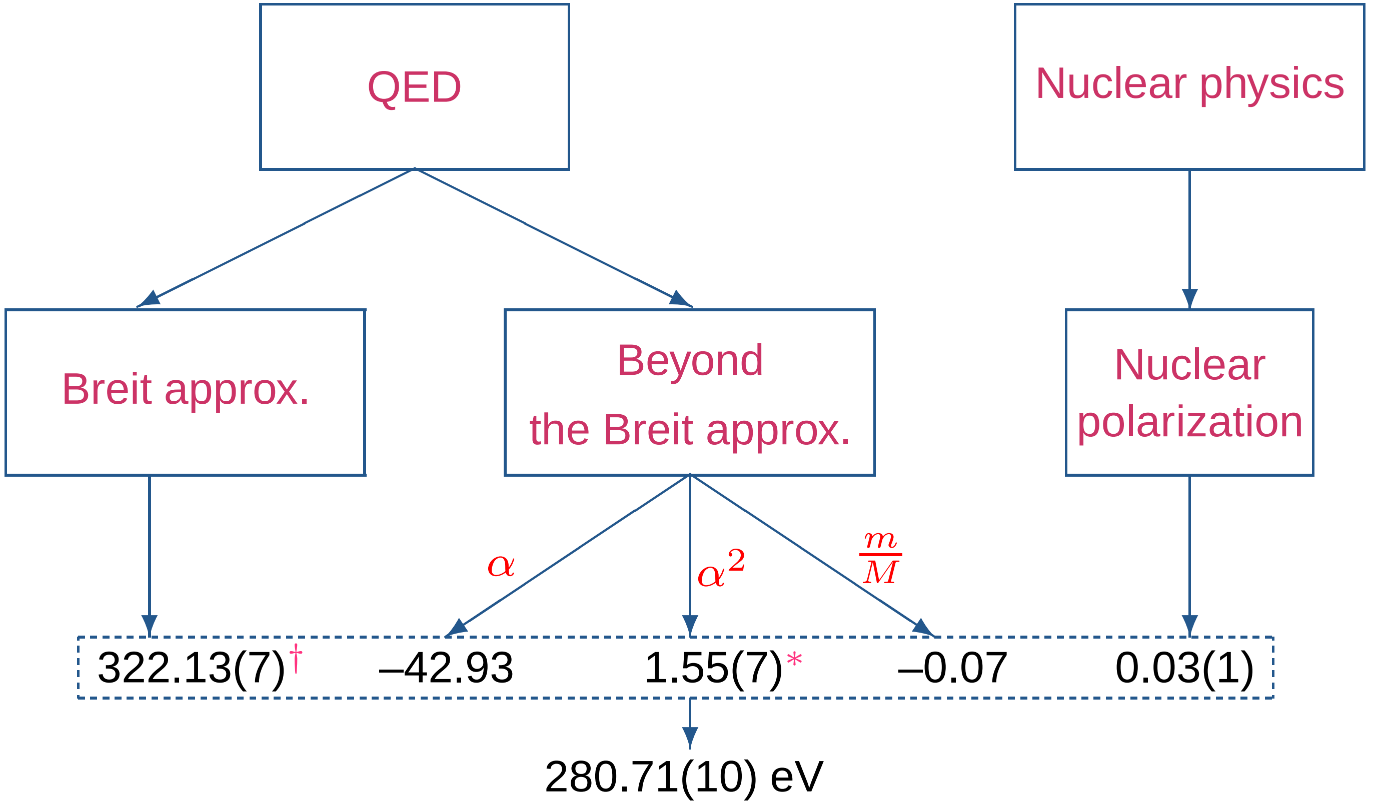


Experiment: 460.2(4.6) eV

(A. Gumberidze, T. Stöhlker, D. Banas et al., PRL, 2005)

Test of QED: $\sim$ 2%

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



Experiment: 280.645(15) eV (P. Beiersdorfer et al., PRL, 2005)

