QED calculations of highly charged ions and heavy atoms

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Outline of the talk

- Introduction
- Bound-state QED with heavy ions and atoms
- Parity nonconservation effects with heavy atoms and ions
- Low-energy heavy-ion collisions and supercritical fields
- Conclusion

Introduction

High-Z few-electron ions

$$N \ll Z\,,$$

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

To zeroth-order approximation:

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

Interelectronic-interaction and QED effects:

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

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

Introduction

Relativistic many-electron atoms and ions

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

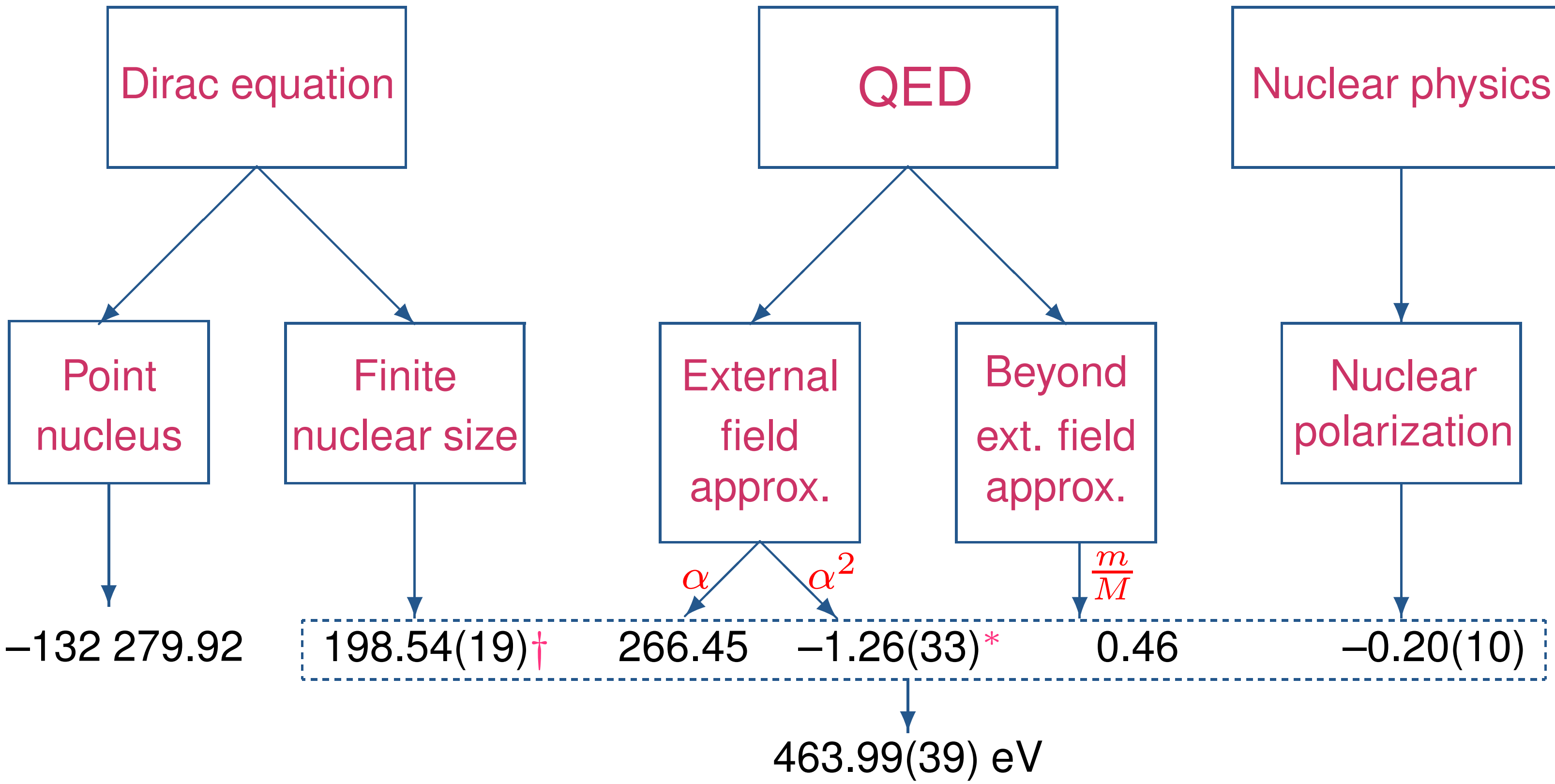
$$V_{\rm C} \to V_{\rm eff} = V_{\rm C} + V_{\rm scr} \,,$$

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

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

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

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



Experiment: 460.2(4.6) eV

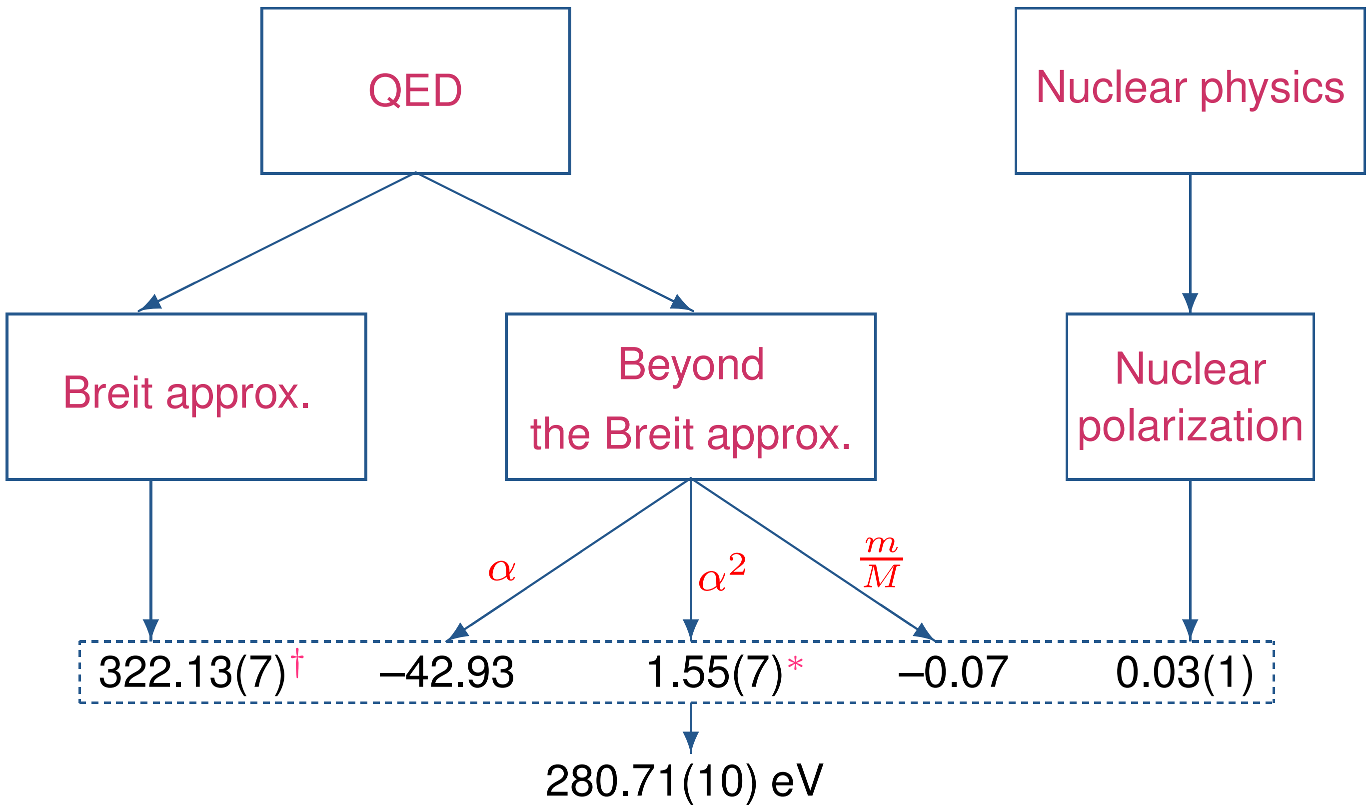
(A. Gumberidze, T. Stöhlker, D. Banas et al., PRL, 2005)

