High Precision Atomic Data as a Measurement Tool for Halo Nuclei: Theory

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"To understand hydrogen is to understand all of physics."
– Victor Weisskopf (cited by Dan Kleppner in *Physics Today*, April 1999).

"There is a reason physicists are so successful with what they do, and that is they study the hydrogen atom and the helium ion and then they stop."
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Helium and lithium now also rank as a fundamental atomic systems. What's new?

- Essentially exact solutions to the quantum mechanical three-body problem.
- Accurate relativistic and QED corrections up to order α^4 Ry for total energies, and α^5 Ry for fine structure splittings.
- Techniques of single-atom spectroscopy.

semin23.tex, March, 2012. Thanks to Randolph Pohl.

OUTLINE

Main Theme: Both theory and experiment continue pushing toward ever higher levels of accuracy. Explore ways that they can be combined to achieve new types of measurements, or measurement techniques.

Examples – Hot Topics:

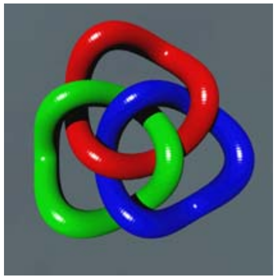
- Properties of exotic "halo" nuclei from atomic isotope shifts
  Theory: Drake (Windsor), Yan & Wang (UNB), Pachucki (Poland)
  Experiment: Argonne (Chicago), GSI (Darmstadt), TRIUMF (Vancouver)

- Atomic fine structure splittings as a means to measure the fine structure constant.
  Theory: Drake (Windsor), Pachucki (Poland), Yerokhin (Russia).
  Experiment: Shiner (North Texas), Hessels (York), Gabrielse (Harvard), Inguscio (Florence)

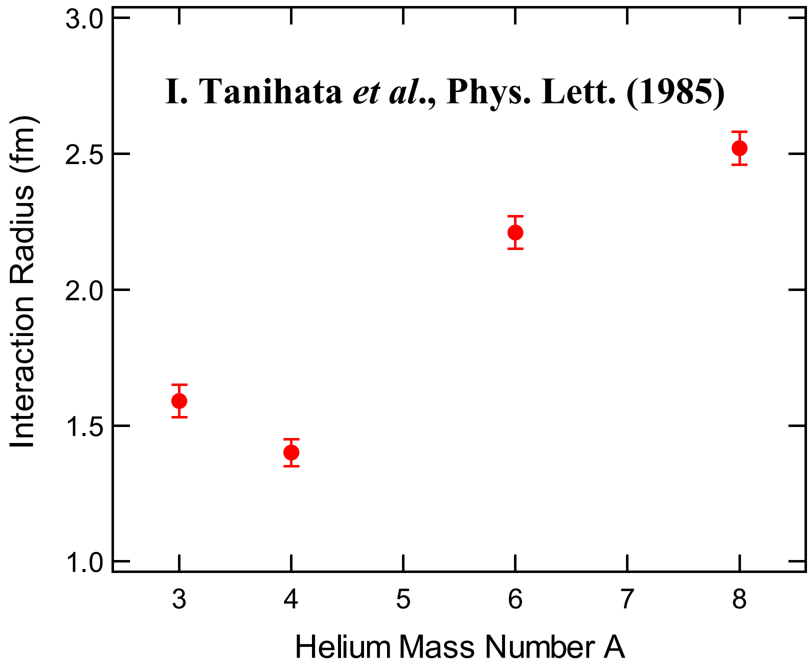
- Proton size anomaly: the electronic and muonic values do not agree for the charge radius (Randolf Pohl, Garching)

Halo Nuclei ^{6}He and ^{8}He

Isotope	Half-life	Spin	Isospin	Core + Valence
He-6	807 ms	0^+	1	α + 2n
He-8	119 ms	0^+	2	α + 4n



Borromean



Core-Halo Structure

$$\sigma_I(6He) - \sigma_I(4He) = \sigma_{-2n}(6He)$$

$$\sigma_I(8He) - \sigma_I(4He) = \sigma_{-2n}(8He) + \sigma_{-4n}(8He)$$

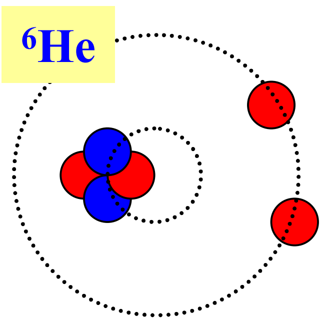
$$\sigma_I(8He) - \sigma_I(6He) \neq \sigma_{-2n}(8He)$$

I. Tanihata *et al.*, Phys. Lett. (1992)

Charge Radii Measurements

Methods of measuring nuclear radii (interaction radii, matter radii, charge radii)