Test of QED: $\sim$ 0.2%

* *V.A. Yerokhin, P. Indelicato, and V.M. Shabaev, PRL, 2006*

† *Y.S. Kozhedub, O.V. Andreev, V.M. Shabaev et al., PRA, 2008*

Hyperfine splitting in H-like ions

Experiment

I. Klaft et al., PRL, 1994:

$^{209}\mathrm{Bi}^{82+}$	ΔE^{exp}=5.0840(8) eV

J. Crespo Lopez-Urritia et al., PRL, 1996; PRA, 1998:

$^{165}\mathrm{Ho}^{66+}$	ΔE^{exp}=2.1645(6) eV
$^{185}\mathrm{Re}^{74+}$	ΔE^{exp}=2.7190(18) eV
$^{187}\mathrm{Re}^{74+}$	ΔE^{exp}=2.7450(18) eV

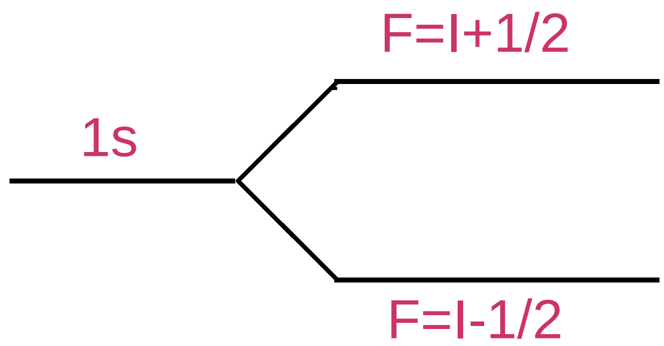
P. Seelig et al., PRL, 1998:

$^{207}\mathrm{Pb}^{81+}$	ΔE^{exp}=1.2159(2) eV

P. Beiersdorfer et al., PRA, 2001:

$^{203}\mathrm{Tl}^{80+}$	ΔE^{exp}=3.21351(25) eV
$^{205}\mathrm{Tl}^{80+}$	ΔE^{exp}=3.24410(29) eV