Test of QED: $\sim$ 2%

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

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

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



Experiment: 280.59(10) eV (J. Schweppe et al., PRL, 1991)
280.52(10) eV (C. Brandau et al., PRL, 2003)
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

$2p_{3/2} - 2p_{1/2}$ *transition energy in B-like uranium, in eV*

Contributions to the energy of the forbidden $2p_{3/2} - 2p_{1/2}$ transition in B-like uranium in different potentials:

Effective potential	$V_{\rm CH}$	$V_{\rm LDF}$	$V_{\rm PZ}$
Breit approximation	4085.4933	4085.4321	4085.4693
First-order QED	1.8786	1.8614	1.7259
Second-order QED	0.3505	0.3726	0.3780
Nucl. recoil	-0.0383	-0.0388	-0.0389
Total theory	4087.6841	4087.6273	4087.5342

Total theoretical value: 4087.59(41) eV *(A.N. Artemyev et al., PRA, 2013)*
Experiment: 4087.02(17) eV *(P. Beiersdorfer et al., PRA, 1998)*

Ionization energy in Be-like uranium, in eV

Contributions to the ground-state ionization energy in Be-like uranium in different potentials *(A.V. Malyshev et al., PRA, 2015)*:

Effective potential	V_{LDF3}	V_{PZ3}	V_{KS4}
Breit approximation	-32433.286	-32433.288	-32433.289
First-order QED	48.427	48.617	47.960
Second-order QED	-1.360	-1.554	-0.888
Nucl. recoil	0.113	0.113	0.113
Nucl. polarization	-0.036	-0.036	-0.036
Total theory	-32386.142	-32386.147	-32386.141

Total theoretical value: $-32386.14(20)$ eV

Lamb shift in many-electron atoms

Relativistic calculations of many-electron atoms are generally based on the Dirac-Coulomb-Breit Hamiltonian:

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

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

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

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

How can we incorporate the QED effects into these calculations?

Model Lamb-shift operator: *V.M. Shabaev, I.I. Tupitsyn, and V.A. Yerokhin, PRA, 2013; CPC, 2015.*

Model self-energy operator for a relativistic atom

The model self-energy operator is given by

$$\begin{aligned} h^{\rm SE} &= V^{\rm SE}_{\rm loc} + \frac{1}{4}\sum_{i,k}\sum_{j,l}(I-(-1)^{s_i}\beta)\rho_{l_i}(r)|\psi_i\rangle \\ &\quad \times((D^t)^{-1})_{ij}\langle\psi_j|\big[\frac{1}{2}(\Sigma(\varepsilon_j)+\Sigma(\varepsilon_l))-V^{\rm SE}_{\rm loc}\big]|\psi_l\rangle \\ &\quad \times(D^{-1})_{lk}\langle\psi_k|\rho_{l_k}(r)(I-(-1)^{s_k}\beta), \end{aligned}$$

where ψ_i are the H-like wave functions and the summations run over ns states with the principal quantum number $n \le 3$ and over $np_{1/2}$, $np_{3/2}$, $nd_{3/2}$, and $nd_{5/2}$ states with $n \le 4$,

$$\begin{aligned} \rho_{l_i}(r) &= \exp\left(-2\alpha Z(r/\lambda_{\rm C})/(1+l_i)\right), \\ D_{ik} &= \frac{1}{2}\langle\psi_i|(I-(-1)^{s_i}\beta)\rho_{l_i}(r)|\psi_k\rangle, \end{aligned}$$

and $s_i = n_i - l_i$.

Self energy in Cu-like ions

Self-energy contribution to the transition energies in Cu-like ions, in eV.

Ion	Transition	Model SE operator	Exact[a]
Yb^{41+}	$4s - 4p_{1/2}$	-1.29	-1.28
	$4s - 4p_{3/2}$	-1.21	-1.21
	$4p_{1/2} - 4d_{3/2}$	-0.10	-0.11
	$4p_{3/2} - 4d_{3/2}$	-0.18	-0.18
	$4p_{3/2} - 4d_{5/2}$	-0.14	-0.14
U^{63+}	$4s - 4p_{1/2}$	-4.24	-4.24
	$4s - 4p_{3/2}$	-4.32	-4.33
	$4p_{1/2} - 4d_{3/2}$	-0.87	-0.88
	$4p_{3/2} - 4d_{3/2}$	-0.79	-0.79
	$4p_{3/2} - 4d_{5/2}$	-0.63	-0.65

[a] *J. Sapirstein and K.T. Cheng, PRA, 2002.*

Isotope shifts with highly charged ions

Measurements of the isotope energy shifts have been performed for few-electron uranium ions *(S. R. Elliott et al., PRC, 1998)*, for Cu-like lead *(R. Schuch et al., PRL, 2005)*, B-like argon *(R. Soria Orts et al., PRL, 2006)*, and Li-like neodymium *(C. Brandau et al., PRL, 2008)*.

The experiment with Li-like Nd provided high-precision determination of the nuclear charge radius difference. The corresponding experiments can be also performed for radioactive isotopes with a lifetime longer than about 10 s *(C. Brandau et al., Hyp. Int., 2010)*.

With the FAIR facilities the measurements of the isotope energy shifts in highly charged ions will be improved in accuracy by an order of magnitude. From the theoretical side, the most precise calculations have been performed in *(N.A. Zubova et al., PRA, 2014; PRA, 2016)*.

Isotope shift in Li-like neodymium

Individual contributions to the isotope shifts for the $2p_{1/2} - 2s$ and $2p_{3/2} - 2s$ transitions in Li-like neodymium, $^{150,142}\mathrm{Nd}^{57+}$, (in meV) with $^{150,142}\delta\langle r^2\rangle = 1.36\,\mathrm{fm}^2$ *(N.A. Zubova et al., PRA, 2014)*.

Contribution	$2\mathrm{p}_{1/2} - 2\mathrm{s}$	$2\mathrm{p}_{3/2} - 2\mathrm{s}$
Field shift: non-QED	-42.57	-44.05
Mass shift: non-QED	1.30	1.50
Field shift: QED	0.22	0.24
Mass shift: QED	0.33	0.30
Nuclear polarization	0.36	0.33
Nuclear deformation	0.27	0.28
Total theory	$-40.1(2)$	$-41.4(2)$
Experiment *(C. Brandau et al., PRL, 2008)*	$-40.2(3)(6)$	$-42.3(12)(20)$

QED recoil effect in hydrogen

The nuclear recoil effect in H-like atom beyond the Breit approximation can be written as

$$\Delta E = \frac{m^2}{M}\frac{(\alpha Z)^5}{n^3}P(\alpha Z),$$

where

$$P(\alpha Z) = \ln(\alpha Z)^{-2}D_{51} + D_{50} + (\alpha Z)D_{60} + (\alpha Z)^2 G_{\rm rec}(\alpha Z).$$

The function $G_{\rm rec}(\alpha Z)$ includes all higher-order correction and can be fitted as

$$G_{\rm rec}(\alpha Z) = \ln^2(\alpha Z)^{-2}D_{72} + \ln(\alpha Z)^{-2}D_{71} + D_{70} + \ldots.$$

QED recoil effect in hydrogen

The numerical calculation of $G_{\rm rec}(\alpha Z)$ for the 1s state of hydrogen ($Z = 1$) *(V.M. Shabaev et al., JPB, 1998)*:

$$G_{\rm rec}(\alpha Z) = 9.7(6)\,, \qquad Z = 1.$$

The analytical calculations of the $\ln^2(\alpha Z)^{-2} D_{72}$ term, which should yield the leading contribution to $G_{\rm rec}(\alpha Z)$, *(K. Pachucki and S. G. Karshenboim, PRA, 1999; K. Melnikov and A. S. Yelkhovsky, PLB, 1999)*:

$$\ln^2(\alpha Z)^{-2} D_{72} = -17.75\,, \qquad Z = 1.$$

Who is right?

