Nuclear recoil effect on the g factor of lithiumlike ions

A. V. Malyshev, V. M. Shabaev, D. A. Glazov, and I. I. Tupitsyn

Department of Physics
Saint-Petersburg State University

May 14, 2018

Nuclear recoil effect on the g factor of lithiumlike ions

A. V. Malyshev, V. M. Shabaev, D. A. Glazov, and I. I. Tupitsyn

Department of Physics
Saint-Petersburg State University

May 14, 2018

Outline:

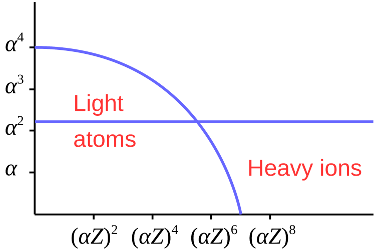
- Introduction and Motivation
- Nuclear recoil effect on the g factor
- Isotope shift of the g factor
- g factor of heavy ions
- Summary and Outlook

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:

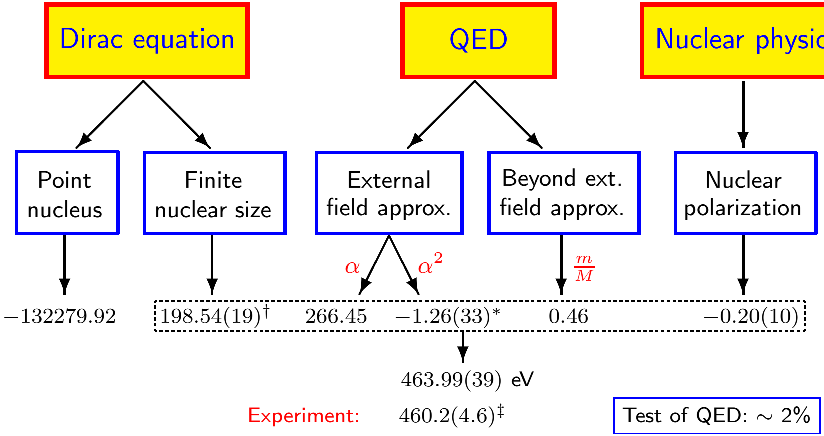
$$[-i\boldsymbol{\alpha}\cdot\nabla + \beta m + V_{\mathrm{nuc}}(\mathbf{r})]\,\psi_n(\mathbf{r}) = \varepsilon_n \psi_n(\mathbf{r})$$

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.

Isotope shifts

Cancellations in the isotope shifts:

- interelectronic-interaction effects;
- one- and two-electron QED corrections.

Two main contributions to the isotope shift:

- mass shift ⇔ nuclear recoil effect;
- field shift ⇔ nuclear size effect.

Measurements of the isotope shifts of:

- transition energies
  - B-like argon: R. S. Orts *et al.*, PRL, 2006;
  - Li-like neodymium: C. Brandau *et al.*, PRL, 2008.
- g-factor
  - Li-like calcium: F. Köhler *et al.*, Nat. Comm., 2016.

Why do we study isotope shifts?

- Access to QED beyond the Furry picture.
- Determination of the isotopic mass and radii differences.

QED theory for the nuclear recoil effect on g factor

Nuclear recoil contribution to the g factor for a state a:

- to first order in m/M;
- to all orders in αZ;
- to zeroth order in α.

$$\mathbf{A}^{\rm cl}(\mathbf{r}) = \mathcal{H}[\mathbf{e}_z \times \mathbf{r}]/2$$

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

where tilde sign indicates that the quantity must be evaluated in presence of $\mathcal{H}$,

$D_k(\omega) = -4\pi\alpha Z \alpha_i D_{ik}(\omega)$,

$D_{ik}(\omega)$ is the transverse part of the photon propagator in the Coulomb gauge,

$\tilde{G}(\omega) = \sum_{\tilde{n}} \frac{|\tilde{n}\rangle\langle\tilde{n}|}{\omega - \tilde{\varepsilon}_n + i\eta(\tilde{\varepsilon}_n - \tilde{\varepsilon}_{\rm F})}$ is the Coulomb Green function.

