Nuclear recoil effect on the g factor of lithiumlike ions

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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
Highly-charged few-electron ions:

$N_e \ll Z$

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

To zeroth-order approximation:

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

Interelectronic interaction and QED effects:

<table>
<thead>
<tr>
<th>Interelectronic interaction</th>
<th>Binding energy</th>
<th>QED</th>
<th>Binding energy</th>
</tr>
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<tbody>
<tr>
<td>Binding energy</td>
<td>$\sim \frac{1}{Z}$</td>
<td>QED</td>
<td>$\sim \alpha(\alpha Z)^2$</td>
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</table>

In uranium: $Z = 92$, $\alpha Z \approx 0.7$
Binding energy of H-like uranium, in eV

\[
\begin{align*}
\text{Dirac equation} & \\
\text{Point nucleus} & \rightarrow -132279.92 \\
\text{Finite nuclear size} & \\
\text{QED} & \\
\text{External field approx.} & \left[198.54(19)^\dagger\right] \rightarrow 266.45 \rightarrow -1.26(33)^* \rightarrow 0.46 \rightarrow -0.20(10) \\
\text{Beyond ext. field approx.} & \\
\text{Nuclear physics} & \\
\text{Nuclear polarization} & \\
\end{align*}
\]

\[
463.99(39) \text{ eV}
\]

Experiment: \[460.2(4.6)^\ddagger\]  
Test of QED: \[\sim 2\%\]

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 $\Leftrightarrow$ nuclear recoil effect;
- field shift $\Leftrightarrow$ nuclear size effect.

Measurements of the isotope shifts of:
- transition energies
  - B-like argon: R. S. Orts et al., PRL, 2006;
- $g$-factor

Why do we study isotope shifts?
- Access to QED beyond the Furry picture.
- Determination of the isotopic mass and radii differences.
Nuclear recoil contribution to the $g$ factor for a state $a$:

- to first order in $m/M$;
- to all orders in $\alpha Z$;
- to zeroth order in $\alpha$.

\[
\Delta g = \frac{1}{\mu_B m_a} \frac{1}{M} \int_{-\infty}^{\infty} d\omega \left[ \frac{\partial}{\partial \mathcal{H}} \langle \tilde{a} | [ p - D(\omega) + eA^{\text{cl}} ] \tilde{a} \rangle \right] \bigg|_{\mathcal{H}=0} \times \tilde{G}(\omega + \tilde{\varepsilon}_a) [ p - D(\omega) + eA^{\text{cl}} ] | \tilde{a} \rangle,
\]

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,

\[
\tilde{G}(\omega) = \sum_{\tilde{n}} \frac{|\tilde{n}\rangle\langle\tilde{n}|}{\omega - \tilde{\varepsilon}_n + i\eta(\tilde{\varepsilon}_n - \tilde{\varepsilon}_F)}
\]

is the Coulomb Green function.

---

One-electron contribution to the recoil effect on \( g \) factor

The one-electron contribution is represented as a sum \( \Delta g = \Delta g_L + \Delta g_H \)

\[
\Delta g_L = \frac{1}{\mu_B \mathcal{H} m_a} \frac{1}{M} \langle \delta a | \left[ p^2 - \frac{\alpha Z}{r} \left( \alpha + \frac{\alpha \cdot r}{r^2} \right) \cdot p \right] | a \rangle \\
- \frac{1}{m_a M} \langle a | \left( [r \times p]_z - \frac{\alpha Z}{2r} [r \times \alpha]_z \right) | a \rangle,
\]

\[
\Delta g_H = \frac{1}{\mu_B \mathcal{H} m_a} \frac{1}{M} \frac{i}{2\pi} \int_{-\infty}^{\infty} d\omega \left\{ \langle a | B^{(-)}_{\omega} G(\omega + \varepsilon_a)(\delta V - \delta \varepsilon_a)G(\omega + \varepsilon_a)B^{(+)}_{\omega} | a \rangle \\
+ \langle \delta a | B^{(-)}_{\omega} G(\omega + \varepsilon_a)B^{(+)}_{\omega} | a \rangle + \langle a | B^{(-)}_{\omega} G(\omega + \varepsilon_a)B^{(+)}_{\omega} | \delta a \rangle \right\}
\]

where

\[
\delta V(\mathbf{r}) = -e\mathbf{\alpha} \cdot \mathbf{A}^cl(\mathbf{r}) \quad \text{and} \quad |\delta a\rangle = \sum_n \frac{|\varepsilon_n \neq \varepsilon_a\rangle}{\varepsilon_a - \varepsilon_n} - 1, \\

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

\[
G(\omega) = \sum_n \frac{|n\rangle\langle n|}{\omega - \varepsilon_n(1 - i0)} \quad \text{is the Coulomb Green function.}
\]
For a point-charge nucleus, the low-order one-electron term $\Delta g_L$ can be evaluated analytically,