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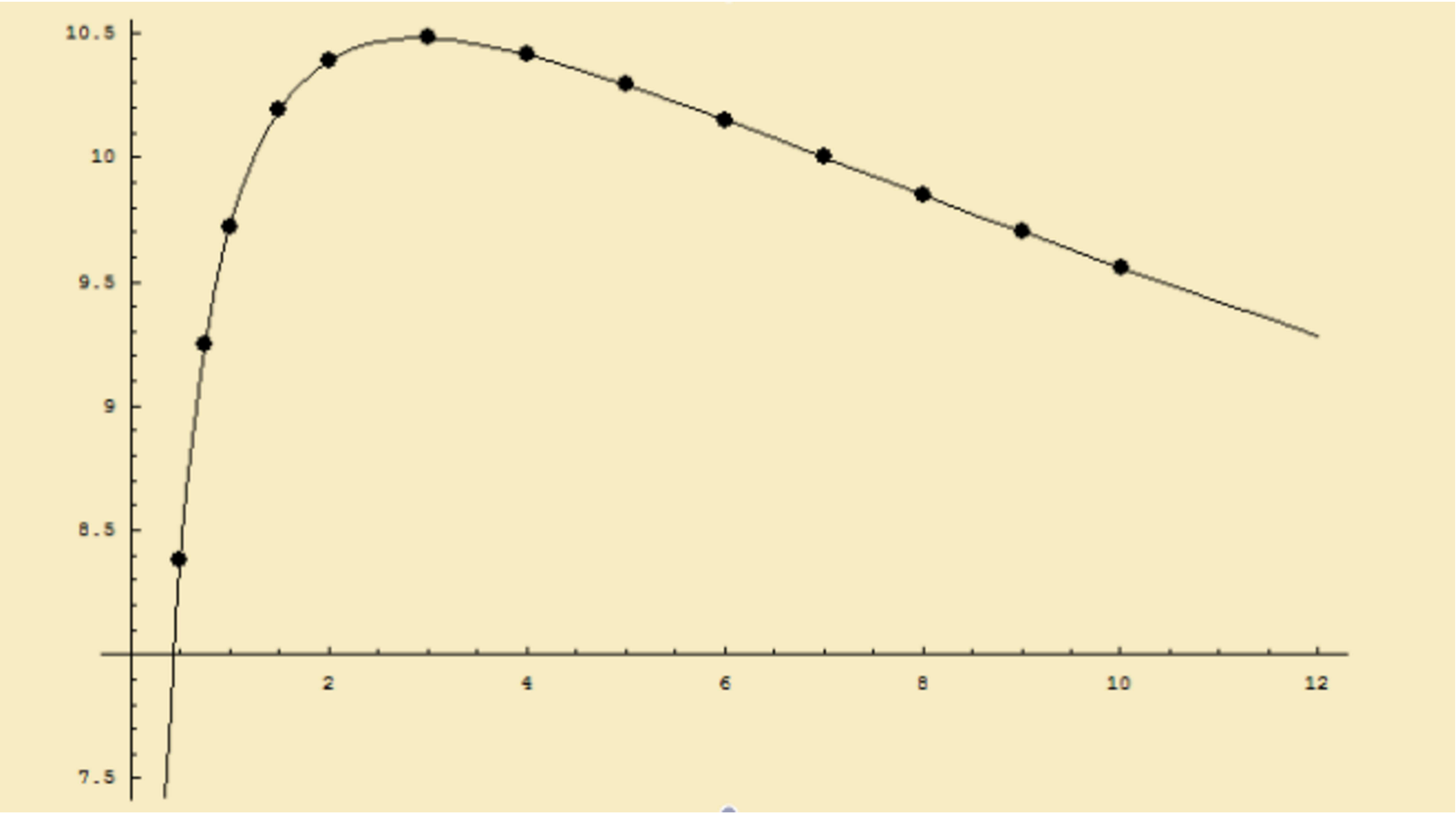
Who is right?

Recent numerical calculation *(V.A. Yerokhin and V.M. Shabaev, PRL, 2015)*:

$$G_{\rm rec}(\alpha Z) = 9.720(3)\,, \quad Z = 1.$$

QED recoil effect in hydrogen

The numerical calculation of the function $G_{\rm rec}(\alpha Z)$ for the 1s state *(V.A. Yerokhin and V.M. Shabaev, PRL, 2015)*:



Hyperfine splitting in H-like ions

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:

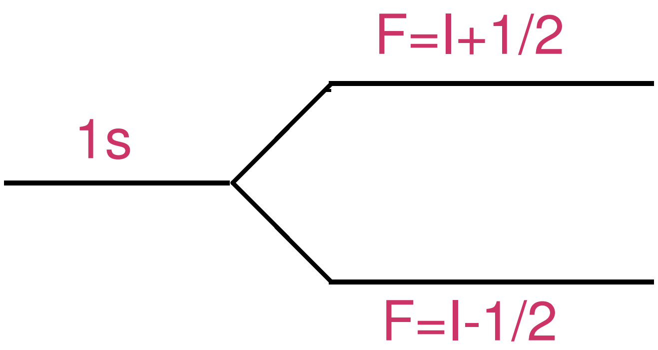
$^{203}\mathrm{Tl}^{80+}$ ΔE^{exp}=3.21351(25) eV

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

J. Ullmann et al., JPB, 2015:

$^{209}\mathrm{Bi}^{82+}$ ΔE^{exp}=5.08505(8) eV

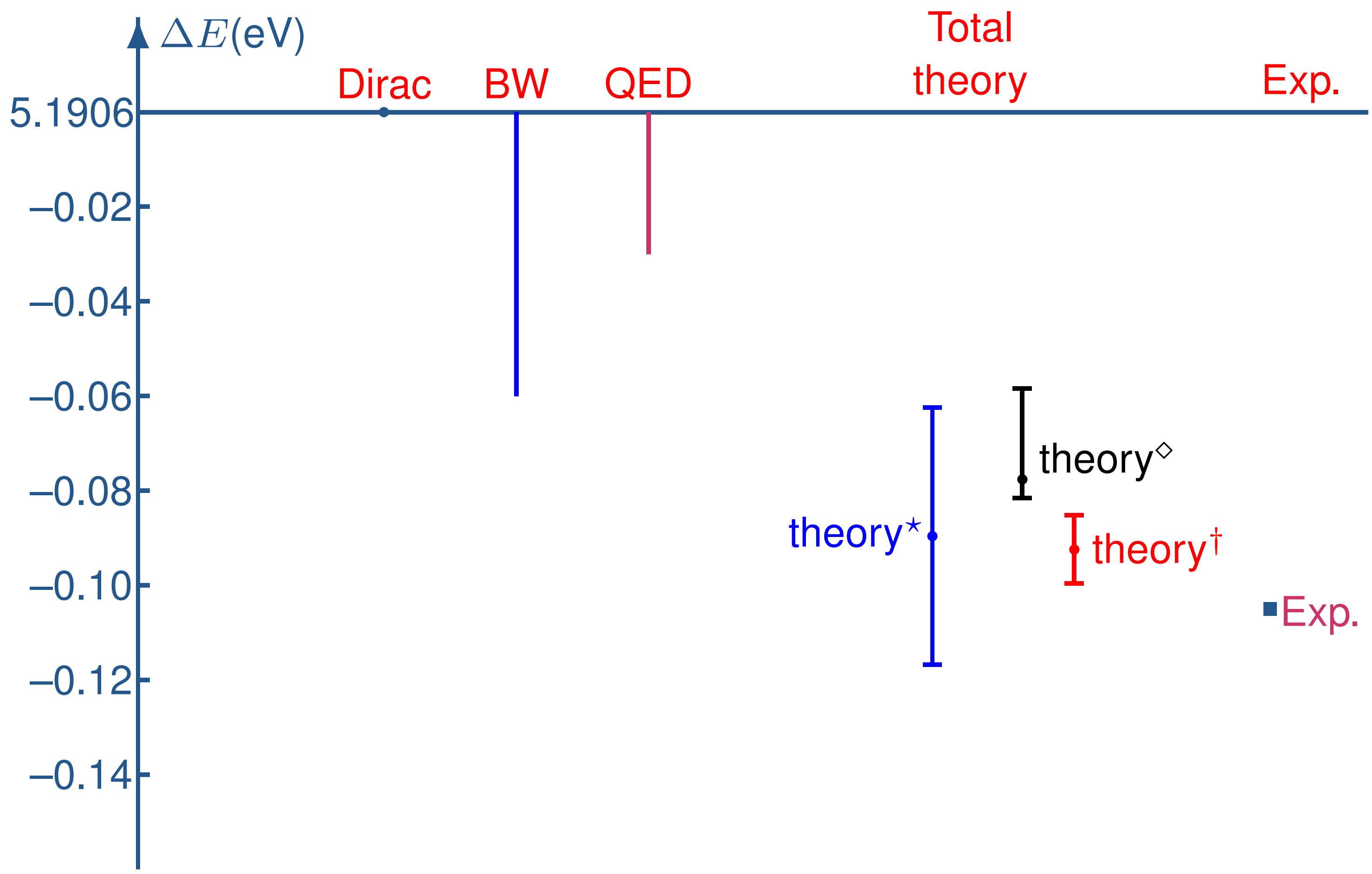
Hyperfine splitting in H-like ions



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

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

Hyperfine splitting in H-like Bi



⋆ V.M. Shabaev et al., PRA, 1997

◇ 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, A.N. Artemyev, V.A. Yerokhin, O.M. Zherebtsov, and G. Soff, PRL, 2001)*