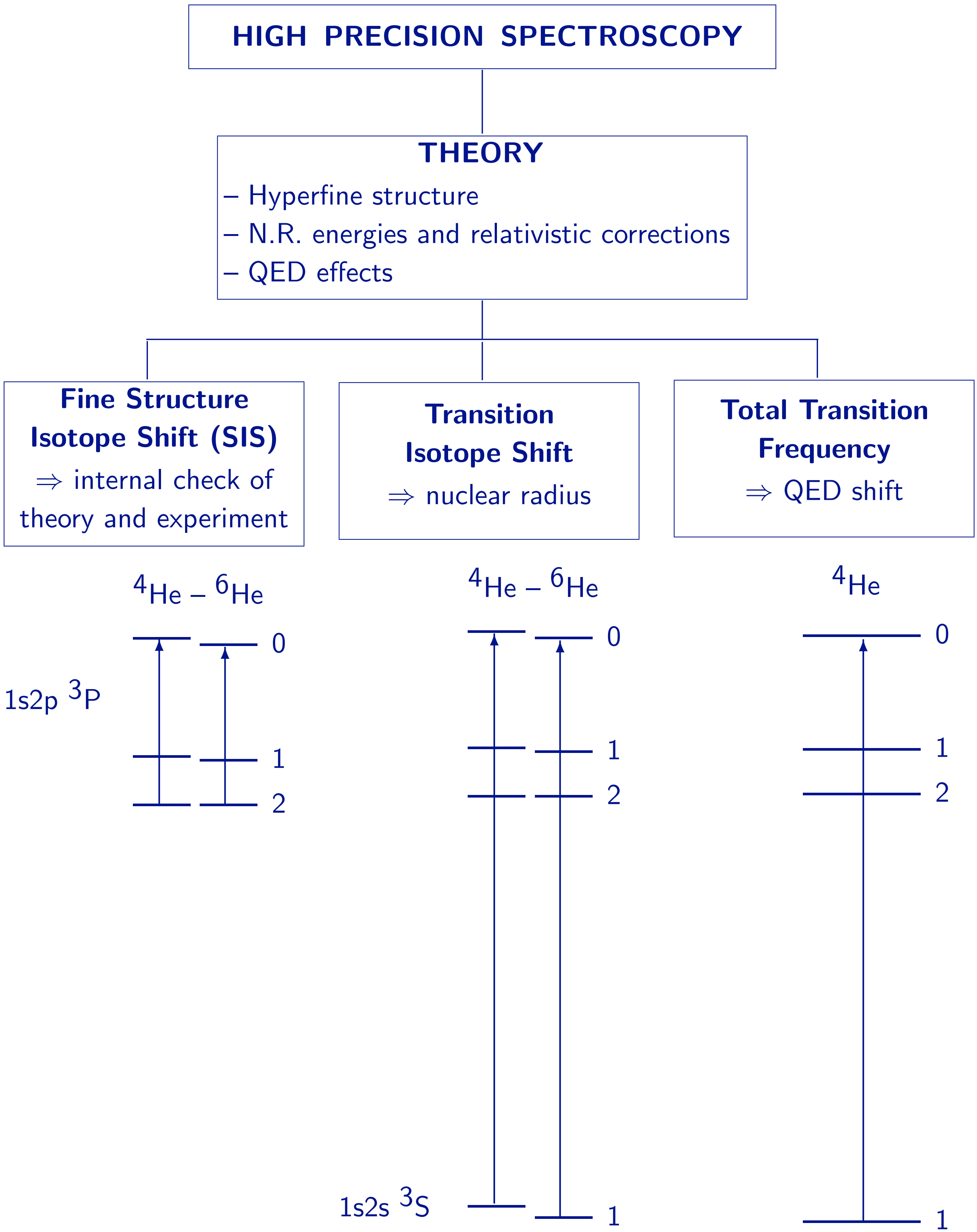
- Nuclear scattering – model dependent
- Electron scattering – stable isotope only
- Muonic atom spectroscopy – stable isotope only
- Atomic isotope shift



RMS point proton radii (fm) from theory and experiment

	He-3	He-4	He-6	He-8
QMC Theory	1.74(1)	1.45(1)	1.89(1)	1.86(1)
μ-He Lamb Shift		1.474(7)		
Atomic Isotope Shift	1.766(6)		**?**	**?**
p-He Scattering			1.95(10) GG 1.81(09) GO	1.68(7) GG 1.42(7) GO

G.D. Alkhazov et al., Phys. Rev. Lett. **78**, 2313 (1997);
D. Shiner et al., Phys. Rev. Lett. **74**, 3553 (1995).



Flow diagram for types of measurements.

Phenomenologically, The isotope shift between isotopes x and y for some atomic transition frequency is

$$(\mathrm{IS})_{x-y} = A + B(\bar{r}^2_{\mathrm{c},\,x} - \bar{r}^2_{\mathrm{c},\,y})$$

where $\bar{r}_{\mathrm{c}}$ = rms nuclear charge radius.

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where $\bar{r}_{\mathrm{c}} =$ rms nuclear charge radius.

