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 8×10^{-12}, $2^3S_1 \rightarrow 2^1S_0$ in ^{3}He [R. van Rooij et al., Science 333, 196 (2011)]

  up to 5×10^{-12}, $2^3P \rightarrow 2^3S$ in ^{3}He [P. Cancio Pastor et al., PRL 108, 143001 (2012)]

  up to 8×10^{-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 2.5×10^{-10})

  α^{-1} = 137.035 999 173 (35) [Aoyama et al., PRL 109, 111807 (2012)]

- atomic recoil velocity measurements (accurate to 7×10^{-10})

  α^{-1} = 137.035 999 037 (91) [Bouchendira et al., PRL 106, 080801 (2011)]

- helium fine structure (accurate to 3×10^{-8})

  α^{-1} = 137.035 999 6 (34)

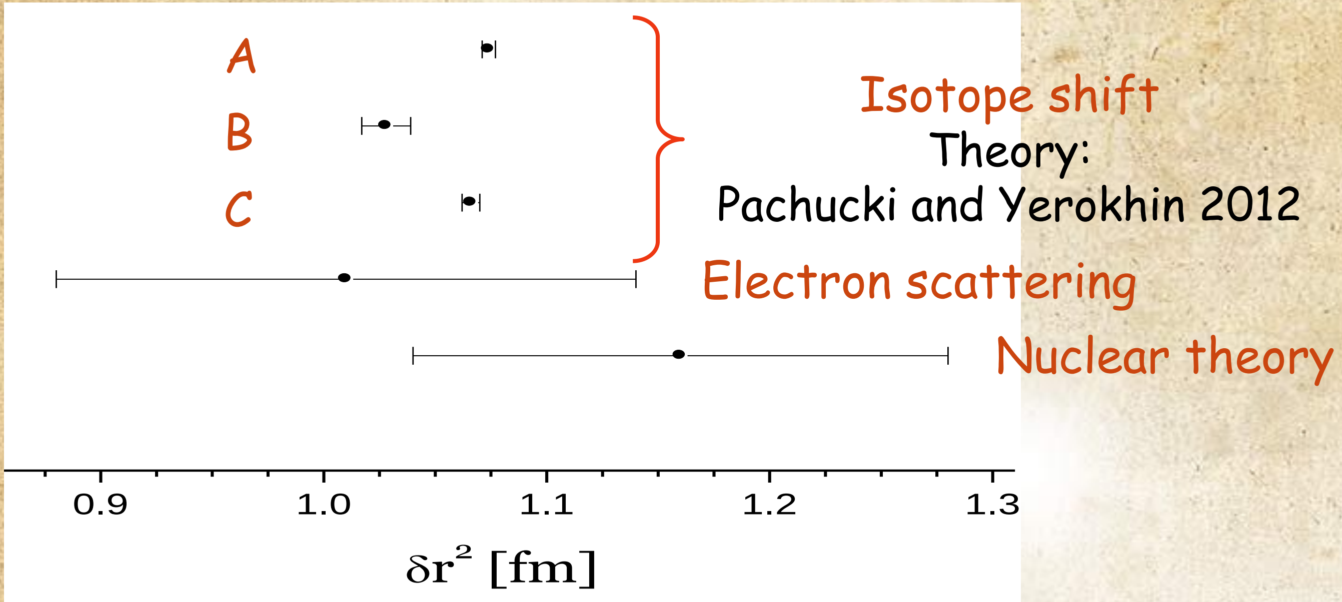
  Theory: Pachucki and Yerokhin, PRL 104, 070403 (2010)

  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}He – ^{4}He isotope shift can be used to determine the difference of the (squares of the) nuclear charge radii δr^2



Experiments:

- A 2^3P-2^3S, Cancio Pastor et al., PRL 108, 143001 (2012)
- B 2^1S-2^3S, van Rooij et al., Science 333, 196 (2011)
- C 2^3P-2^3S, Shiner et al., PRL 74, 3553 (1995)