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

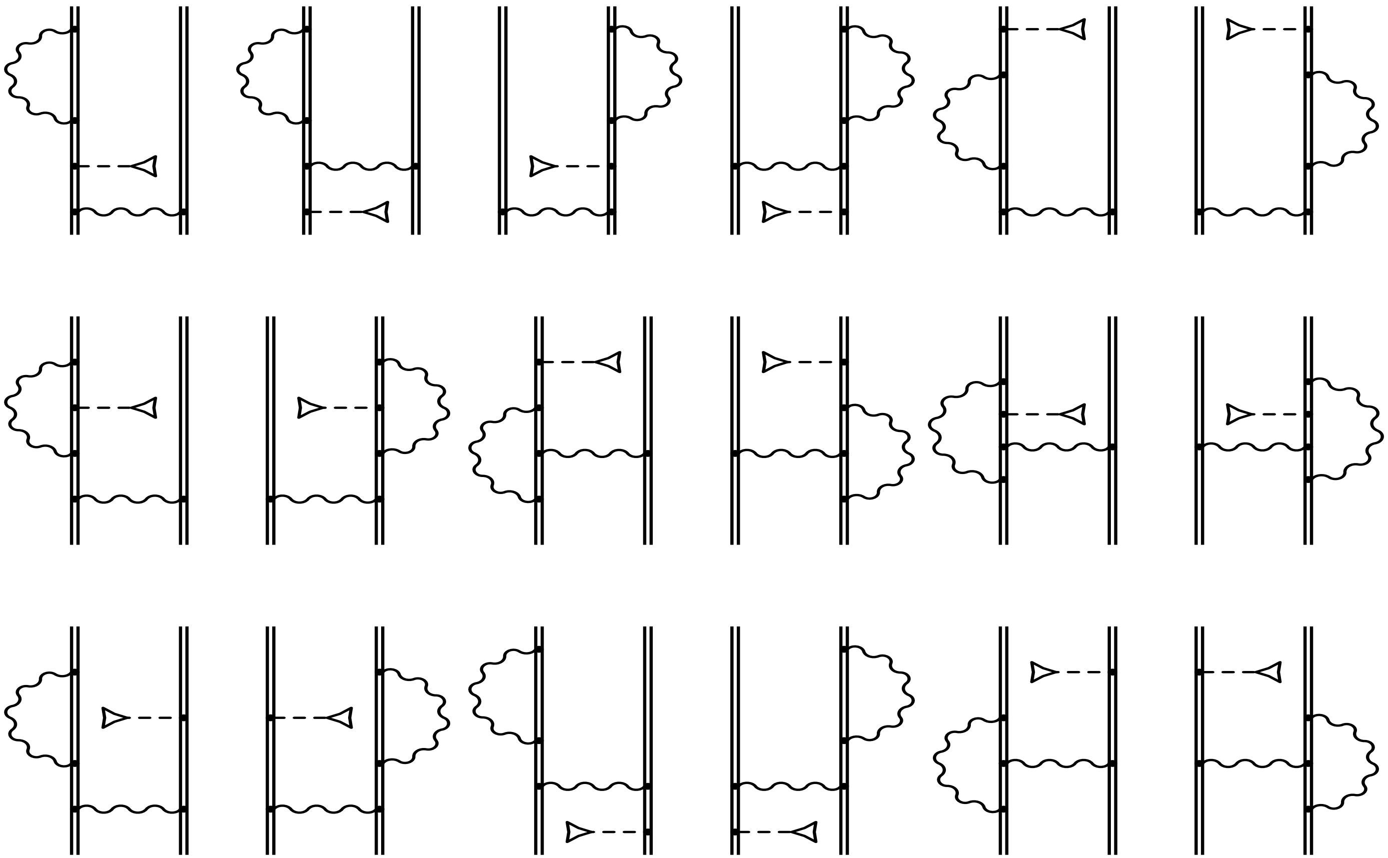
where $\Delta E^{(1s)}$ is the HFS in H-like ion, $\Delta E^{(2s)}$ is the HFS in Li-like ion, and ξ is chosen to cancel the Bohr-Weisskopf effect. In the case of Bi, ξ = 0.16886.

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

Calculations of the screened QED and higher-order interelectronic-interaction corrections to the HFS in Li-like ions are needed.