Measure $(\mathrm{IS})_{x-y}$, and calculate A and B from atomic theory.

History

1. G.W.F. Drake in *Long-range Casimir Forces: Theory and Recent Experiments in Atomic Systems*, Edited by F.S. Levin and S.A. Micha (Plenum, New York, 1993).

^{3}He – ^{4}He Isotope shift (MHz)

Transition	Theory [a]	Experiment [b]	Difference
$2\ ^3S_1 - 2\ ^3P_0$	33 667.734(1)	33 667.968(38)	–0.234(38)
$2\ ^3S_1 - 2\ ^3P_1$	33 667.459(1)	33 667.693(38)	–0.234(38)
$2\ ^3S_1 - 2\ ^3P_2$	33 668.447(1)	33 668.670(38)	–0.223(38)

[a]Assuming $r_c(^3\text{He}) = 1.875 \pm 0.05$ fm. (from nuclear scattering)

[b]Zhao, Lawell, and Pipkin, Phys. Rev. Lett. **66**, 592 (1991).

Adjust $r_c(^3\text{He}) = 1.925 \pm 0.008$ fm. (revised to 1.963 fm.)

2. Riis, Sinclair, Poulsen, Drake, Rowley and Levick, "Lamb shifts and hyperfine structure in $^6\text{Li}^+$ and $^7\text{Li}^+$: theory and experiment," Phys. Rev. A **49**, 207–220 (1993).

   Showed that the ^{6}Li – ^{7}Li difference in r_c is in good agreement with nuclear scattering data.

Time-Line for Isotope Shift Measurements

1993 — Pipkin/Drake [1, 2]: ^{3}He-^{4}He $2\,^3\mathrm{S}$-$2\,^3\mathrm{P} \Longrightarrow \bar{r}_{\mathrm{c}}(^3\mathrm{He}) = 1.963 \pm 0.006$ fm (revised 2006 [3]).

— Riis [4]: ^{6}Li$^+$-^{7}Li$^+$ agrees with $\Delta\bar{r}_{\mathrm{c}}^2$ from nuclear scattering data.

1994 — Inguscio [5]: ^{3}He-^{4}He $2\,^3\mathrm{S}$-$3\,^3\mathrm{P} \Longrightarrow \bar{r}_{\mathrm{c}}(^3\mathrm{He}) = 1.985 \pm 0.041$ fm (revised/06).

1995 — Shiner [6]: ^{3}He-^{4}He $2\,^3\mathrm{S}$-$2\,^3\mathrm{P} \Longrightarrow \bar{r}_{\mathrm{c}}(^3\mathrm{He}) = 1.9643 \pm 0.0011$ fm (revised/06).

1996 — GSI: Andreas Dax suggests the ^{11}Li halo nucleus experiment.

2000 — GSI [7]: Schmitt, Dax, Kirchner, Kluge, Kühl, Tanihata, Wakasugi, Wang, and Zimmermann: Formal ^{11}Li proposal in Hyperfine Interactions.

— GSI: Wilfried Nörtershäuser begins work on the ^{11}Li experiment.

— Drake & Goldman [8]: Bethe logs and QED corrections for He $\Longrightarrow$ control of theoretical uncertainties up to order $\alpha^3\mu/M$ Ry ($\sim$1 part in 10^{10}).

2001 Argonne: Z.-T. Lu suggests ^{6}He experiment.
Pieper & Wiringa [9]: $\bar{r}_c$ from QMC calculations.

2003 Yan & Drake [10]: Bethe logs and QED shift for Li and Be^+.
Pachucki & Komasa [11] confirm QED result for the ground state.

2004 Argonne [12]: ^{6}He experiment completed.

2006 Feldmeier, Neff and Roth [13]: Fermionic molecular dynamics calculations.
GSI/TRIUMF [14]: ^{9}Li and ^{11}Li experiment completed.