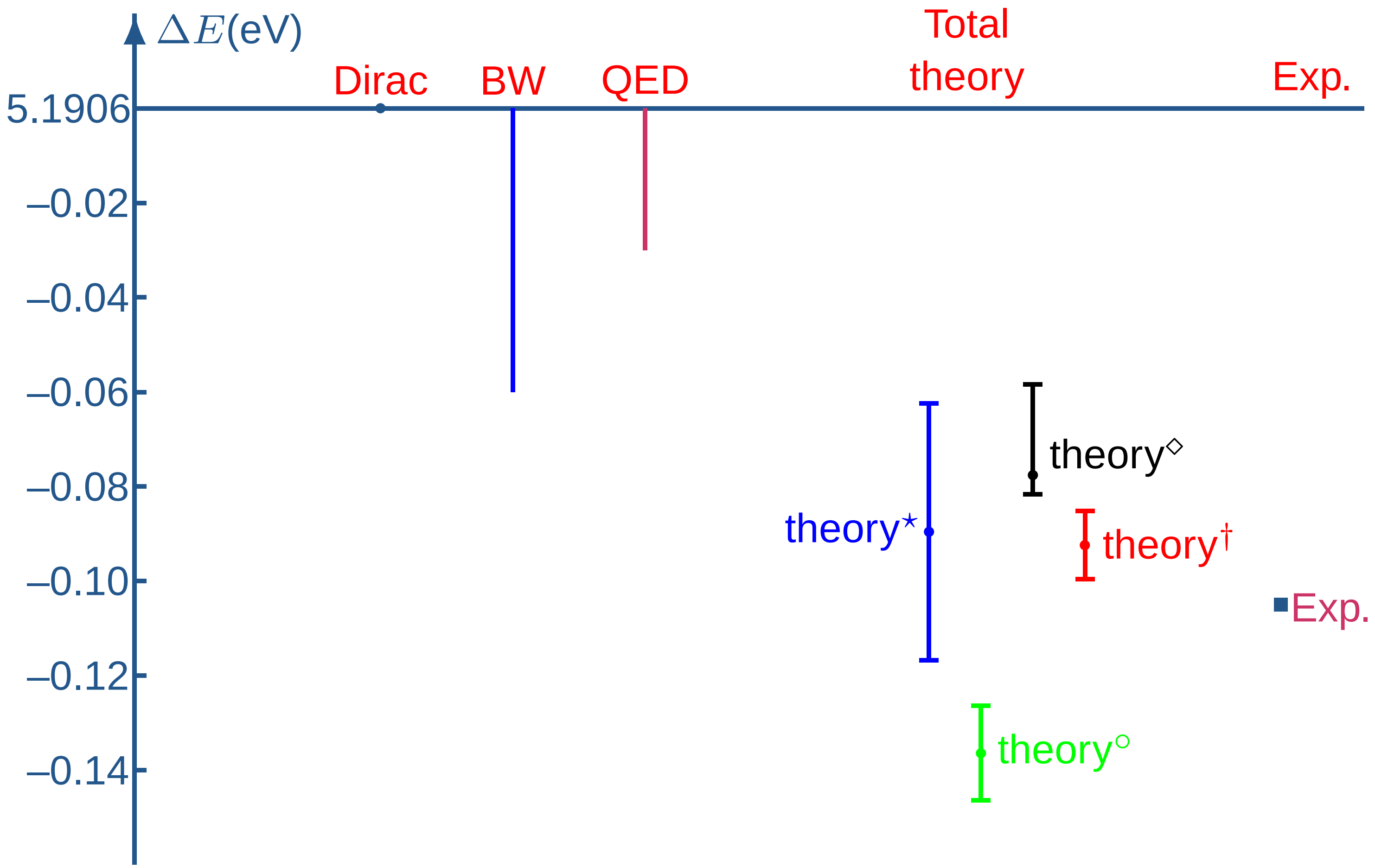
Hyperfine splitting in H-like ions



$$\Delta E = \Delta E_{\mathrm{Dirac}}(1-\varepsilon) + \Delta E_{\mathrm{QED}} \,,$$

where ε is the nuclear magnetization distribution correction
(the Bohr-Weisskopf effect)

Hyperfine splitting in H-like Bi



$^{\circ}$ M. Tomaselli et al., PRC, 1995

* V.M. Shabaev et al., PRA, 1997

$^{\diamond}$ R.A. Sen'kov and V.F. Dmitriev, Nuc. Phys. A, 2002

† A.A. Elizarov et al., NIMB, 2005

Exp.: I. Klaft et al., PRL, 1994

Tests of QED in HFS study

We consider *(V.M. Shabaev et al., PRL, 2001)*

$$\Delta' E = \Delta E^{(2s)} - \xi \Delta E^{(1s)},$$

$\Delta E^{(1s)}$ is the HFS in H-like ion and $\Delta E^{(2s)}$ is the HFS in Li-like ion. In the case of Bi, ξ = 0.16885.

Theoretical contributions to $\Delta' E$, in meV, for Bi

non-QED	-61.52(4)
QED	0.24(1)
Total	-61.27(4)
Experiment	?

This method has a potential to test QED on level of a few percent, provided the HFS is measured to accuracy $\sim 10^{-6}$.

g factor of H-like ions

Definition: $\Delta E = g\,(|e|\hbar/2m_e)BM_z\,.$

High-precision measurement of the g-factor of $^{12}\mathrm{C}^{5+}$ using a single ion confined in a Penning ion trap *(H. Häffner et al., PRL, 2000)*:

$$g_{\mathrm{exp}} = 2(\omega_L/\omega_c)(m_e/M)(q/|e|) = 2.001\,041\,596\,3\,(10)(44)\,.$$

Here $\omega_c = (q/M)B$ is the cyclotron frequency, $\omega_L = \Delta E/\hbar$, M is the ion mass, and q is the ion charge. The second uncertainty (44) is due to the uncertainty of the (m_e/M) ratio.