Recent progress on the QED calculations of the HFS

Screened self-energy corrections to the HFS in Li-like ions

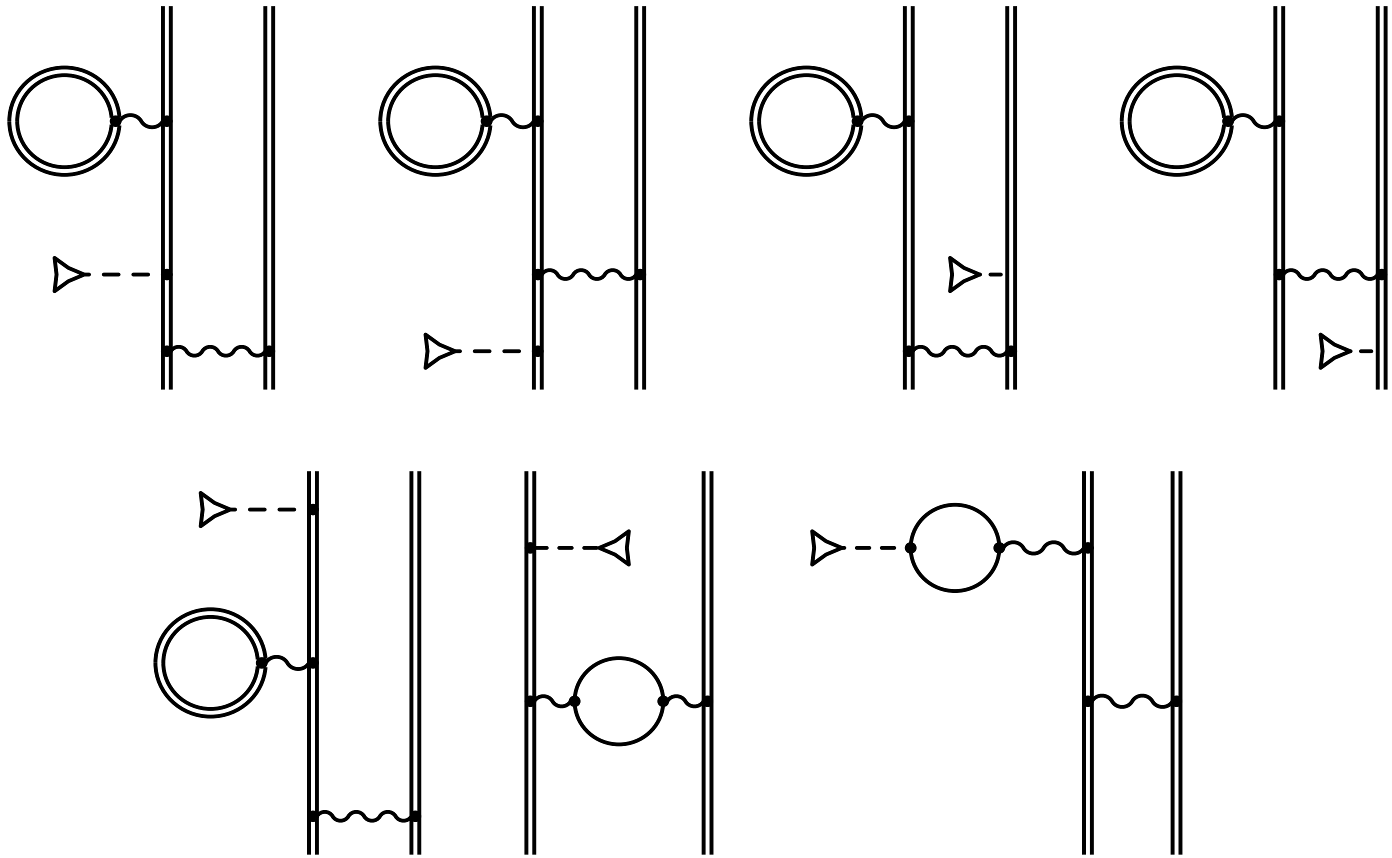


36 diagrams

A.V. Volotka et al., PRL, 2009; D.A. Glazov et al., PRA, 2010.

Recent progress on the QED calculations of the HFS

Screened vacuum-polarization corrections to the HFS in Li-like ions

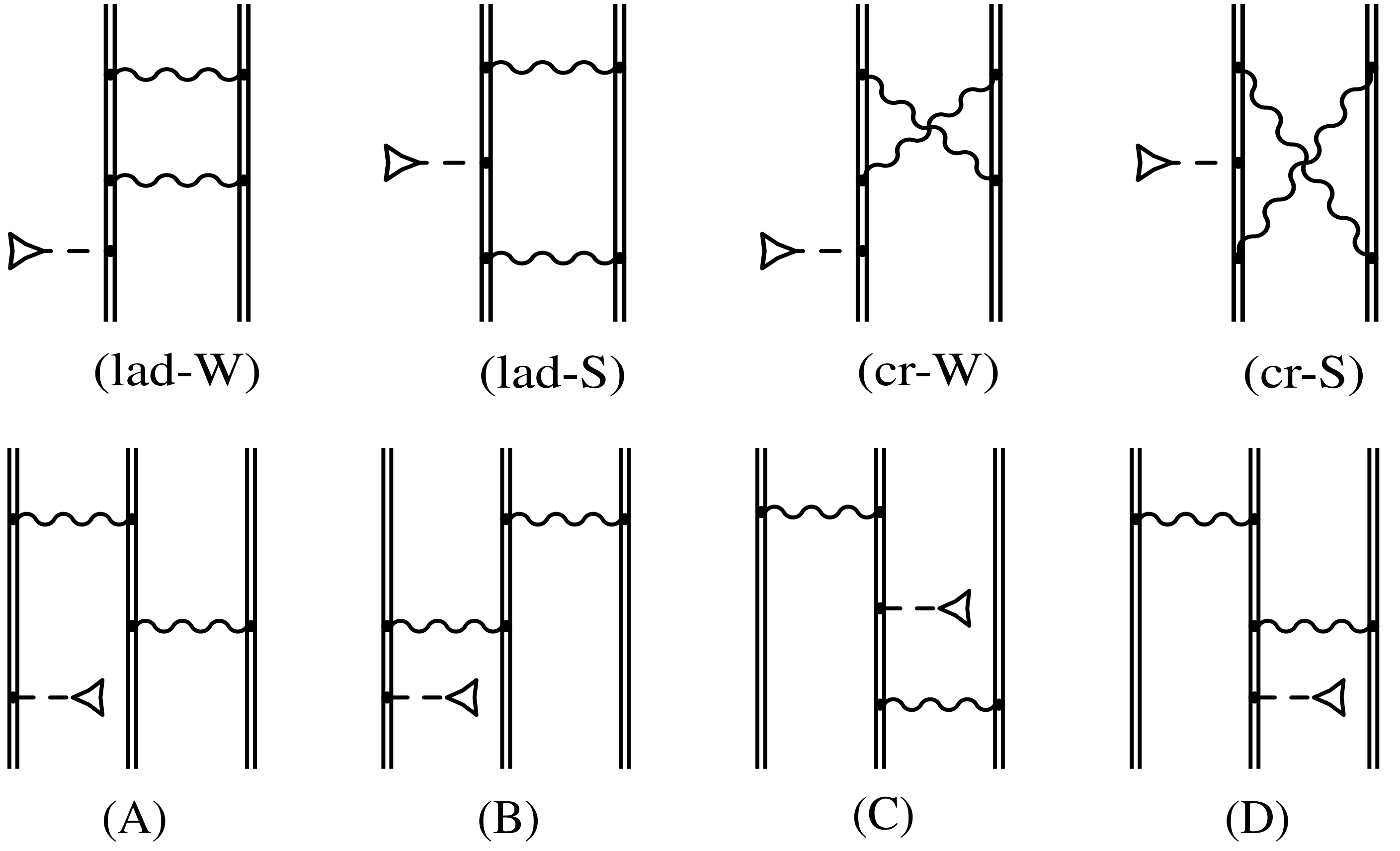


28 diagrams

O.V. Andreev et al., PRA, 2012.

Recent progress on the QED calculations of the HFS

Two-photon exchange corrections to the HFS in Li-like ions



A.V. Volotka et al., PRL, 2012.

Current value for the specific HFS difference in Bi

Theoretical contributions to $\Delta' E = \Delta E^{(2s)} - \xi \Delta E^{(1s)}$ (in meV)
for $\mu/\mu_N = 4.1106(2)$

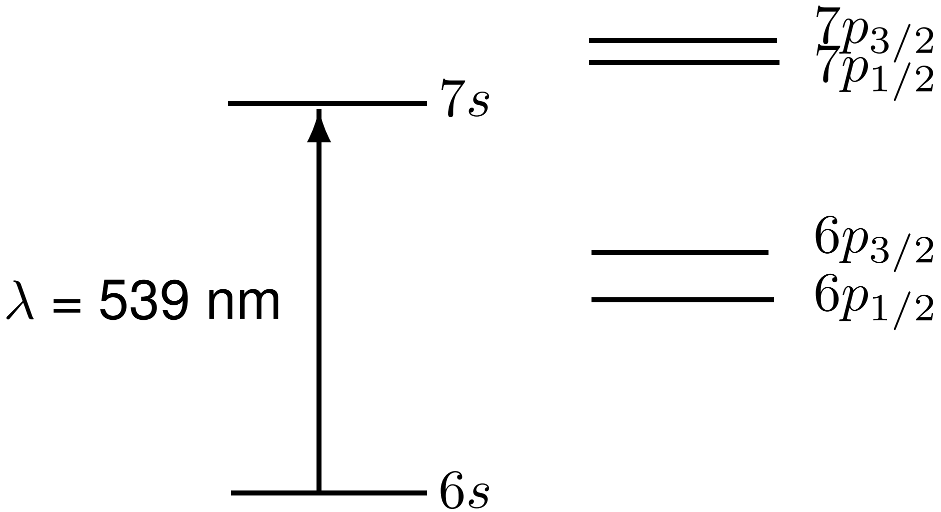
(A.V. Volotka et al., PRL, 2012; O.V. Andreev et al., PRA, 2012)

Dirac value	-31.809
Interel. inter., $\sim 1/Z$	-29.995
Interel. inter., $\sim 1/Z^2$ and h.o.	0.255(3)
One-electron QED	0.036
Screened QED	0.193(2)
Total	-61.320(6)
Experiment [1]	-61.012 (5)(21)

[1] *J. Ullmann et al., Nature Communications, 2017*

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

Most precise experiment: *C.S. Wood et al., Science, 1997; S.C. Bennett and C.E. Wieman, PRL, 1999.*