2007 Pachucki & Moro [15]: nuclear polarization correction.

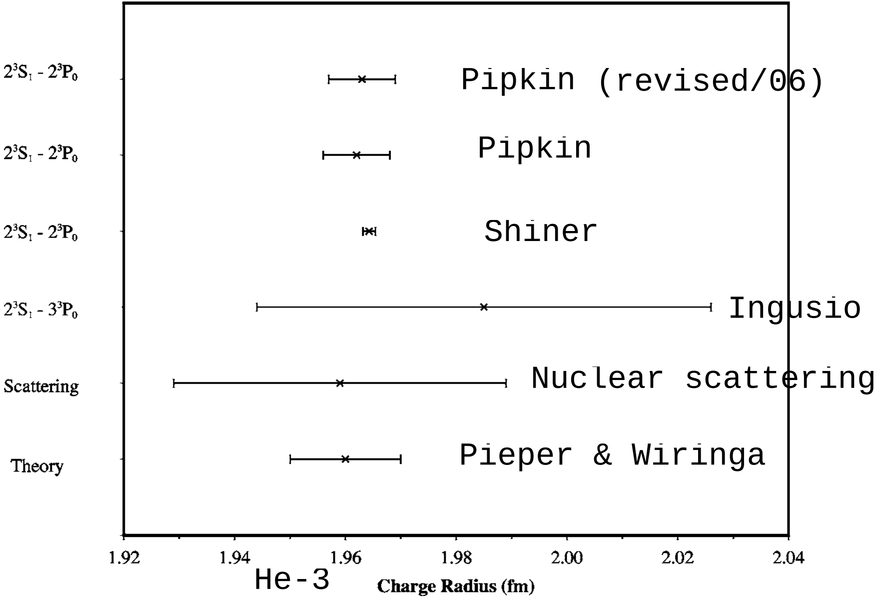
2008 Puchalski & Pachucki [16]: independent calculations for Li and Be^+.
Argonne [17]: ^{8}He experiment completed.
TRIUMF [18]: Penning trap mass measurement for ^{11}Li.
GSI/Mainz/ISOLDE [19]: ^{11}Be experiment completed.

2009 Pulchalski and Pachucki [20]: hyperfine splittings for Li and Be^+
TRIUMF [21]: Penning trap mass measurement for ^{11}Be

2011 GSI [22, 23]: Nuclear structure calculations and interpretation
Neff, Sick, Nördershäuser, Sanchez [24].

2012 TRIUMF: Penning trap mass measurement for ^{6}He and ^{8}He
GSI/ISOLDE [25]: ^{12}Be experiment completed.

2013 Argonne/GSI: Proposed boron proton-halo experiment ^{8}B.



Morton et al. PRA 73, 034502 (2006) 034502-2

Also van Rooij et al. (2011): r_c = 1.961 fm.

Science

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- REPORT

Frequency Metrology in Quantum Degenerate Helium: Direct Measurement of the $2\ ^3S_1 \rightarrow 2\ ^1S_0$ Transition

R. van Rooij[1], J. S. Borbely[1], J. Simonet[2], M. D. Hoogerland[3], K. S. E. Eikema[1], R. A. Rozendaal[1], W. Vassen[1,*]

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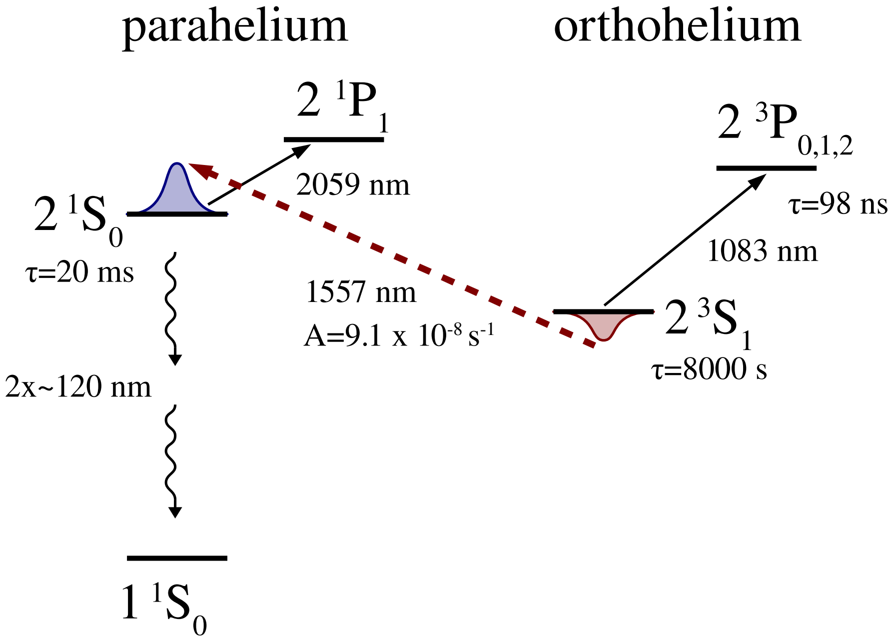
ABSTRACT

Precision spectroscopy of simple atomic systems has refined our understanding of the fundamental laws of quantum physics. In particular, helium spectroscopy has played a crucial role in describing two-electron interactions, determining the fine-structure constant and extracting the size of the helium nucleus. Here we present a measurement of the doubly forbidden 1557-nanometer transition connecting the two metastable states of helium (the lowest energy triplet state $2\ ^3S_1$ and first excited singlet state $2\ ^1S_0$), for which quantum electrodynamic and nuclear size effects are very strong. This transition is weaker by 14 orders of magnitude than the most predominantly measured transition in helium. Ultracold, submicrokelvin, fermionic ^{3}He and bosonic ^{4}He atoms are used to obtain a precision of 8×10^{-12}, providing a stringent test of two-electron quantum electrodynamic theory and of nuclear few-body theory.

r_c = 1.961(4) fm.


