Fine and hyperfine structure of helium atom

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Helium: Introduction

- The simplest few-body system. Three-body bound-state QED.

- Very accurately measured
  - accuracy $8 \times 10^{-12}$, $2^3S_1 \rightarrow 2^1S_0$ in $^3$He [R. van Rooij et al., Science 333, 196 (2011)]
  - up to $5 \times 10^{-12}$, $2^3P \rightarrow 2^3S$ in $^3$He [P. Cancio Pastor et al., PRL 108, 143001 (2012)]
  - up to $8 \times 10^{-12}$, $2^3P \rightarrow 2^3S$ in $^4$He [P. Cancio Pastor et al., PRL 92, 023001 (2004)]

- Determination of fine-structure constant and nuclear charge radius
Determination of the fine-structure constant

• free-electron $g$ factor (accurate to $2.5 \times 10^{-10}$)
  \[ \alpha^{-1} = 137.035 \, 999 \, 173 \, (35) \] [Aoyama et al., PRL 109, 111807 (2012)]

• atomic recoil velocity measurements (accurate to $7 \times 10^{-10}$)
  \[ \alpha^{-1} = 137.035 \, 999 \, 037 \, (91) \] [Bouchendira et al., PRL 106, 080801 (2011)]

• helium fine structure (accurate to $3 \times 10^{-8}$)
  \[ \alpha^{-1} = 137.035 \, 999 \, 6 \, (34) \]
  
  Theory: Pachucki and Yerokhin, PRL 104, 070403 (2010)
  Exp.: Smiciklas and Shiner, PRL 105, 123001 (2010)

Highly sensitive test of consistency of different theories across a wide range of energy scales.
Determination of the nuclear charge radius

$^3\text{He} - ^4\text{He}$ isotope shift can be used to determine the difference of the (squares of the) nuclear charge radii $\delta r^2$

Experiments:

A  $^2\text{P} - ^2\text{S}$, Cancio Pastor et al., PRL 108, 143001 (2012)
B  $^1\text{S} - ^2\text{S}$, van Rooij et al., Science 333, 196 (2011)
C  $^2\text{P} - ^2\text{S}$, Shiner et al., PRL 74, 3553 (1995)

Electron scattering
Nuclear theory

Isotope shift
Theory:
Pachucki and Yerokhin 2012

Nuclear charge radium from muonic helium coming soon (talk of Randolph Pohl)
NRQED Expansion

Small parameters:

\( \alpha (\approx Z \alpha) \) == fine-structure constant (relativistic effects, QED effects)

\( m/M \) == electron-to-nucleus mass ratio (nuclear recoil effects)

Expansion for energy levels:

\[
E = E^{(2)}_{\text{NR}} + E^{(4)}_{\text{Breit}} + E^{(5)}_{\text{QED}} + E^{(6)} + E^{(7)} + \ldots
\]

\[
E^{(n)} = \langle H^{(n)} \rangle \sim m \alpha^n
\]

- \( E^{(2)} \) — nonrelativistic energy
- \( E^{(4)}_{\text{Breit}} \) — leading relativistic (Breit) correction
- \( E^{(5)}_{\text{QED}} \) — leading QED (Araki-Sucher) correction

Expansion is non-alalytic in \( \alpha \) == contains log's
Nonrelativistic wave function

All matrix elements are calculated with the nonrelativistic wave function.
Singular operators => high accuracy wave function is required.
Fully correlated basis sets that depend explicitly on \( r_1, r_2, r_{12} \) and satisfy the cusp condition.

\[ E(2^3P) = -2.133\, 164\, 190\, 779\, 283\, 205\, 146\, 96^{+0.10}_{-10} \]

The spatial part of the triplet \( P \) wave function is represented as

\[ \bar{\phi}(\vec{r}_1, \vec{r}_2) = \sum_i c_i \left[ \vec{r}_1 \exp(-\alpha_i r_1 - \beta_i r_2 - \gamma_i r_{12}) - (1 \leftrightarrow 2) \right]. \]

Real nonlinear parameters \( \alpha_i, \beta_i, \) and \( \gamma_i \) are chosen quasirandomly from the intervals \( \alpha_i \in [A_1, A_2], \beta_i \in [B_1, B_2], \gamma_i \in [C_1, C_2], \) with the parameters \( A_{1,2}, \) \( B_{1,2}, \) and \( C_{1,2} \) determined by a variational optimization.