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

These experiments stimulated improvements of the theory by evaluations of the Breit and QED corrections and by new calculations of the electron-correlation contribution. As the result, comparing the total theoretical value for the PNC amplitude with the experiment yielded *(V.M. Shabaev, K. Pachucki, I.I. Tupitsyn and V.A. Yerokhin, PRL, 2005)*:

$$Q_W = -72.57(29)_{\rm exp}(36)_{\rm th}$$

that was in a reasonable agreement with the prediction of the Standard Model (2005):

$$Q_W^{\rm SM} = -73.16(3) \, .$$

Later, a new calculation of the electron-correlation contribution *(S.G. Porsev, K. Beloy, and A. Derevianko, PRL, 2009)* gave

$$Q_W = -73.16(29)_{\rm exp}(20)_{\rm th}$$

that was in the perfect agreement with the SM prediction. However, a revision of this calculation *(V.A. Dzuba et al., PRL, 2012)* resulted in

$$Q_W = -72.58(29)_{\rm exp}(32)_{\rm th} \, .$$

Parity nonconservation effects with heavy ions

Recent studies:

PNC effect with laser-induced $2^3S_1 - 2^1S_0$ transition in He-like Gd (*V.M. Shabaev et al., PRA, 2010*): $\sigma = (1 \pm \varepsilon_{\rm PNC})\sigma_0\,.$

$$\sigma_0 = 4086.3 \ {\rm barn}\,,\, \varepsilon_{\rm PNC} = -0.05\%\,.$$

Photon-photon polarization correlations as a tool for studying PNC in He-like uranium (*F. Fratini et al., PRA, 2011*)

Hyperfine transitions in He-like ions as a tool for nuclear-spin-dependent PNC studies (*F. Ferro et al., PRA, 2011*)

PNC effects on the radiative recombination of heavy H-like ions (*J. Gunst et al., PRA, 2013*)

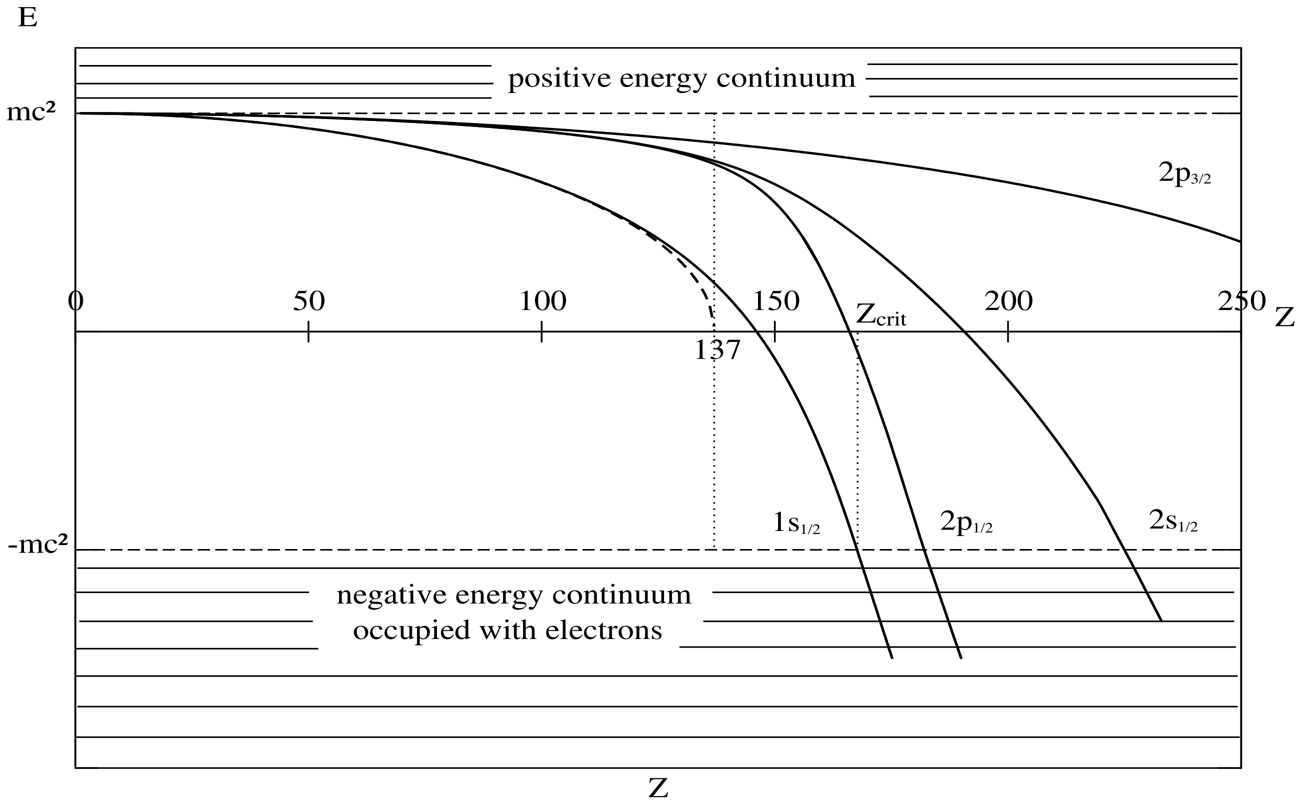
PNC effect in the dielectronic recombination of polarized electrons with heavy He-like ions (*V.A. Zaytsev et al., PRA, 2014*)

PNC effect in the resonance elastic electron scattering on heavy He-like ions (*V. A. Zaytsev et al., JPB, 2015*)

Low-energy heavy-ion collisions

Access to supercritical fields

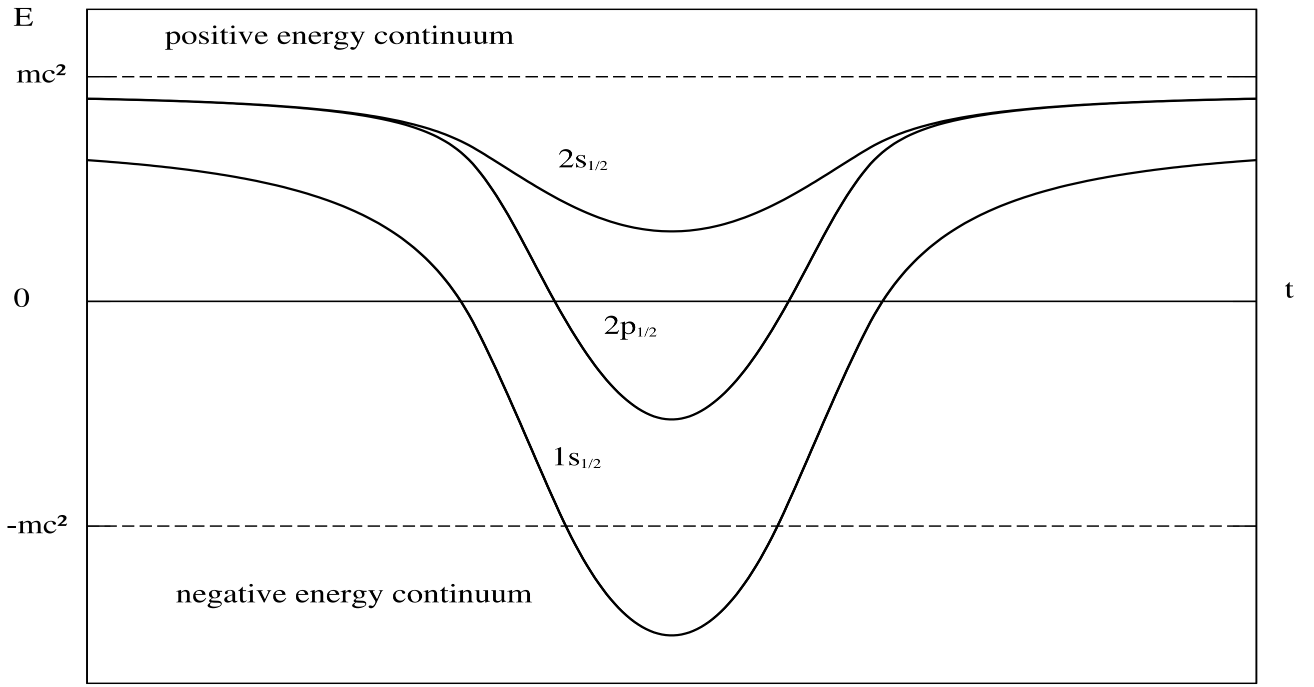
S.S. Gershtein, Ya.B. Zel'dovich, 1969; W. Pieper, W. Greiner, 1969



The $1s$ level dives into the negative-energy continuum at $Z_{\rm crit} \approx 173$.