parahelium
orthohelium
2 1P1
2 3P0,1,2
2059 nm
τ=98 ns
2 1S0
1083 nm
τ=20 ms
1557 nm
A=9.1 x 10-8 s-1
2 3S1
τ=8000 s
2x~120 nm
1 1S0

Frequency Metrology of Helium around 1083 nm and Determination of the Nuclear Charge Radius

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[2]*European Laboratory for Non-Linear Spectroscopy (LENS) and Dipartimento di Fisica, Universitá di Firenze, Via Nello Carrara 1, I-50019 Sesto Fiorentino, Italy*

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We measure the absolute frequency of seven out of the nine allowed transitions between the $2\,^3S$ and $2\,^3P$ hyperfine manifolds in a metastable ^{3}He beam by using an optical frequency comb synthesizer-assisted spectrometer. The relative uncertainty of our measurements ranges from 1×10^{-11} to 5×10^{-12}, which is, to our knowledge, the most precise result for any optical ^{3}He transition to date. The resulting $2\,^3P$–$2\,^3S$ centroid frequency is 276 702 827 204.8(2.4) kHz. Comparing this value with the known result for the ^{4}He centroid and performing *ab initio* QED calculations of the ^{4}He-^{3}He isotope shift, we extract the difference of the squared nuclear charge radii δr^2 of ^{3}He and ^{4}He. Our result for $\delta r^2 = 1.074(3)$ fm^2 disagrees by about 4σ with the recent determination [R. van Rooij *et al.*, Science **333**, 196 (2011)].

DOI: 10.1103/PhysRevLett.108.143001 PACS numbers: 31.30.Gs, 21.10.Ft, 31.30.J−, 42.62.Eh

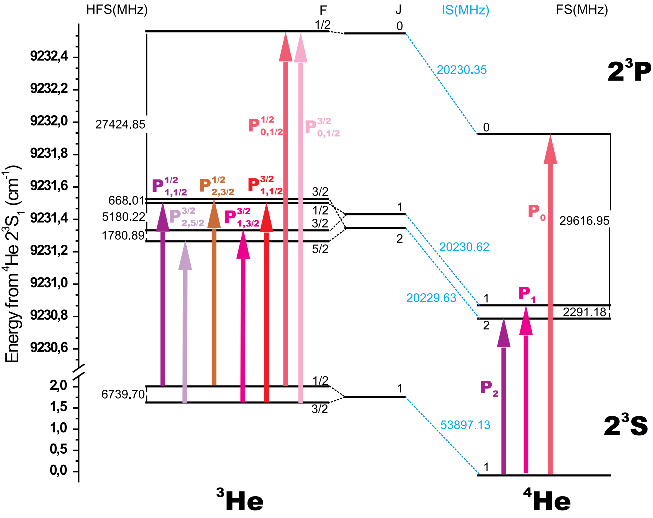


FIG. 1: (color online) . Level scheme of the 2^3S and 2^3P

TABLE III. ^{4}He-^{3}He isotope shift of the centroid energies, for the pointlike nucleus, in kHz. m_r is the reduced mass, and M is the nuclear mass.

Contribution	$2\,^3P$–$2\,^3S$	$2\,^1S$–$2\,^3S$
$m_r\alpha^2$	12 412 458.1	8 632 567.86
$m_r\alpha^2(m_r/M)$	21 243 041.3	−608 175.58
$m_r\alpha^2(m_r/M)^2$	13 874.6	7319.80
$m_r\alpha^2(m_r/M)^3$	4.6	−0.30
$m_r\alpha^4$	17 872.8	8954.22
$m_r\alpha^4(m_r/M)$	−20 082.4	−6458.23
$m_r\alpha^4(m_r/M)^2$	−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	−80.69
Total	33 667 143.2(3.9)	8 034 065.69(69)
Other theory [13,16][a]	33 667 146.2(7)	8 034 067.8(1.1)

[a]Corrected by adding the triplet-singlet HFS mixing.

Determinations of $\Delta r_c^2 = r_c^2(^3\mathrm{He}) - r_c^2(^4\mathrm{He})$. Units are fm^2.

Δr_c^2	Method	Authors	Ref.
1.059(3)	$2\ ^3\mathrm{P}_0 - 2\ ^3\mathrm{S}_1$	Shiner et al. (1995)	[1]
1.019(11)	$2\ ^1\mathrm{S}_0 - 2\ ^3\mathrm{S}_1$	van Rooij et al. (2011)	[2]
1.028(11)	$2\ ^1\mathrm{S}_0 - 2\ ^3\mathrm{S}_1$	Pachucki & Yerokhin revision (2012)	[3]
1.074(3)	$2\ ^3\mathrm{P}_{\mathrm{cg}} - 2\ ^3S_1$	Cancio Pastor et al. (2012)	[3]
1.16(12)	Nuclear few-body theory	Kievsky et al. (2008)	[4]
1.01(13)	Electron-nuclear scattering	Sick (2008)	[5]