The single master integral is

\[ \frac{1}{16\pi^2} \int d^3r_1 \, d^3r_2 \, \frac{e^{\alpha r_1 - \beta r_2 - \gamma r_{12}}}{r_1 \, r_2 \, r_{12}} = \frac{1}{(\alpha + \beta)(\beta + \gamma)(\gamma + \alpha)}. \]

The nonrelativistic energy of the \( 2^3P \) state of helium is obtained with a 23-digit accuracy. Octuple arithmetics (appr. 72 digits) is required for calculations.
Fine structure
Structure of 2P states of $^4$He

$1s2p \ ^1P$

$1s2p \ ^3P$

$J=0$

$J=1$

$J=2$

$\nu_{01} = 29616.9 \text{ MHz}$

$\nu_{12} = 2291.2 \text{ MHz}$

$\nu_{02} = \nu_{01} + \nu_{12} = 31908.1 \text{ MHz}$

61 THz
Fine structure: NRQED expansion

\[ \langle H_{fs} \rangle = \langle H_{\text{Breit}}^{(4+)} \rangle + \langle H_{\text{DK}}^{(6)} \rangle + \langle H_{\text{Breit}}^{(4)} \rangle \frac{1}{(E - H)^2} H_{\text{Breit}}^{(4)} \] + \langle H^{(7)} \rangle + 2 \langle H_{\text{Breit}}^{(4)} \rangle \frac{1}{(E - H)^2} H^{(5)} + E_L^{(7)}.

- \( m^4 \) and \( m^5 \) corrections
- \( m^6 \) corrections
- \( m^7 \) corrections

Lewis and Serafino 1978
Yan and Drake 1995

- Second-order perturbative corrections induced by local operators
- Bethe-logarithm type corrections (non-local operators) \( E_L^{(7)} \)

Pachucki 2006
Pachucki and Yerokhin 2009,2010
Table 2. Summary of individual contributions to the fine-structure intervals in helium, in kHz. The parameters [25] are $\alpha^{-1} = 137.035999679(94)$, $cR_\infty = 3289.841960361(22)$ kHz, and $m/M = 1.37093355570 \times 10^{-4}$. The label $(+m/M)$ indicates that the corresponding entry comprises both the non-recoil and recoil contributions of the specified order in $\alpha$.

<table>
<thead>
<tr>
<th>Term</th>
<th>$\nu_{01}$</th>
<th>$\nu_{12}$</th>
<th>$\nu_{02}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$m\alpha^4 (+m/M)$</td>
<td>29563 765.45</td>
<td>2320 241.43</td>
<td></td>
</tr>
<tr>
<td>$m\alpha^5 (+m/M)$</td>
<td>54 704.04</td>
<td>-22 545.00</td>
<td></td>
</tr>
<tr>
<td>$m\alpha^6$</td>
<td>-1 607.52(2)</td>
<td>-6 506.43</td>
<td></td>
</tr>
<tr>
<td>$m\alpha^6 m/M$</td>
<td>-9.96</td>
<td>9.15</td>
<td></td>
</tr>
<tr>
<td>$m\alpha^7 \log(Z\alpha)$</td>
<td>81.43</td>
<td>-5.87</td>
<td></td>
</tr>
<tr>
<td>$m\alpha^7$, nlog</td>
<td>18.86</td>
<td>-14.38</td>
<td></td>
</tr>
<tr>
<td>$m\alpha^8$</td>
<td>±1.7</td>
<td>±1.7</td>
<td></td>
</tr>
<tr>
<td>Total theory</td>
<td>29 616 952.29 ± 1.7</td>
<td>2 291 178.91 ± 1.7</td>
<td>31 908 131.20 ± 1.7</td>
</tr>
<tr>
<td>Experiment</td>
<td>29 616 951.66(70)$^a$</td>
<td>2 291 177.53(35)$^d$</td>
<td>31 908 131.25(30)$^f$</td>
</tr>
<tr>
<td></td>
<td>29 616 952.7(10)$^b$</td>
<td>2 291 175.59(51)$^a$</td>
<td>31 908 126.78(94)$^a$</td>
</tr>
<tr>
<td></td>
<td>29 616 950.9(9)$^c$</td>
<td>2 291 175.9(10)$^e$</td>
<td></td>
</tr>
</tbody>
</table>