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:

$$E = E^{(2)}_{\rm NR} + E^{(4)}_{\rm Breit} + E^{(5)}_{\rm QED} + E^{(6)} + E^{(7)} + \ldots$$

$$E^{(n)} = \langle H^{(n)} \rangle \sim m\,\alpha^n$$

$E^{(2)} -$ nonrelativistic energy

$E^{(4)}_{\rm Breit} -$ leading relativistic (Breit) correction

$E^{(5)}_{\rm QED} -$ leading QED (Araki-Sucher) correction

Expansion is non-alalytic in α == 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.

Vladimir Korobov 2000, 2002

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

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

Real nonlinear parameters α_i, β_i, and γ_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

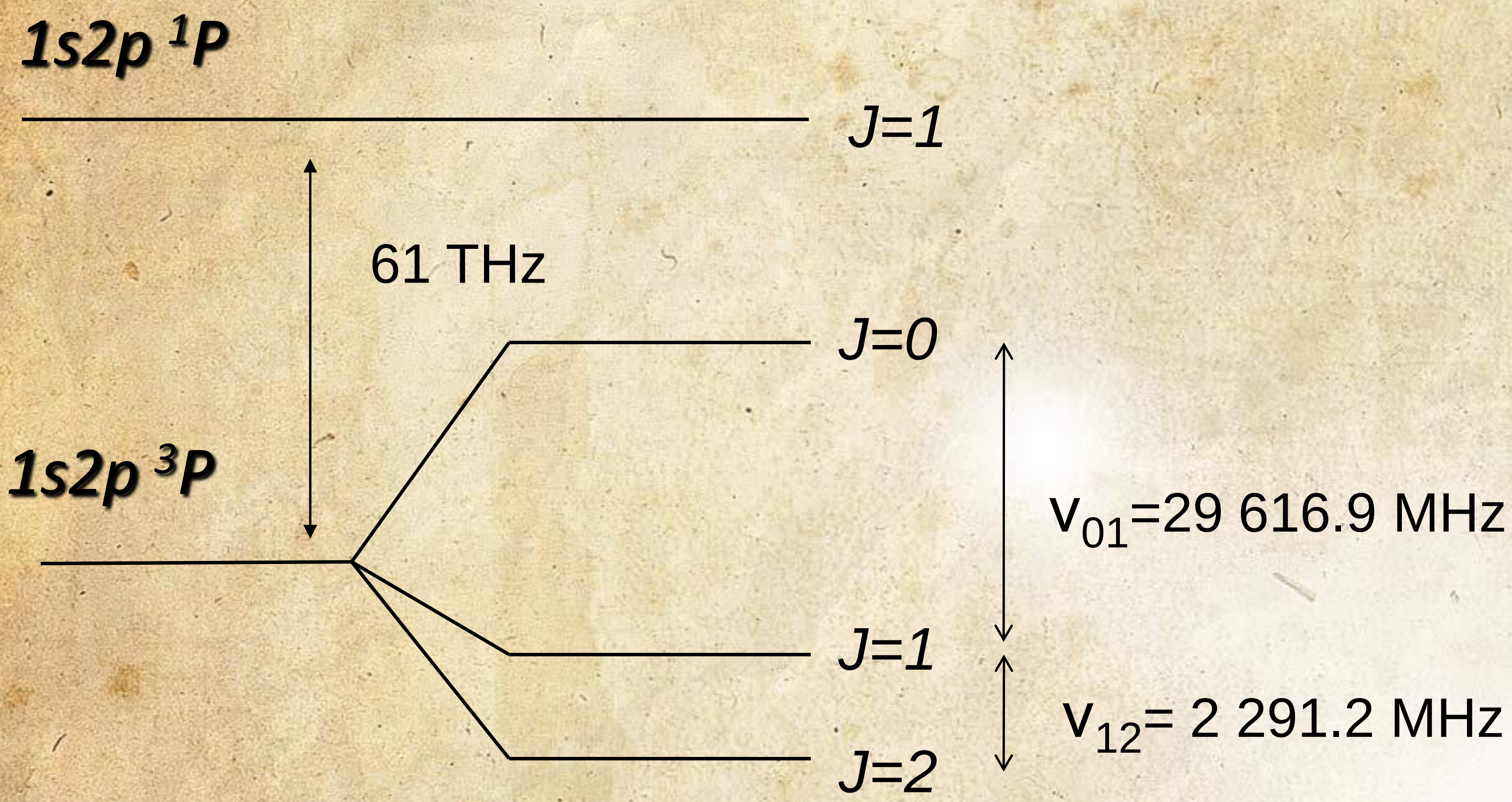
$$\frac{1}{16\pi^2} \int d^3r_1\, d^3r_2\, \frac{e^{-\alpha r_1 - \beta r_2 - \gamma r_{12}}}{r_1\, r_2\, r_{12}} = \frac{1}{(\alpha+\beta)(\beta+\gamma)(\gamma+\alpha)} .$$