V. M. Shabaev, PRA, 2001.

One-electron contribution to the recoil effect on g factor

The one-electron contribution is represented as a sum $\Delta g = \Delta g_{\rm L} + \Delta g_{\rm H}$

$$\Delta g_{\rm L} = \frac{1}{\mu_{\rm B}\mathcal{H}m_a}\frac{1}{M}\langle\,\delta a\,|\Big[\mathbf{p}^2 - \frac{\alpha Z}{r}\Big(\boldsymbol{\alpha} + \frac{(\boldsymbol{\alpha}\cdot\mathbf{r})\mathbf{r}}{r^2}\Big)\cdot\mathbf{p}\Big]|\,a\,\rangle$$
$$-\frac{1}{m_a}\frac{m}{M}\langle\,a\,|\Big([\mathbf{r}\times\mathbf{p}]_z - \frac{\alpha Z}{2r}[\mathbf{r}\times\boldsymbol{\alpha}]_z\Big)|\,a\,\rangle\,,$$

$$\Delta g_{\rm H} = \frac{1}{\mu_{\rm B}\mathcal{H}m_a}\frac{1}{M}\frac{i}{2\pi}\int_{-\infty}^{\infty}d\omega\,\Big\{\langle\,a\,|\,\mathbf{B}_\omega^{(-)}G(\omega+\varepsilon_a)(\delta V - \delta\varepsilon_a)G(\omega+\varepsilon_a)\mathbf{B}_\omega^{(+)}\,|\,a\,\rangle$$
$$+\langle\,\delta a\,|\,\mathbf{B}_\omega^{(-)}G(\omega+\varepsilon_a)\mathbf{B}_\omega^{(+)}\,|\,a\,\rangle + \langle\,a\,|\,\mathbf{B}_\omega^{(-)}G(\omega+\varepsilon_a)\mathbf{B}_\omega^{(+)}\,|\,\delta a\,\rangle\Big\}$$

where

$\delta V(\mathbf{r}) = -e\boldsymbol{\alpha}\cdot\mathbf{A}^{\rm cl}(\mathbf{r})$ and $|\delta a\rangle = \sum_n^{\varepsilon_n\neq\varepsilon_a} |n\rangle\langle n|\delta V|a\rangle(\varepsilon_a - \varepsilon_n)^{-1}$,

$\mathbf{B}_\omega^{(\pm)} = \mathbf{D}(\omega) \pm [\mathbf{p}, V]/(\omega + i0)$,

$G(\omega) = \sum_n \dfrac{|n\rangle\langle n|}{\omega - \varepsilon_n(1 - i0)}$ is the Coulomb Green function.

Low-order one-electron term $\Delta g_{\rm L}$

For a point-charge nucleus, the low-order one-electron term $\Delta g_{\rm L}$ can be evaluated analytically,

$$\Delta g_{\rm L} = -\frac{m}{M}\frac{2\kappa^2\varepsilon^2 + \kappa m\varepsilon - m^2}{2m^2 j(j+1)}\,.$$

To leading order in αZ:

$$\Delta g_{\rm L} = -\frac{m}{M}\frac{1}{j(j+1)}\left[\kappa^2 + \frac{\kappa}{2} - \frac{1}{2} - \left(\kappa^2 + \frac{\kappa}{4}\right)\frac{(\alpha Z)^2}{n^2} + \dots\right]\,.$$

For an S state ($\kappa = -1$), this term is of pure relativistic origin:

$$\Delta g_{\rm L} = \frac{m}{M}\frac{(\alpha Z)^2}{n^2} + \dots\,.$$

Isotope shift of the g factor of Li-like ions

F. Köhler *et al.*, Nat. Commun., 2016.

Effect	Contribution $[\Delta g \times 10^9]$
One-electron non-QED nuclear recoil	12.240
Two-electron non-QED nuclear recoil	$-2.051(25)$
QED nuclear recoil: $\sim m/M$	0.123
QED nuclear recoil: $\sim \alpha(m/M)$	$-0.009(1)$
Finite nuclear size	$0.004(10)$
Total theory	$10.305(27)$
Experiment	$11.70(1.39)$

Individual contributions to the shift $\Delta g = g(^{40}\mathrm{Ca}^{17+}) - g(^{48}\mathrm{Ca}^{17+})$

The calculation of two-electron non-QED nuclear recoil effect is based on the extrapolation of the results from [Z.-C. Yan, PRL, 2001; JPB, 2002] which were obtained within the two-component approach [R. A. Hegstrom, PRA, 1975].