1. D. Shiner, R. Dixson, V. Vedantham, Phys. Rev. Lett. **74**, 3553 (1995).
2. R. van Rooij, J.S. Borbely, J. Simonet, M.D. Hoogerland, K.S.E. Eikema, R.A. Rozendaal and W. Vassen, Science **333**, 196 (2011).
3. P. Cancio Pastor, L. Consolino, G. Giusfredi, P. De Natale, M. Inguscio, V. A. Yerokhin, and K. Pachucki, Phys. Rev. Lett. **108**, 143001 (2012).
4. A. Kievsky, S. Rosati, M. Viviani, L. E. Marcucc, L. Girlanda, J. Phys. G **35**, 063101 (2008).
5. I. Sick, Phys. Rev. C **77**, 041302 (2008) ($r_c(^4\mathrm{He}) = 1.681 \pm 0.004$ fm.); Lect. Notes Phys. **745**, 57 (2008).

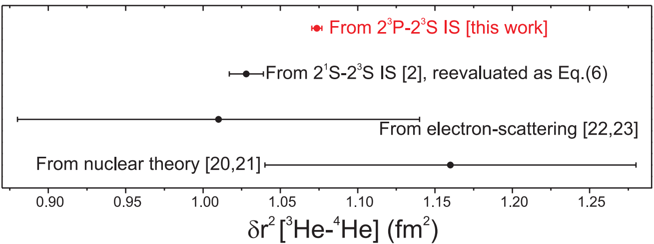


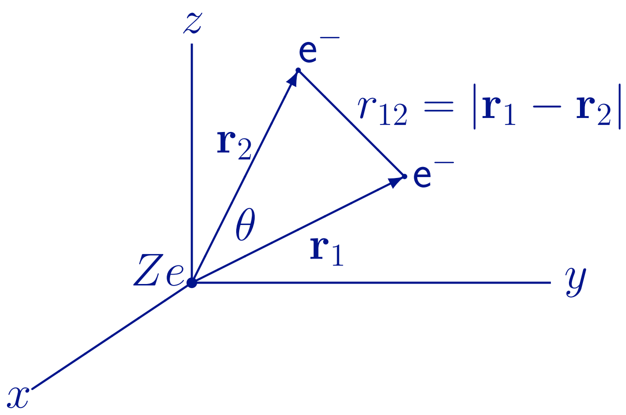
FIG. 3 (color online). Different determinations of the difference of the squared nuclear charge radii for ^{3}He and ^{4}He.

Contributions to the energy and their orders of magnitude in terms of Z, $\mu/M = 1.370\,745\,624 \times 10^{-4}$, and $\alpha^2 = 0.532\,513\,6197 \times 10^{-4}$.

Contribution	Magnitude
Nonrelativistic energy	Z^2
Mass polarization	$Z^2\mu/M$
Second-order mass polarization	$Z^2(\mu/M)^2[1 + O(\mu/M) + \cdots]$
Relativistic corrections	$Z^4\alpha^2$
Relativistic recoil	$Z^4\alpha^2\mu/M[1 + O(\mu/M) + \cdots]$
Anomalous magnetic moment	$Z^4\alpha^3$
Hyperfine structure	$Z^3 g_I \mu_0^2$
Lamb shift	$Z^4\alpha^3 \ln\alpha + \cdots$
Radiative recoil	$Z^4\alpha^3(\ln\alpha)\mu/M$
Finite nuclear size	$Z^4\langle\bar{r}_\mathrm{c}/a_0\rangle^2$
Nuclear polarization	$Z^3 e^2 \alpha_{\mathrm{d,nuc}}/(\alpha a_0)$

Isotope shift: $\Delta\nu = \Delta\nu^{(0)} + C\langle\bar{r}_\mathrm{c}\rangle^2$

Nonrelativistic Eigenvalues



The Hamiltonian in atomic units is

$$H = -\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 - \frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{r_{12}}$$

Expand

$$\Psi(\mathbf{r}_1, \mathbf{r}_2) = \sum_{i,j,k} a_{ijk}\, r_1^i r_2^j r_{12}^k\, e^{-\alpha r_1 - \beta r_2}\, \mathcal{Y}_{l_1 l_2 L}^{M}(\hat{\mathbf{r}}_1, \hat{\mathbf{r}}_2)$$

(Hylleraas, 1929). Pekeris shell: $i + j + k \leq \Omega, \quad \Omega = 1, 2, \ldots$.

Methods of Theoretical Atomic Physics.

Method	Typical Accuracy for the Energy
Many Body Perturbation Theory	$\geq 10^{-6}$ a.u.
Configuration Interaction	10^{-6} – 10^{-8} a.u.
Explicitly Correlated Gaussians[a]	$\sim 10^{-10}$ a.u.
Hylleraas Coordinates (He)[b,c]	$\leq 10^{-35}$ – 10^{-40} a.u.
Hylleraas Coordinates (Li)[d]	$\sim 10^{-15}$ a.u.