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.

$E(2^3P) = -2.133\,164\,190\,779\,283\,205\,146\,96\,^{+0}_{-10}$

Fine structure

Structure of 2P states of ^4He



$\nu_{02} = \nu_{01} + \nu_{12} = 31\,908.1$ MHz

Fine structure: NRQED expansion

$$\langle H_{\rm fs}\rangle = \boxed{\langle H^{(4+)}_{\rm Breit}\rangle} + \boxed{\langle H^{(6)}_{\rm DK}\rangle + \langle H^{(4)}_{\rm Breit}\frac{1}{(E-H)'}H^{(4)}_{\rm Breit}\rangle} + \boxed{\langle H^{(7)}\rangle + 2\,\langle H^{(4)}_{\rm Breit}\frac{1}{(E-H)'}H^{(5)}\rangle + E^{(7)}_L}$$

mα^4 and mα^5 corrections

mα^6corrections

mα^7corrections

Lewis and Serafino 1978

Yan and Drake 1995

Pachucki 2006

Pachucki and Yerokhin 2009,2010

- Second-order perturbative corrections induced by local operators
- Bethe-logarithm type corrections (non-local operators) $E^{(7)}_L$

Fine structure of helium: present status

Table 2. Summary of individual contributions to the fine-structure intervals in helium, in kHz. The parameters [25] are $\alpha^{-1} = 137.035\,999\,679(94)$, $cR_\infty = 3\,289\,841\,960\,361(22)$ kHz, and $m/M = 1.370\,933\,555\,70 \times 10^{-4}$. The label $(+m/M)$ indicates that the corresponding entry comprises both the non-recoil and recoil contributions of the specified order in α.

Term	ν_{01}	ν_{12}	ν_{02}
$m\alpha^4(+m/M)$	29 563 765.45	2 320 241.43	
$m\alpha^5(+m/M)$	54 704.04	−22 545.00	
$m\alpha^6$	−1 607.52(2)	−6 506.43	
$m\alpha^6 m/M$	−9.96	9.15	
$m\alpha^7 \log(Z\alpha)$	81.43	−5.87	
$m\alpha^7$, nlog	18.86	−14.38	
$m\alpha^8$	±1.7	±1.7	
Total theory	29 616 952.29 ± 1.7	2 291 178.91 ± 1.7	31 908 131.20 ± 1.7
Experiment	29 616 951.66(70)[a]	2 291 177.53(35)[d]	31 908 131.25(30)[f]
	29 616 952.7(10)[b]	2 291 175.59(51)[a]	31 908 126.78(94)[a]
	29 616 950.9(9)[c]	2 291 175.9(10)[e]	

Experiments:

a Zelevinsky *et al.* PRL 95, 203001 (2005) [Gabrielse]

b Guisfredi *et al.* Can. J. Phys. 83, 301 (2005) [Inguscio]