Effective two-component Hamiltonian (for S states)

R. A. Hegstrom, PRA, 1973; PRA, 1975.
The Hamiltonian for a many-particle system in a homogeneous magnetic field [anomalous moments, g_e + nuclear motion]

Magnetic-field-dependent spin-dependent part of the Hegstrom's Hamiltonian:

$$H_{\rm eff} = \mu_{\rm B}\mathcal{H}\Bigg\{ g_e \sum_i s_{iz} + \frac{1}{3}(1-g_e)\alpha \sum_{i\neq j} \frac{\mathbf{r}_i\cdot\mathbf{r}_{ij}}{r_{ij}^3} s_{iz} - \frac{1}{3} g_e \alpha \sum_{i\neq j} \frac{\mathbf{r}_i\cdot\mathbf{r}_{ij}}{r_{ij}^3} s_{jz}$$

$$+\left(\frac{2}{3}+\frac{g_e}{6}\right)\sum_i \nabla_i^2 s_{iz} - \frac{\alpha Z}{3}(1-g_e)\sum_i \frac{1}{r_i} s_{iz} - \frac{1}{3}\alpha Z \frac{m}{M} g_e \sum_i \frac{1}{r_i} s_{iz}$$

$$-\frac{1}{3}\alpha Z \frac{m}{M} g_e \sum_{i<j}\left(\frac{\mathbf{r}_i\cdot\mathbf{r}_j}{r_i^3} s_{iz} + \frac{\mathbf{r}_i\cdot\mathbf{r}_j}{r_j^3} s_{jz}\right)\Bigg\}\,.$$

The g factor for lithiumlike ions in an S state ($J=1/2$):

$$g = \frac{\langle H_{\rm eff}\rangle}{\mu_{\rm B}\mathcal{H}J}\,.$$

Recoil effect on the g factor within the Breit approximation

Within the lowest-order relativistic (Breit) approximation

- Effective non-magnetic recoil operator (the combined interaction):
  - $H_M = \frac{1}{2M} \sum_{i,k} \left[\mathbf{p}_i \cdot \mathbf{p}_k - \frac{\alpha Z}{r_i} \left(\boldsymbol{\alpha}_i + \frac{(\boldsymbol{\alpha}_i \cdot \mathbf{r}_i)\mathbf{r}_i}{r_i^2} \right) \cdot \mathbf{p}_k \right]$
  - $\delta V(\mathbf{r}) = -e\boldsymbol{\alpha} \cdot \mathbf{A}^{\mathrm{cl}}(\mathbf{r})$
- Effective magnetic recoil operator:
  - $H_M^{\mathrm{magn}} = -\mu_{\mathrm{B}} \mathcal{H} \frac{m}{M} \sum_{i,k} \left\{ [\mathbf{r}_i \times \mathbf{p}_k] - \frac{\alpha Z}{2r_k} \left[\mathbf{r}_i \times \left(\boldsymbol{\alpha}_k + \frac{(\boldsymbol{\alpha}_k \cdot \mathbf{r}_k)\mathbf{r}_k}{r_k^2} \right) \right] \right\}$

To take into account the interelectronic-interaction effects: DCB Hamiltonian

- $H_{\mathrm{DCB}} = \Lambda^{(+)} \left[\sum_i h_i^{\mathrm{D}} + \sum_{i<k} V_{ik} \right] \Lambda^{(+)}$, where

$$V_{ik} = \frac{\alpha}{r_{ik}} - \alpha \left[\frac{\boldsymbol{\alpha}_i \cdot \boldsymbol{\alpha}_k}{r_{ik}} + \frac{1}{2} (\boldsymbol{\alpha}_i \cdot \boldsymbol{\nabla}_i)(\boldsymbol{\alpha}_k \cdot \boldsymbol{\nabla}_k) r_{ik} \right]$$