Theory, 2000:

$$g_{\mathrm{theo}} = 2.001\,041\,589\,8\,(38)(10)\,,$$

where the first entry (38) is due to the higher-order relativistic recoil effect and the second one (10) is due to the QED correction.

g factor of H-like ions

Formula for the nuclear recoil effect on the g-factor of an H-like ion to first order in m/M and to all orders in αZ *(V.M. Shabaev, PRA, 2001)*:

$$\Delta g = \frac{1}{\mu_0 m_a} \frac{i}{2\pi M} \int_{-\infty}^{\infty} d\omega \left[\frac{\partial}{\partial \mathcal{H}} \langle a | [\vec{p} - \vec{D}(\omega) + e\vec{A}_{\rm cl}] \times G(\omega + E_a) [\vec{p} - \vec{D}(\omega) + e\vec{A}_{\rm cl}] | a \rangle \right]_{\mathcal{H}=0} .$$

Here μ_0 is the Bohr magneton, m_a is the angular momentum projection, $\vec{A}_{\rm cl} = [\vec{\mathcal{H}} \times \vec{r}]/2$ is the vector potential of the homogeneous magnetic field $\vec{\mathcal{H}}$ directed along the z axis. It is implied that all quantities are calculated in the presence of the magnetic field.

Numerical evaluation: *V.M. Shabaev and V.A. Yerokhin, PRL, 2002.*

g factor of H-like ions

g factor of $^{12}\mathrm{C}^{5+}$

Dirac value (point nucleus)	1.998 721 354 39(1)
Free QED	0.002 319 304 37(1)
Binding QED [1]	0.000 000 843 40(3)
Recoil [2]	0.000 000 087 62
Nuclear size	0.000 000 000 41
Total theory	2.001 041 590 18(3)
Experiment [3]	2.001 041 596 3(10)(44)

[1] *K. Pachucki et al., PRA, 2005; V.A. Yerokhin et al., PRL, 2002.*

[2] *V.M. Shabaev, PRA, 2001; V.M. Shabaev and V.A. Yerokhin, PRL, 2002.*

[3] *H. Häffner et al., PRL, 2000.*

Determination of the electron mass: m_e=0.000 548 579 909 32(29) u.

g-factor of heavy ions: a new access to α

We consider a specific difference of the g-factors of B- and H-like lead *(V.M. Shabaev, D.A. Glazov, N.S. Oreshkina, A.V. Volotka et al., PRL, 2006)*:

$$g' = g^{[(1s)^2(2s)^2 2p_{1/2}]} - \xi g^{[1s]} \,,$$

where $\xi = 0.0097416$ is chosen to cancel the nuclear size effect.

The uncertainties of $g' \approx 0.585$ for Pb due to various effects:

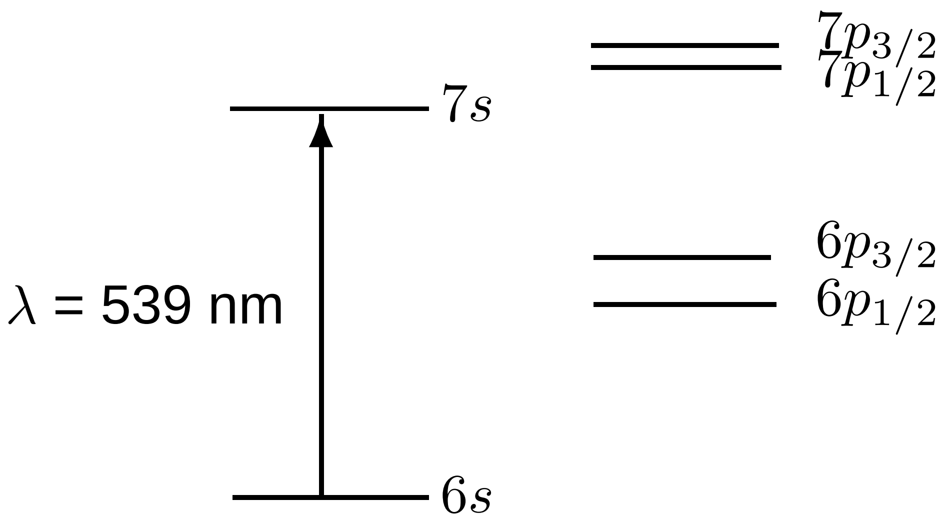
Effect	$\delta g'$	$\delta g'/g'$
$1/\alpha = 137.035999084(51)^{*}$	0.6×10^{-10}	1.0×10^{-10}
Nuc. polarization	0.6×10^{-10}	1.0×10^{-10}

* *D. Hanneke, S. Foqwell, G. Gabrielse, PRL, 2008*

This method can provide a determination of α to an accuracy which is comparable to that of the value recently obtained by G. Gabrielse et al.