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]

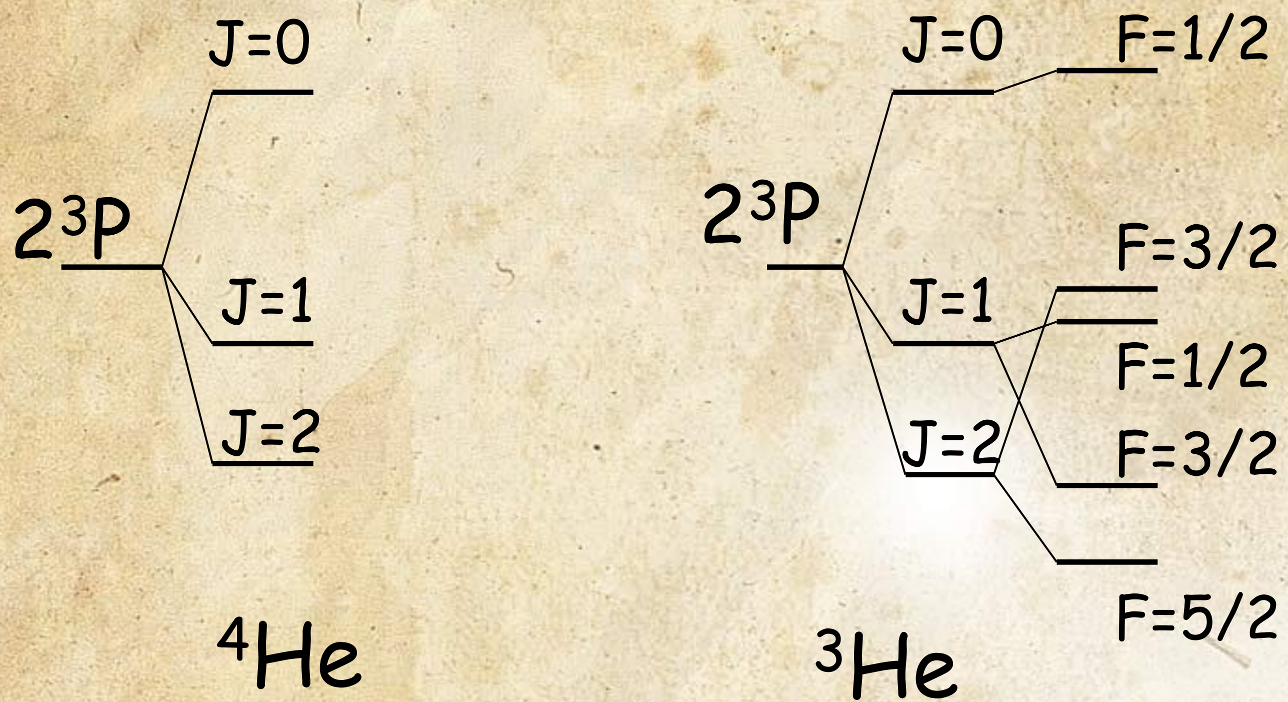
f Smiciklas and Shiner, PRL 105, 123001 (2010) [Shiner]

Theory:

Pachucki and Yerokhin, PRL 104, 070403 (2010)

Hyperfine structure

^4He and ^3He: energy level scheme



(not to scale)

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:

$$|FJ\rangle \equiv |2^3P_J^F\rangle, \text{with } J = 0, 1, 2 \text{ and } F = J \pm 1/2$$

5x5 matrix of the effective Hamiltonian:

$$E_{JJ'}^F = \langle FJ|H|FJ'\rangle$$

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

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

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

All effects that do not depend on electron or nuclear spin do not contribute.