The $1/Z$ recoil contribution to the g factor

Nuclear recoil correction to the g factor to lowest order relativistic approximation

$$\Delta g = \frac{m}{M}(\alpha Z)^2 \left(A + \frac{B}{Z} + \frac{C}{Z^2} + \dots \right)$$

From the 4-C approach: PT with H_M, H_M^{magn}, and H_{DCB} including δV.

$$B_{\text{4-C}} = -0.5155(2)\,.$$

From the 2-C approach: PT with H_{eff} and α/r.

$$B_{\text{2-C}} = -0.8603\,.$$

Omitted term for 2-C approach: $-\mu_{\mathrm{B}}\mathcal{H}\frac{m}{M}\sum_{i,k}[\mathbf{r}_i \times \mathbf{p}_k]$, SO or S-other-O, and α/r.

$$\Delta B_{\text{2-C}} = 0.3447\,.$$

Total 2-C result:

$$B_{\text{2-C}}^{\mathrm{tot}} = B_{\text{2-C}} + \Delta B_{\text{2-C}} = -0.5156\,.$$

Isotope shift of the g factor of Li-like ions

V. M. Shabaev *et al.*, PRL, 2017.

Effect	Contribution $\left[\Delta g \times 10^9\right]$
One-electron non-QED nuclear recoil	12.240
Two-electron non-QED nuclear recoil, 2-C	$-2.051(25)$
Two-electron non-QED nuclear recoil, 4-C	$-1.302(12)$
QED nuclear recoil: $\sim m/M$	0.123
QED nuclear recoil: $\sim \alpha(m/M)$	$-0.009(1)$
Finite nuclear size	$0.004(10)$
Total theory, 2-C	$10.305(27)$
Total theory, 4-C	$11.056(16)$
Experiment	$11.70(1.39)$

Individual contributions to the shift $\Delta g = g(^{40}\mathrm{Ca}^{17+}) - g(^{48}\mathrm{Ca}^{17+})$

The calculation of the two-electron non-QED nuclear recoil effect is based on the four-component approach.

Specific difference

The QED recoil effect for S states

$$\Delta g_{\rm H}^{(ns)} = \frac{m}{M}\frac{(\alpha Z)^5}{n^3} P^{(ns)}(\alpha Z)\,.$$

The uncertainty due to the nuclear size and polarization effects masks the recoil effect for heavy ions.

The specific differences between different ions of the same isotope

- HFS: V. M. Shabaev *et al.*, PRL, 2001.

$$\Delta E' = \Delta E_{(1s)^2 2s} - \xi_{\rm HFS}\, \Delta E_{1s}\,.$$

- g factor: V. M. Shabaev *et al.*, PRA, 2002.

$$g' = g_{(1s)^2 2s} - \xi_g\, g_{1s}\,.$$

The parameters ξ must be chosen to cancel the nuclear size corrections.

Specific difference of the g-factor values for $^{208}\mathrm{Pb}$

The specific difference between the g factors of Li- and H-like ions

$$g' = g_{(1s)^2 2s} - \xi_g \, g_{1s} \, .$$

For lead ($Z = 82$), one obtains $\xi_g = 0.1670264$.

A. V. Malyshev *et al.*, JETP Lett., 2017.

Effect	Contribution $\left[g' \times 10^9\right]$
Nuclear shape variation	~ 1
Nuclear radius dependence	~ 0.1
Nuclear polarization	$-0.13(6)$
QED recoil	8.7

Individual contributions to the specific difference between the g factors of Li- and H-like lead

Tests of the QED recoil effect on the g factor of heavy ions are possible on a few-percent level.

Summary and Outlook

Main results:

- The most precise to-date theoretical values for the recoil effect on the g factor of Li-like ions have been obtained.
- The discrepancy was found between the present result for the two-electron contribution and its previous evaluation within the 2-C approach. The reason of the discrepancy is revealed.
- The QED recoil effect on the g factor can be probed in experiments with heavy ions studying the specific difference of the g factors of H- and Li-like ions.

Future plans:

- extension to B-like ions [the QED recoil effect behaves as $(\alpha Z)^3$].
- further improvement of the bound-state QED calculations of the g factor of highly charged ions.


Thank You for Your attention

The work was supported by

RSF