PNC 6s-7s transition amplitude in neutral ^{133}Cs

Basic idea *(M.A. Bouchiat and C. Bouchiat, J. Phys. (Paris), 1974)*:



The nuclear spin-independent weak interaction:

$$H_W = -\frac{G_{\mathrm{F}}}{2\sqrt{2}} Q_W \rho_N(r) \gamma_5 \, .$$

Wave function: $\psi \to \psi + i\eta\psi'$.

Transition amplitude: $A \to A + i\eta A'$.

PNC 6s-7s transition amplitude in neutral ^{133}Cs

The most precise measurement of the ratio of the PNC amplitude to the Stark-induced amplitude β *(C.S. Wood et al., Science, 1997.)*:

$$\frac{\mathrm{Im}E1_{\mathrm{PNC}}}{\beta} = -1.5939(56)\frac{mV}{cm} \,.$$

Accurate measurement of β: *S.C. Bennett and C.E. Wieman, PRL, 1999.*

These experiments stimulated improvements of the theory:

Breit interaction: *A. Derevianko, PRL, 2000, M.G. Kozlov et al., PRL, 2001.*

New atomic structure calculations: *V.A. Dzuba et al., PRD, 2002.*

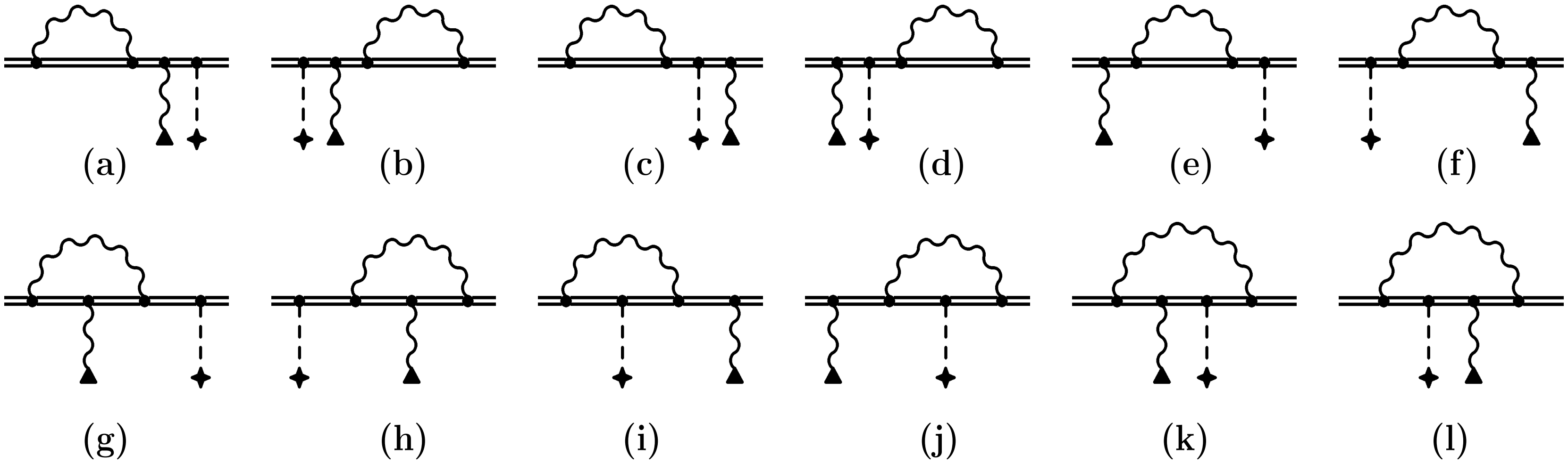
Vacuum polarization correction: *W.R. Johnson et al., PRL, 2002.*

Comparison of this theory with the experiment gave the weak charge of ^{133}Cs which deviated by 2σ from the SM prediction.