Low-energy heavy-ion collisions

Creation of the supercritical field in heavy-ion collisions, with $Z_1 + Z_2 > 173$



The ground state dives into the negative-energy continuum for about 10^{-21} sec.

Low-energy heavy-ion collisions

New method for solving the time-dependent two-center Dirac equation (*I.I. Tupitsyn, Y.S. Kozhedub, V.M. Shabaev et al., PRA, 2010*):

$$i\frac{\partial\Psi(\vec{r},t)}{\partial t} = c(\vec{\alpha}\cdot\vec{p}) + \beta\, mc^2 + V^{(A)}_{\rm nucl}(\vec{r}_A) + V^{(B)}_{\rm nucl}(\vec{r}_B)\,,$$

where $\vec{r}_A = \vec{r} - \vec{R}_A$, $\vec{r}_B = \vec{r} - \vec{R}_B$.

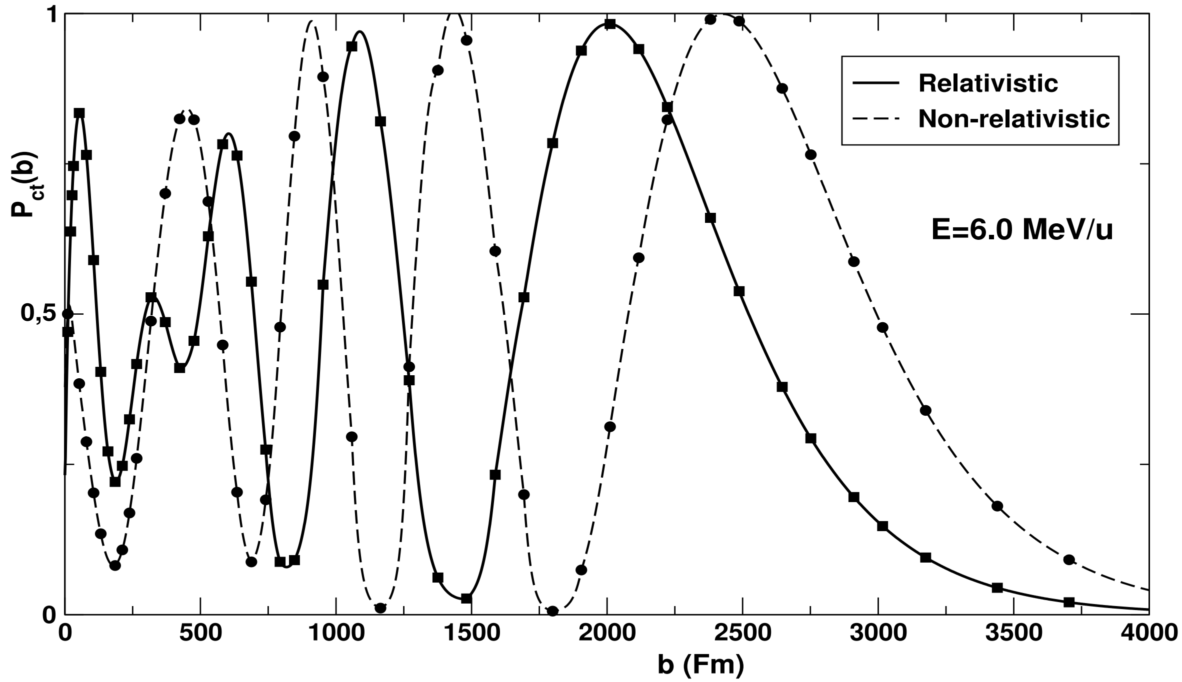
The time-dependent Dirac wave function is presented as a sum of atomic-like Dirac-Sturm orbitals localized at the ions.

The method has been tested by calculation of the charge-transfer and ionization probabilities for low-Z systems and comparison with the related nonrelativistic results.

Extention of the method to collisions of neutral atoms with H-like ions and comparison with related experiments: *I.I. Tupitsyn et al., PRA, 2012*.

Low-energy heavy-ion collisions

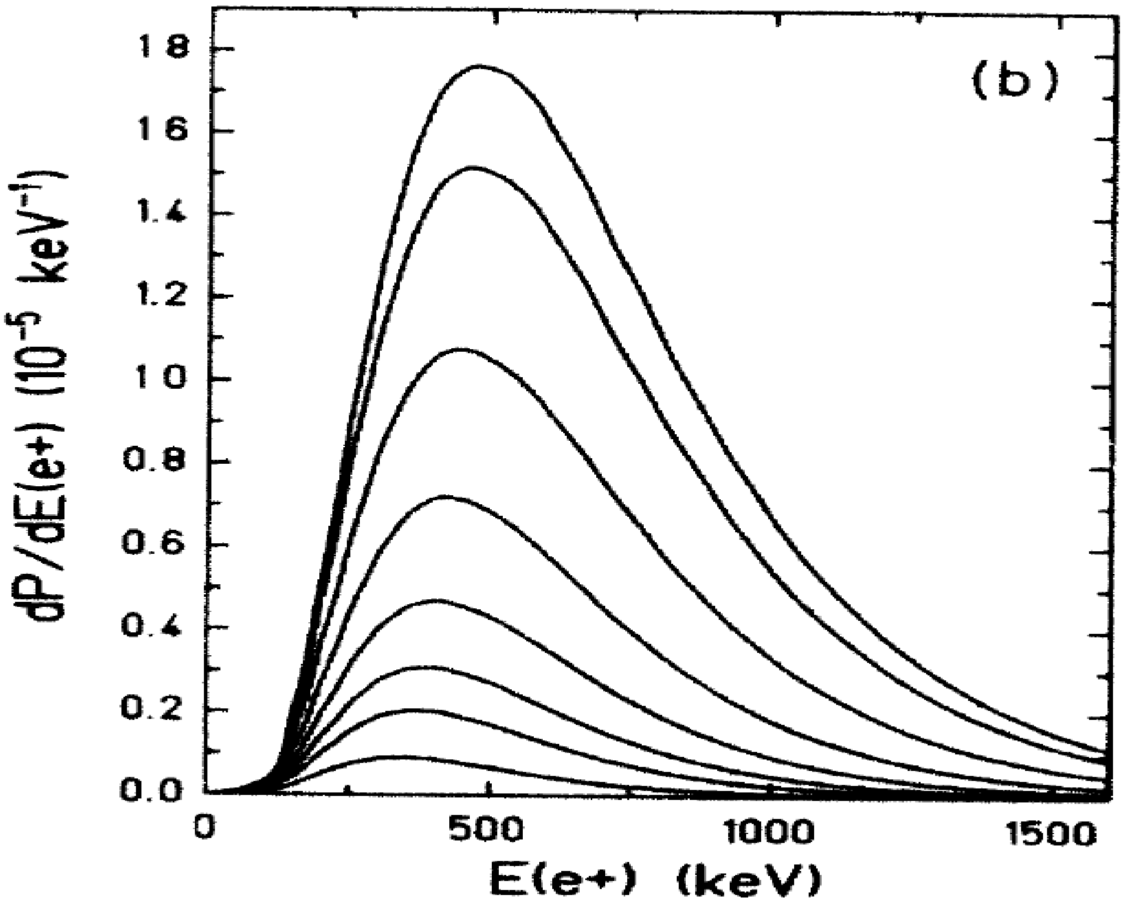
Charge-transfer probability for the $U^{91+}(1s)-U^{92+}$ collision



Charge-transfer probability as a function of the impact parameter b for the projectile energy of 6 MeV/u *(I.I. Tupitsyn et al., PRA, 2012)*. The same results are obtained by a different method *(I.A. Maltsev et al., Phys. Scr., 2013)*.