Experiments:

a Zelevinsky et al. PRL 95, 203001 (2005) [Gabrielse]
c George et al. PRL 84, 4321 (2000) [Hessels]
d Borbely et al. PRA 79, 0605030(R) (2009) [Hessels]
e Castillega et al. PRL 84, 4321 (2000) [Shiner]
f Smiciklas and Shiner, PRL 105, 123001 (2010) [Shiner]

Theory:

Pachucki and Yerokhin, PRL 104, 070403 (2010)
Hyperfine structure
Fine and hyperfine structure in helium are of the same order of magnitude!
Combined fine and hyperfine structure

Basis of strongly interacting quasi-degenerate states:

\[ |FJ\rangle \equiv |2^3 P^F_J\rangle, \text{ with } J = 0, 1, 2 \text{ and } F = J \pm 1/2 \]

5x5 matrix of the effective Hamiltonian:

\[ E^F_{J,J'} = \langle FJ | H | FJ' \rangle \]

Energy levels are obtained as the eigenvalues of the Hamiltonian matrix.

Energy levels are calculated relative to the centroid (center-of-mass) energy:

\[ E(2^3 P) = \frac{\sum_{F,J} (2F + 1) E(2^3 P^F_J)}{(2I + 1)(2S + 1)(2L + 1)} \]

All effects that do not depend on electron or nuclear spin do not contribute.
Fine + Hyperfine structure: NRQED expansion

\[ \langle H \rangle = \langle H_{fs} \rangle + \langle H_{hfs}^{(4+)} \rangle + \langle H_{hfs}^{(6)} \rangle + 2 \langle H_{hfs}^{(4)} \frac{1}{E - H} H_{\text{Breit}} \rangle + \langle H_{hfs}^{(4)} \frac{1}{(E - H)^2} H_{\text{Breit}}^{(4)} \rangle + \langle H_{\text{nucl}} \rangle \]

**ma^6 corrections**

Pachucki and Yerokhin 2012

\( H_{fs} \) - fine-structure effective Hamiltonian (operators depend on electron spins)

\( H_{hfs} \) - hyperfine-structure effective Hamiltonian (operators depend on nuclear spin)

\( H_{\text{Breit}} \) - Breit Hamiltonian (operators do not depend on spin)

\( H_{\text{nucl}} \) - effective Hamiltonian of nuclear effects
Nuclear effects

Hyperfine interaction $1/r^2 \Rightarrow$ nuclear effects are significant.

Cannot be (accurately) calculated from first principles.

One can claim that

$$H_{\text{nucl}} = C \delta^3(r)$$

The constant $C$ can be extracted by comparing theory and experiment for 1s He$^+$ hyperfine splitting.
\[ \delta E_{\text{reg}}(^3P) = \sum_{n>2} \frac{1}{E(2^3P) - E(n^3P)} \left[ \langle 2^3 \bar{P}|Q|n^3 \bar{P} \rangle \langle n^3 \bar{P}|\bar{T}|2^3 \bar{P} \rangle \left( \frac{2}{3} \bar{T} \cdot \bar{L} + I^i L^j (S^i S^j)^{(2)} \right) \\ + \langle 2^3 \bar{P}|Q|n^3 \bar{P} \rangle \langle n^3 \bar{P}|T|2^3 \bar{P} \rangle \left( \frac{1}{3} \bar{T} \cdot \bar{S} + \frac{1}{2} I^i S^j (L^i L^j)^{(2)} \right) \right] \]
## $2^3P$ hyperfine structure in He

<table>
<thead>
<tr>
<th>$(J, F) - (J', F')$</th>
<th>Value [kHz]</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>$(0, 1/2) - (1, 1/2)$</td>
<td>28 092 855.9 (1.8)</td>
<td>Theory, present</td>
</tr>
<tr>
<td></td>
<td>28 092 870 (60)</td>
<td>Theory, previous</td>
</tr>
<tr>
<td></td>
<td>28 092 858 (3)</td>
<td>Experiment, Texas</td>
</tr>
<tr>
<td></td>
<td>28 092 858.6 (2.1)</td>
<td>Experiment, Florence</td>
</tr>
<tr>
<td>$(1, 1/2) - (1, 3/2)$</td>
<td>4 512 214.1 (0.9)</td>
<td>Theory, present</td>
</tr>
<tr>
<td></td>
<td>4 512 191 (12)</td>
<td>Theory, previous</td>
</tr>
<tr>
<td></td>
<td>4 512 213 (3)</td>
<td>Experiment, Texas</td>
</tr>
<tr>
<td></td>
<td>4 512 211.9 (2.7)</td>
<td>Experiment, Florence</td>
</tr>
</tbody>
</table>