Calculations of the self-energy corrections to the $6s - 7s$ PNC transition ampitude became very urgent !

PNC 6s-7s transition amplitude in neutral ^{133}Cs

Self-energy corrections to the PNC 6s-7s transition amplitude



The wavy line terminated with a triangle indicates the absorbed photon. The dashed line terminated with a cross indicates the electron-nucleus weak interaction.

PNC 6s-7s transition amplitude in neutral ^{133}Cs

Self-energy corrections to the PNC 6s-7s amplitude in ^{133}Cs, in %.

(V.M. Shabaev, K. Pachucki, I.I. Tupitsyn, and V.A. Yerokhin, PRL, 2005)

Contribution	Length gauge	Velocity gauge
Diagrams “a-f”	3.78	2.80
Diagrams “g-h”	-2.71	-1.83
Diagrams “i-j”	-3.12	-2.24
Diagrams “k-l”	1.26	0.38
Non-diagr. term	0.00	0.10
Total SE	-0.79	-0.79
Binding SE	-0.67	-0.67

Total binding QED = Binding SE+VP = -0.67%+0.41% = -0.27(3)%

Previous results: -0.5(1)% *(M.Y. Kuchiev and V.V. Flambaum, JPB, 2003)*
-0.43(4)% *(A.I. Milstein et al., PRL, 2002)*

Semiempirical revision of the previous results: -0.32(3)%

(V.V. Flambaum and J.S.M. Ginges, PRA, 2005)

PNC 6s-7s transition amplitude in neutral ^{133}Cs

Comparing the total theoretical value for the PNC amplitude with the experiment yields:

$$Q_W = -72.65(29)_{\rm exp}(36)_{\rm th}$$

This value deviates by 1.1σ from the prediction of the Standard Model,

$$Q_W^{\rm SM} = -73.19(13)\,.$$

From strong to supercritical fields

Charge transfer in low-energy U^{92+} - U^{91+} collision

Head-on collision approximation:

$$i(\partial/\partial t)\,\psi(\mathbf{r},t)=\{\,\alpha\cdot\mathbf{p}+\beta m+U(r)+V(r_p(t)\}\,\psi(\mathbf{r},t),$$

where $r_p(t)$ is the electron-projectile distance,

$U(r)$ is the target potential, $V(r_p(t))$ is the projectile potential.

In cylindrical coordinates:

$$\psi(\rho,z,\varphi)=\begin{pmatrix} p_1(\rho,z)e^{i(\mu-1/2)\varphi} \\ p_2(\rho,z)e^{i(\mu+1/2)\varphi} \\ iq_1(\rho,z)e^{i(\mu-1/2)\varphi} \\ iq_2(\rho,z)e^{i(\mu+1/2)\varphi} \end{pmatrix}$$