Low-energy heavy-ion collisions

Electron-positron pair production in low-energy U-U collisions

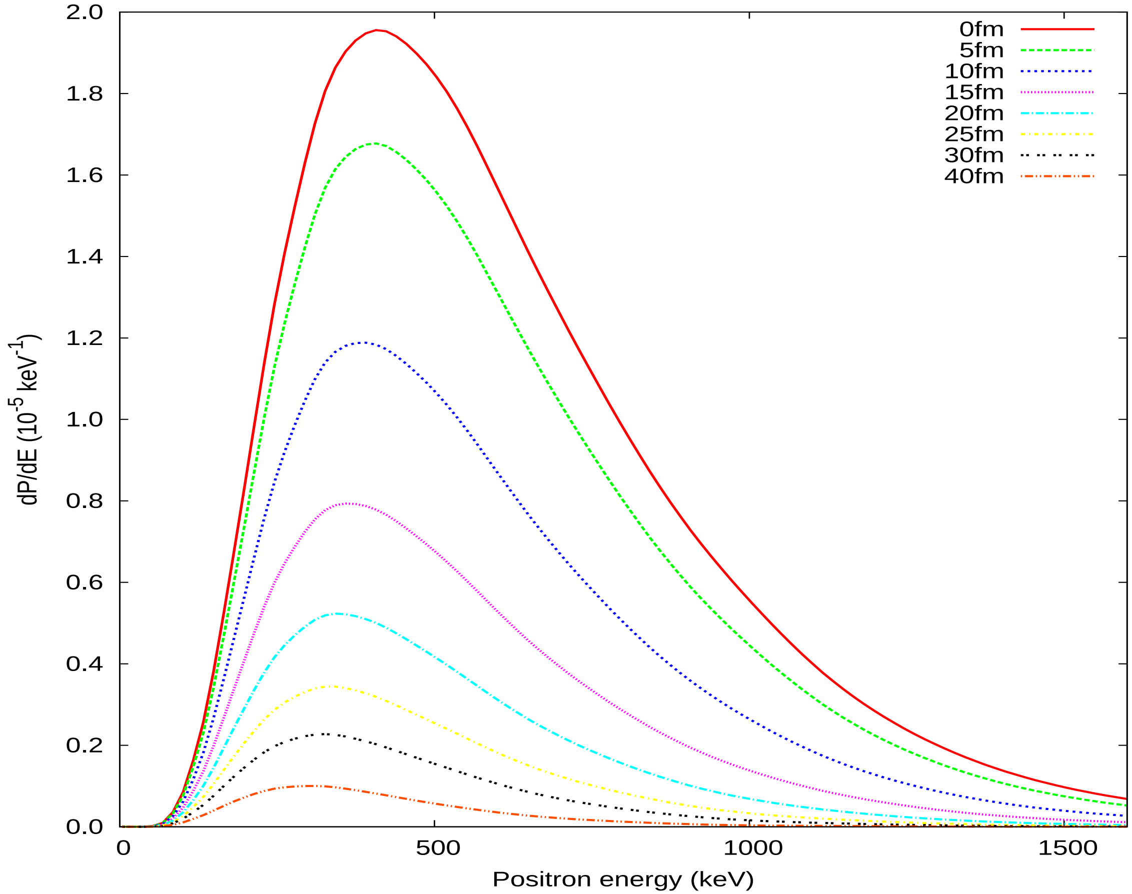


Energy distribution of positrons emitted in U-U collisions at energy E=6.2 MeV/u for the impact parameter in the range: $b = 0 - 40$ fm

(U. Müller, T. de Reus, J. Reinhardt et al., Phys. Rev. A, 1988).

Low-energy heavy-ion collisions

Electron-positron pair production in low-energy U-U collisions



Energy distribution of positrons emitted in U-U collisions at energy E=6.2 MeV/u for the impact parameter in the range: $b = 0 - 40$ fm *(I.A. Maltsev et al., PRA, 2015)*.

Low-energy heavy-ion collisions

Pair creation beyond the monopole approximation

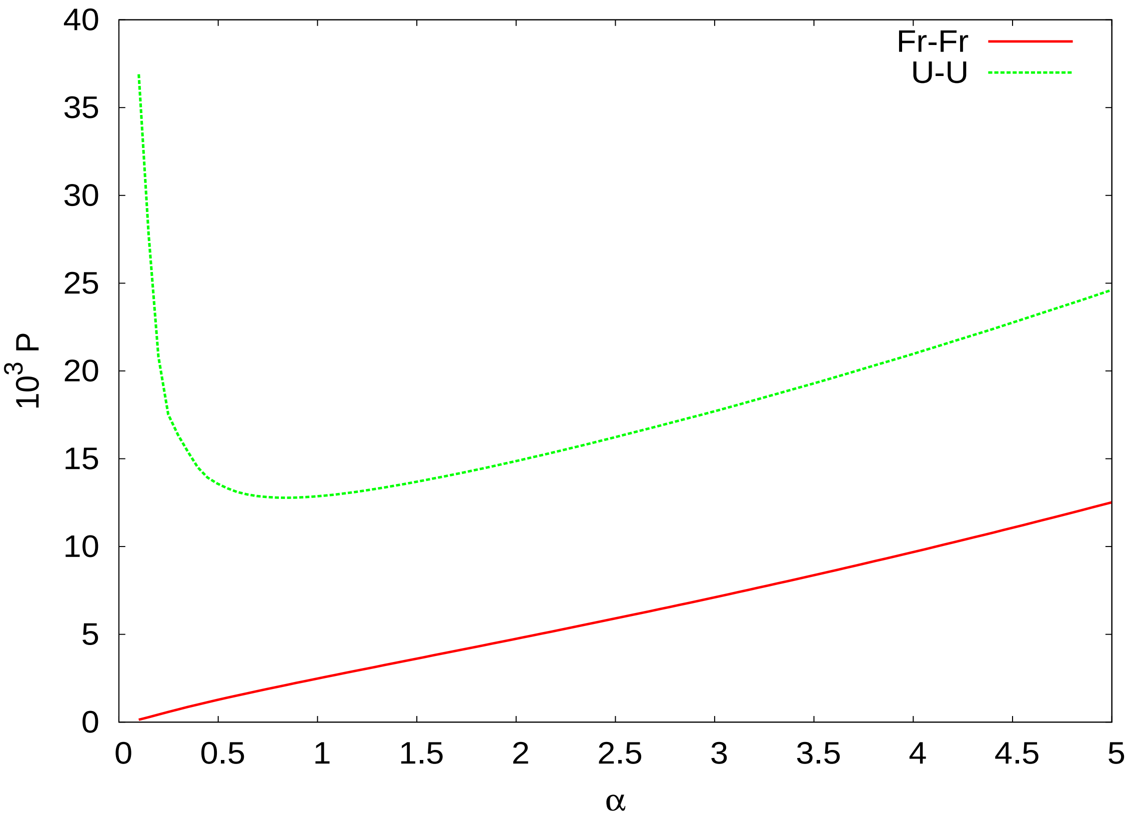
U-U, $E_{\rm cm}$ = 740 MeV

Expected number of created pairs with an electron captured into a bound state as a function of the impact parameter b

(I.A. Maltsev et al., NIMB, 2017) .

b (fm)	Two-center approach	Monopole approximation
0	1.33 $\times 10^{-2}$	1.25 $\times 10^{-2}$
10	7.71 $\times 10^{-3}$	7.03 $\times 10^{-3}$
20	3.12 $\times 10^{-3}$	2.70 $\times 10^{-3}$
30	1.28 $\times 10^{-3}$	1.03 $\times 10^{-3}$
40	5.66 $\times 10^{-4}$	4.09 $\times 10^{-4}$

Low-energy heavy-ion collisions



Pair creation with artificial trajectories for the supercritical U−U and subcritical Fr−Fr collisions at $E_{\rm cm} = 674.5$ and $E_{\rm cm} = 740$ MeV, respectively. The trajectory $R_\alpha(t)$ is defined by $\dot{R}_\alpha(t) = \alpha \dot{R}(t)$, where $R(t)$ is the classical Rutherford trajectory *(I.A. Maltsev et al., PRA, 2015)*.

Conclusion

Investigations of heavy ions at low-energy regime can provide:

- Tests of QED in strong and supercritical fields
- Tests of QED at strong coupling regime beyond the Furry picture
- Determination of the fundamental constants
- Tests of the Standard Model at the low-energy regime