[a]S. Bubin and Adamowicz J. Chem. Phys. **136**, 134305 (2012).

[b]C. Schwartz, Int. J. Mod. Phys. E–Nucl. Phys. **15**, 877 (2006).

[c]H. Nakashima, H. Nakatsuji, J. Chem. Phys. **127**, 224104 (2007).

[d]Present work: L.M. Wang et al., Phys. Rev. A **85**, 052513 (2012) .

Rayleigh-Schrödinger Variational Principle

Diagonalize H in the

$$\chi_{ijk} = r_1^i r_2^j r_{12}^k \, e^{-\alpha r_1 - \beta r_2} \, \mathcal{Y}_{l_1 l_2 L}^M(\hat{\mathbf{r}}_\mathbf{1}, \hat{\mathbf{r}}_\mathbf{2})$$

basis set to satisfy the variational condition

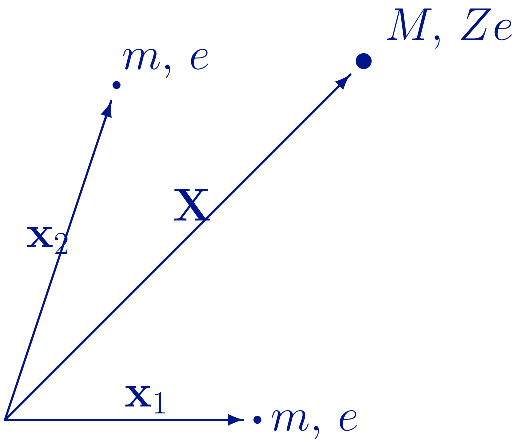
$$\delta \int \Psi \, (H - E) \, \Psi \, d\tau = 0.$$

For finite nuclear mass M,

$$H = -\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 - \frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{r_{12}} - \frac{\mu}{M}\nabla_1 \cdot \nabla_2$$

in reduced mass atomic units e^2/a_μ, where $a_\mu = (m/\mu)a_0$ is the reduced mass Bohr radius, and $\mu = mM/(m+M)$ is the electron reduced mass.

Mass Scaling



$$H = -\frac{\hbar^2}{2M}\nabla_X^2 - \frac{\hbar^2}{2m}\nabla_{x_1}^2 - \frac{\hbar^2}{2m}\nabla_{x_2}^2 - \frac{Ze^2}{|\mathbf{X}-\mathbf{x}_1|} - \frac{Ze^2}{|\mathbf{X}-\mathbf{x}_2|} + \frac{e^2}{|\mathbf{x_1}-\mathbf{x}_2|}$$

Transform to centre-of-mass plus relative coordinates $\mathbf{R}$, $\mathbf{r}_1$, $\mathbf{r}_2$

$$\begin{aligned} \mathbf{R} &= \frac{M\mathbf{X} + m\mathbf{x}_1 + m\mathbf{x}_2}{M+2m} \\ \mathbf{r}_1 &= \mathbf{X} - \mathbf{x}_1 \\ \mathbf{r}_2 &= \mathbf{X} - \mathbf{x}_2 \end{aligned}$$

and ignore centre-of-mass motion. Then

$$H = -\frac{\hbar^2}{2\mu}\nabla_{r_1}^2 - \frac{\hbar^2}{2\mu}\nabla_{r_2}^2 - \frac{\hbar^2}{M}\nabla_{r_1}\cdot\nabla_{r_2} - \frac{Ze^2}{r_1} - \frac{Ze^2}{r_2} + \frac{e^2}{|\mathbf{r_1}-\mathbf{r}_2|}$$

Expand

$$\begin{aligned}\Psi &= \Psi_0 + \frac{\mu}{M}\Psi_1 + \left(\frac{\mu}{M}\right)^2 \Psi_2 + \cdots \\ \mathcal{E} &= \mathcal{E}_0 + \frac{\mu}{M}\mathcal{E}_1 + \left(\frac{\mu}{M}\right)^2 \mathcal{E}_2 + \cdots\end{aligned}$$

The zero-order problem is the Schrödinger equation for infinite nuclear mass

$$\left\{-\frac{1}{2}\nabla^2_{\rho_1} - \frac{1}{2}\nabla^2_{\rho_2} - \frac{Z}{\rho_1} - \frac{Z}{\rho_2} + \frac{1}{|\boldsymbol{\rho}_1 - \boldsymbol{\rho}_2|}\right\}\Psi_0 = \mathcal{E}_0\Psi_0$$

The “normal” isotope shift is

$$\Delta E_{\mathsf{normal}} = -\frac{\mu}{M}\left(\frac{\mu}{m}\right)\mathcal{E}_0 \quad 2R_\infty$$

The first-order “specific” isotope shift is

$$\Delta E^{(1)}_{\mathsf{specific}} = -\frac{\mu}{M}\left(\frac{\mu}{m}\right)\langle\Psi_0|\nabla_{\rho_1}\cdot\nabla_{\rho_2}|\Psi_0\rangle \quad 2R_\infty$$

The second-order “specific” isotope shift is

$$\Delta E^{(2)}_{\mathsf{specific}} = \left(-\frac{\mu}{M}\right)^2\left(\frac{\mu}{m}\right)\langle\Psi_0|\nabla_{\rho_1}\cdot\nabla_{\rho_2}|\Psi_1\rangle \quad 2R_\infty$$

Convergence study for the ground state of helium [1].