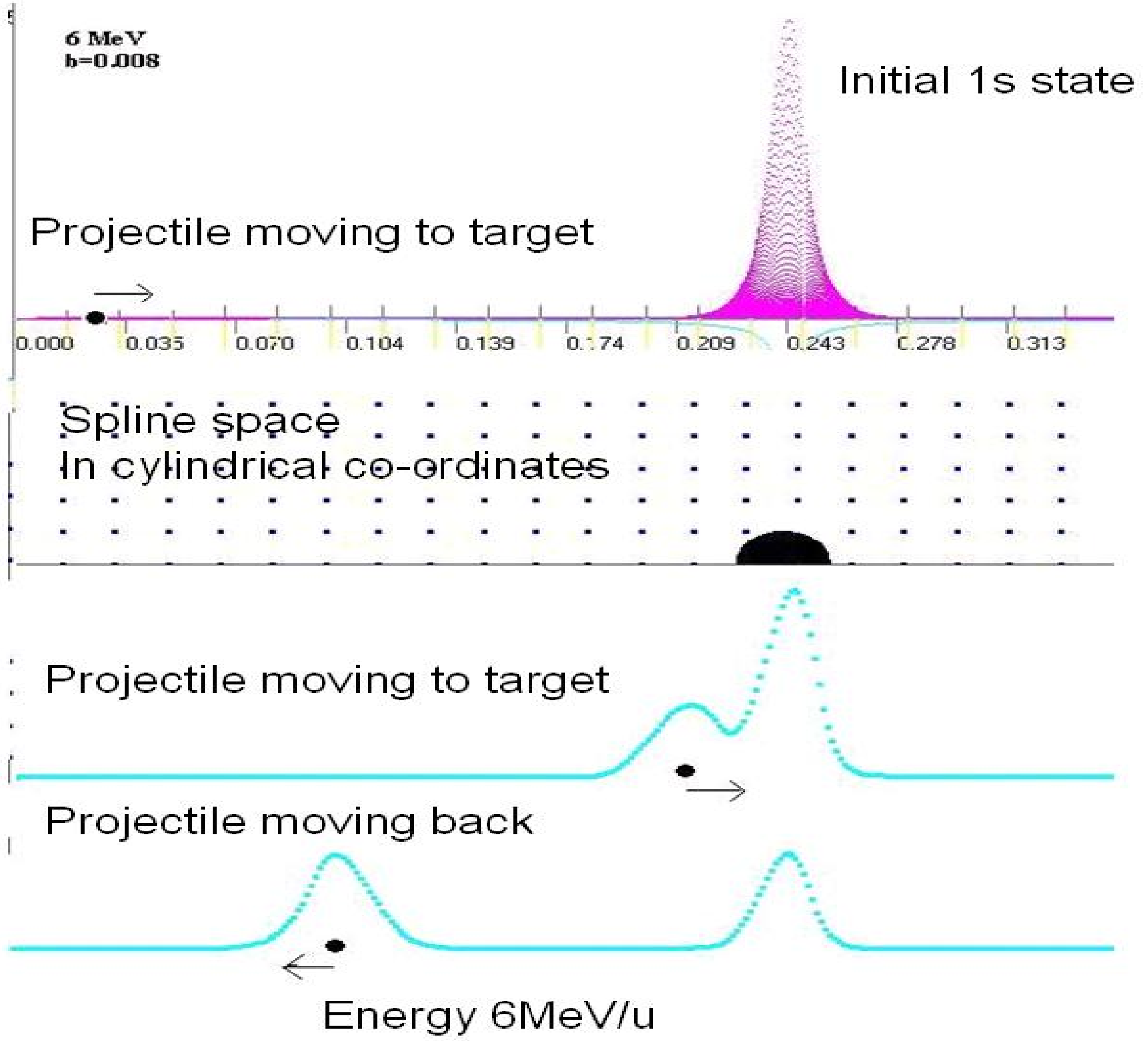
The calculations are performed using the B-spline basis set method.

From strong to supercritical fields

Head-on collision approximation for U^{92+} - U^{91+}

Probability P of the charge transfer at the impact parameter 0.008 a.u. (R(1s) U^{91+} =0.0135a.u.):

E_p =3MeV/u	P =0.22
E_p =4MeV/u	P =0.36
E_p =5MeV/u	P =0.24
E_p =6MeV/u	P =0.68



Collaborators

St.Petersburg

O.V. Andreev, A.N. Artemyev, G.B. Deyneka, A.A. Elizarov, D.A. Glazov, Y.S. Kozhedub, A.V. Maiorova, D.L. Moskovkin, N.S. Oreshkina, I.I. Tupitsyn, A.V. Volotka, V.A. Yerokhin, O.M. Zherebtsov

TU Dresden

G. Plunien, G. Soff

GSI, Darmstadt

H.-J. Kluge, C. Kozhuharov, W. Quint, T. Stöhlker

Laboratoire Kastler-Brossel, Paris

P. Indelicato

Warsaw University

K. Pachucki