Fine + Hyperfine structure: NRQED expansion

$$\langle H\rangle = \langle H_{\rm fs}\rangle + \langle H_{\rm hfs}^{(4+)}\rangle + \boxed{\langle H_{\rm hfs}^{(6)}\rangle + 2\,\langle H_{\rm hfs}^{(4)}\frac{1}{(E-H)'}H_{\rm Breit}^{(4)}\rangle} + \langle H_{\rm hfs}^{(4)}\frac{1}{(E-H)'}H_{\rm hfs}^{(4)}\rangle + \langle H_{\rm nucl}\rangle$$

$m\alpha^6$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_{Breit} – Breit Hamiltonian (operators do not depend on spin)

H_{nucl} – effective Hamiltonian of nuclear effects

Nuclear effects

Hyperfine interaction $1/r^2$ => nuclear effects are significant.

Cannot be (accurately) calculated from first principles.

One can claim that

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

The constant C can be extracted by comparing theory and experiment for 1s He^+ hyperfine splitting.

An example of second-order contributions

$$
\begin{aligned}
\delta E_{\rm reg}(^3P) \;=\; \sum_{n>2} \frac{1}{E(2^3P)-E(n^3P)} \Big[& \langle 2^3\vec{P}|Q|n^3\vec{P}\rangle\,\langle n^3\vec{P}|\vec{T}|2^3\vec{P}\rangle\,\langle \frac{2}{3}\,\vec{I}\cdot\vec{L} + I^i\,L^j\,(S^i\,S^j)^{(2)}\rangle \\
& + \langle 2^3\vec{P}|Q|n^3\vec{P}\rangle\,\langle n^3\vec{P}|\hat{T}|2^3\vec{P}\rangle\,\langle -\frac{3}{5}\,I^i\,S^j\,(L^i\,L^j)^{(2)}\rangle \\
& + \langle 2^3\vec{P}|\vec{Q}|n^3\vec{P}\rangle\,\langle n^3\vec{P}|T|2^3\vec{P}\rangle\,\langle \vec{I}\cdot\vec{L}\rangle \\
& + \langle 2^3\vec{P}|\vec{Q}|n^3\vec{P}\rangle\,\langle n^3\vec{P}|\vec{T}|2^3\vec{P}\rangle\,\langle \frac{1}{3}\,\vec{I}\cdot\vec{S} + \frac{1}{2}\,I^i\,S^j\,(L^i\,L^j)^{(2)}\rangle \\
& + \langle 2^3\vec{P}|\vec{Q}|n^3\vec{P}\rangle\,\langle n^3\vec{P}|\hat{T}|2^3\vec{P}\rangle\,\langle -\frac{3}{10}\,I^i\,L^j\,(S^i\,S^j)^{(2)}\rangle \\
& + \langle 2^3\vec{P}|\hat{Q}|n^3\vec{P}\rangle\,\langle n^3\vec{P}|T|2^3\vec{P}\rangle\,\langle -\frac{6}{5}\,I^i\,S^j\,(L^i\,L^j)^{(2)}\rangle \\
& + \langle 2^3\vec{P}|\hat{Q}|n^3\vec{P}\rangle\,\langle n^3\vec{P}|\vec{T}|2^3\vec{P}\rangle\,\langle -\frac{1}{3}\,\vec{I}\cdot\vec{L} + \frac{9}{20}\,I^i\,S^j\,(L^i\,L^j)^{(2)} - \frac{1}{20}\,I^i\,L^j\,(S^i\,S^j)^{(2)}\rangle \\
& + \langle 2^3\vec{P}|\hat{Q}|n^3\vec{P}\rangle\,\langle n^3\vec{P}|\hat{T}|2^3\vec{P}\rangle\,\langle \frac{1}{5}\,\vec{I}\cdot\vec{S} - \frac{21}{100}\,I^i\,S^j\,(L^i\,L^j)^{(2)} - \frac{27}{100}\,I^i\,L^j\,(S^i\,S^j)^{(2)}\rangle \Big]\,.
\end{aligned}
$$