Theory, present: Pachucki and Yerokhin, PRA 85, 042517 (2012)
Experiment, Texas: Smiciklas, 2003, xxx.lanl.gov/abs/1203.2830
Experiment, Florence, Cancio Pastor et al., PRL 108, 143001 (2012)
Isotope shift
4\(^\text{He} \) - 3\(^\text{He} \) Isotope shift

Isotope shift == the difference between the centroids of the energy levels.

\[ E(2^3 P) = \frac{\sum_J (2J + 1) E(2^3 P_J)}{(2S + 1)(2L + 1)} \]

\[ E(2^3 P) = \frac{\sum_{F,J} (2F + 1) E(2^3 P^F_J)}{(2I + 1)(2S + 1)(2L + 1)} \]
<table>
<thead>
<tr>
<th>Contribution</th>
<th>$^2!{}^3!P - ^2!{}^3!S$ transition</th>
<th>$^2!{}^1!S - ^2!{}^3!S$ transition</th>
</tr>
</thead>
<tbody>
<tr>
<td>$m_r \alpha^2$</td>
<td>124 124 458.1</td>
<td>8 632 567.86</td>
</tr>
<tr>
<td>$m_r \alpha^2 (m_r / M)$</td>
<td>21 243 041.3</td>
<td>-608 175.58</td>
</tr>
<tr>
<td>$m_r \alpha^2 (m_r / M)^2$</td>
<td>13 874.6</td>
<td>7 319.80</td>
</tr>
<tr>
<td>$m_r \alpha^2 (m_r / M)^3$</td>
<td>4.6</td>
<td></td>
</tr>
<tr>
<td>$m_r \alpha^4$</td>
<td>17 872.8</td>
<td>8 954.22</td>
</tr>
<tr>
<td>$m_r \alpha^4 (m_r / M)$</td>
<td>-20 082.4</td>
<td>-6 458.23</td>
</tr>
<tr>
<td>$m_r \alpha^4 (m_r / M)^2$</td>
<td>-3.0</td>
<td>-1.84</td>
</tr>
<tr>
<td>$m \alpha^5 (m / M)$</td>
<td>-60.7</td>
<td>-56.61</td>
</tr>
<tr>
<td>$m \alpha^6 (m / M)$</td>
<td>-15.5 (3.9)</td>
<td>-2.75 (69)</td>
</tr>
<tr>
<td>Nuclear polarizability</td>
<td>-1.1 (1)</td>
<td>-0.20 (2)</td>
</tr>
<tr>
<td>HFS mixing</td>
<td>54.6</td>
<td>-80.72</td>
</tr>
<tr>
<td>Total theory</td>
<td>33 667 143.2 (3.9)</td>
<td>8 034 065.66 (69)</td>
</tr>
<tr>
<td>Other theory [1,2]a</td>
<td>33 667 146.2 (7)</td>
<td>8 034 067.8 (1.1)</td>
</tr>
</tbody>
</table>


a Corrected by adding the triplet-singlet HFS mixing.

**Theory:** Pachucki and Yerokhin, from [Cancio Pastor, PRL 108 143001 (2012)]
Difference of the squares of charge radii of $^3$He and $^4$He

$$\delta r^2 = r^2( ^3\text{He} ) - r^2( ^4\text{He} )$$

$^3P-^3S$, Cancio Pastor et al., PRL 108, 143001 (2012); theory by Pachucki and Yerokhin (2012)

$$\delta r^2 = 1.074 (3) \text{ fm}^2$$

$^1S-^3S$, van Rooij et al., Science 333, 196 (2011) + theory by Pachucki and Yerokhin (2012)

$$\delta r^2 = 1.028 (11) \text{ fm}^2$$


$$\delta r^2 = 1.066 (4) \text{ fm}^2$$
### Experiment versus Theory in He

<table>
<thead>
<tr>
<th></th>
<th>Experiment, accuracy</th>
<th>Theory, accuracy</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Lamb shift</strong></td>
<td>2 kHz</td>
<td>3000 kHz</td>
</tr>
<tr>
<td><strong>Fine structure</strong></td>
<td>0.2 kHz</td>
<td>2 kHz</td>
</tr>
<tr>
<td><strong>Hyperfine structure</strong></td>
<td>2 kHz</td>
<td>2 kHz</td>
</tr>
</tbody>
</table>