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

To leading order in $\alpha Z$:

$$\Delta g_L = -\frac{m}{M} \frac{1}{j(j+1)} \left[ \kappa^2 + \frac{\kappa}{2} - \frac{1}{2} - \left( \kappa^2 + \frac{3}{4} \right) \frac{(\alpha Z)^2}{n^2} + \ldots \right] .$$

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

$$\Delta g_L = \frac{m}{M} \frac{(\alpha Z)^2}{n^2} + \ldots .$$
### Isotope shift of the $g$ factor of Li-like ions


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<td>Finite nuclear size</td>
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<td><strong>Total theory</strong></td>
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<td><strong>Experiment</strong></td>
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Individual contributions to the shift $\Delta g = g(^{40}\text{Ca}^{17+}) - g(^{48}\text{Ca}^{17+})$

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)


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:

$$
H_{\text{eff}} = \mu_B \mathcal{H} \left\{ g_e \sum_i s_{iz} + \frac{1}{3} (1 - g_e) \alpha \sum_{i \neq j} \frac{r_i \cdot r_{ij}}{r_{ij}^3} s_{iz} - \frac{1}{3} g_e \alpha \sum_{i \neq j} \frac{r_i \cdot r_{ij}}{r_{ij}^3} s_{jz} + \left( \frac{2}{3} + \frac{g_e}{6} \right) \sum_i \nabla_i^2 s_{iz} - \frac{\alpha Z}{3} (1 - g_e) \sum_i \frac{1}{r_i} s_{iz} - \frac{1}{3} \alpha Z \frac{m}{M} g_e \sum_i \frac{1}{r_i} s_{iz} - \frac{1}{3} \alpha Z \frac{m}{M} g_e \sum_{i < j} \left( \frac{r_i \cdot r_j}{r_i^3} s_{iz} + \frac{r_i \cdot r_j}{r_j^3} s_{jz} \right) \right\}.
$$

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

$$
g = \frac{\langle H_{\text{eff}} \rangle}{\mu_B \mathcal{H} J}.
$$
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):
  \[ H_M = \frac{1}{2M} \sum_{i,k} \left[ p_i \cdot p_k - \frac{\alpha Z}{r_i} \left( \alpha_i + \frac{(\alpha_i \cdot r_i) r_i}{r_i^2} \right) \cdot p_k \right] \]

- \[ \delta V(r) = -e \alpha \cdot A^{cl}(r) \]

- Effective magnetic recoil operator:
  \[ H_{M}^{\text{magn}} = -\mu_B H \frac{m}{M} \sum_{i,k} \left\{ [r_i \times p_k] - \frac{\alpha Z}{2r_k} \left[ r_i \times \left( \alpha_k + \frac{(\alpha_k \cdot r_k) r_k}{r_k^2} \right) \right] \right\} \]

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

- \[ H_{DCB} = \Lambda^{(+)} \left[ \sum_i h_i^D + \sum_{i<k} V_{ik} \right] \Lambda^{(+)}, \quad \text{where} \]
  \[ V_{ik} = \frac{\alpha}{r_{ik}} - \alpha \left[ \frac{\alpha_i \cdot \alpha_k}{r_{ik}} + \frac{1}{2} (\alpha_i \cdot \nabla_i)(\alpha_k \cdot \nabla_k) r_{ik} \right] \]
The $1/Z$ recoil contribution to the $g$ factor

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

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

From the 4-C approach: PT with $H_M$, $H_M^{\text{magn}}$, and $H_{\text{DCB}}$ including $\delta V$.

\[ B_{4-C} = -0.5155(2). \]

From the 2-C approach: PT with $H_{\text{eff}}$ and $\alpha/r$.

\[ B_{2-C} = -0.8603. \]

Omitted term for 2-C approach: $-\mu_B H \frac{m}{M} \sum_{i,k} [r_i \times p_k]$, SO or S-other-O, and $\alpha/r$.

\[ \Delta B_{2-C} = 0.3447. \]

Total 2-C result:

\[ B_{2-C}^{\text{tot}} = B_{2-C} + \Delta B_{2-C} = -0.5156. \]
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Individual contributions to the shift $\Delta g = g(^{40}\text{Ca}^{17+}) - g(^{48}\text{Ca}^{17+})$

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

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

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

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

- **$g$ factor**: V. M. Shabaev et al., PRA, 2002.
  $$g' = g_{(1s)^2 2s} - \xi_g g_{1s}.$$  

The parameters $\xi$ must be chosen to cancel the nuclear size corrections.
Specific difference of the $g$-factor values for $^{208}$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 $\xi_g = 0.1670264$.


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<tr>
<td>Nuclear radius dependence</td>
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</tr>
<tr>
<td>Nuclear polarization</td>
<td>$-0.13(6)$</td>
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<tr>
<td>QED recoil</td>
<td>8.7</td>
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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