2^3P hyperfine structure in He

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

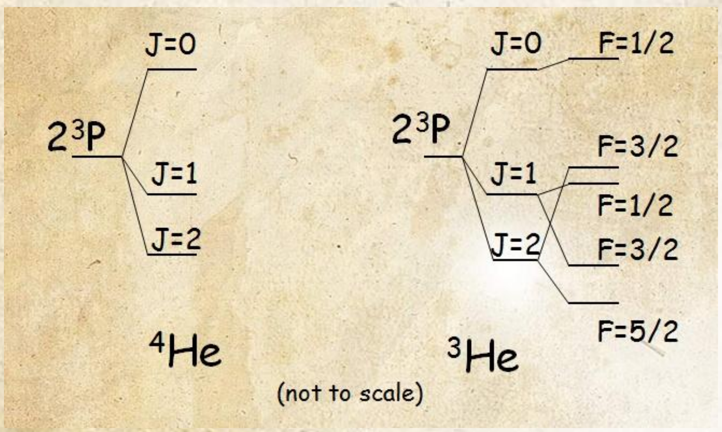
Theory, present: Pachucki and Yerokhin, PRA 85, 042517 (2012)

Theory, previous: Wu and Drake, J. Phys. B 40, 393 (2007)

Experiment, Texas: Smiciklas, 2003, xxx.lanl.gov/abs/1203.2830

Experiment, Florence, Cancio Pastor et al., PRL 108, 143001 (2012)

Isotope shift



^{4}He – ^{3}He Isotope shift

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

^{4}He, Centroid energy:

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

^{3}He, Centroid energy:

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

^{4}He – ^{3}He Isotope shift, results

TABLE I: ^{4}He–^{3}He isotope shift of the centroid energies, for the point-like nucleus, in kHz.

Contribution	2^3P-2^3S transition	2^1S-2^3S transition
$m_r\,\alpha^2$	12412458.1	8 632 567.86
$m_r\,\alpha^2\,(m_r/M)$	21 243 041.3	−608 175.58
$m_r\,\alpha^2\,(m_r/M)^2$	13874.6	7319.80
$m_r\,\alpha^2\,(m_r/M)^3$	4.6	−0.30
$m_r\,\alpha^4$	17872.8	8 954.22
$m_r\,\alpha^4\,(m_r/M)$	−20 082.4	−6 458.23
$m_r\,\alpha^4\,(m_r/M)^2$	−3.0	−1.84
$m\,\alpha^5\,(m/M)$	−60.7	−56.61
$m\,\alpha^6\,(m/M)$	−15.5 (3.9)	−2.75 (69)
Nuclear polarizability	−1.1 (1)	−0.20 (2)
HFS mixing	54.6	−80.72
Total theory	33667143.2 (3.9)	8 034 065.66 (69)
Other theory [1,2][a]	33667146.2 (7)	8 034 067.8 (1.1)

[1] D. C. Morton, Q. Wu, and G. W. F. Drake, Can. J. Phys. **84**, 83 (2006),
[2] G. W. F. Drake, priv. comm. from R. van Rooij *et al.* Science **333**, 196 (2011).
[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

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

2^3P-2^3S, Cancio Pastor et al., PRL 108, 143001 (2012); theory by Pachucki and Yerokhin (2012)

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

2^1S-2^3S, van Rooij et al., Science 333, 196 (2011) + theory by Pachucki and Yerokhin (2012)

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

2^3P-2^3S, Shiner et al., PRL 74, 3553 (1995) + theory by Pachucki and Yerokhin (2012)

$\delta r^2 = 1.066\ (4)\ \mathrm{fm}^2$

Conclusion

Experiment versus Theory in He

	Experiment, accuracy	Theory, accuracy
Lamb shift	2 kHz	3000 kHz
Fine structure	0.2 kHz	2 kHz
Hyperfine structure	2 kHz	2 kHz