Ω	N	$E(\Omega)$	$R(\Omega)$
8	269	−2.903 724 377 029 560 058 400	
9	347	−2.903 724 377 033 543 320 480	
10	443	−2.903 724 377 034 047 783 838	7.90
11	549	−2.903 724 377 034 104 634 696	8.87
12	676	−2.903 724 377 034 116 928 328	4.62
13	814	−2.903 724 377 034 119 224 401	5.35
14	976	−2.903 724 377 034 119 539 797	7.28
15	1150	−2.903 724 377 034 119 585 888	6.84
16	1351	−2.903 724 377 034 119 596 137	4.50
17	1565	−2.903 724 377 034 119 597 856	5.96
18	1809	−2.903 724 377 034 119 598 206	4.90
19	2067	−2.903 724 377 034 119 598 286	4.44
20	2358	−2.903 724 377 034 119 598 305	4.02
Extrapolation	∞	−2.903 724 377 034 119 598 311(1)	
Korobov [2]	5200	−2.903 724 377 034 119 598 311 158 7	
Korobov extrap.	∞	−2.903 724 377 034 119 598 311 159 4(4)	
Schwartz [3]	10259	−2.903 724 377 034 119 598 311 159 245 194 404 4400	
Schwartz extrap.	∞	−2.903 724 377 034 119 598 311 159 245 194 404 446	
Goldman [4]	8066	−2.903 724 377 034 119 593 82	
Bürgers *et al.* [5]	24 497	−2.903 724 377 034 119 589(5)	
Baker *et al.* [6]	476	−2.903 724 377 034 118 4	

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Variational Basis Set for Lithium

Solve for Ψ_0 and Ψ_1 by expanding in Hylleraas coordinates

$$r_1^{j_1}\, r_2^{j_2}\, r_3^{j_3}\, r_{12}^{j_{12}}\, r_{23}^{j_{23}}\, r_{31}^{j_{31}}\, e^{-\alpha r_1 - \beta r_2 - \gamma r_3}\, \mathcal{Y}^{LM}_{(\ell_1 \ell_2)\ell_{12},\ell_3}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3)\, \chi_1\,, \tag{1}$$

where $\mathcal{Y}^{LM}_{(\ell_1 \ell_2)\ell_{12},\ell_3}$ is a vector-coupled product of spherical harmonics, and χ_1 is a spin function with spin angular momentum $1/2$.

Include all terms from (1) such that

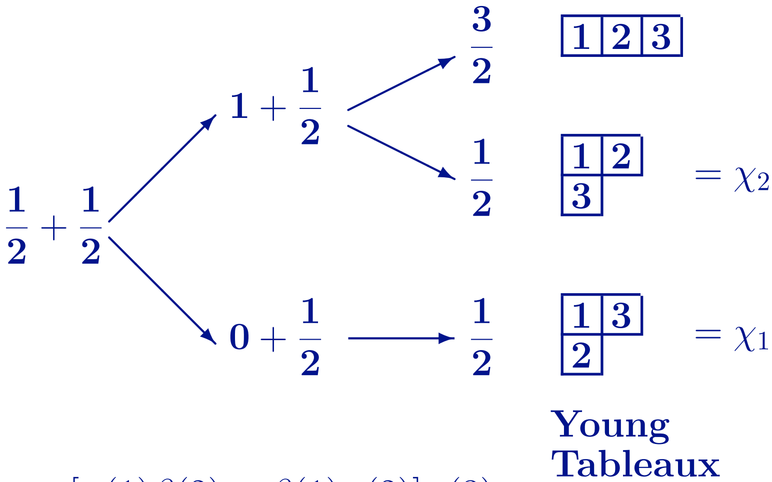
$$j_1 + j_2 + j_3 + j_{12} + j_{23} + j_{31} \;\le\; \Omega\,, \tag{2}$$

and study the eigenvalues as Ω is progressively increased.

The explicit mass-dependence of E is

$$E \;=\; \varepsilon_0 + \lambda\varepsilon_1 + \lambda^2\varepsilon_2 + O(\lambda^3)\,, \quad \text{in units of } 2R_M = 2(1+\lambda)R_\infty\,.$$

Alternative Spin Coupling Chains.



$$\chi_1 = [\alpha(1)\beta(2) - \beta(1)\alpha(2)]\alpha(3)$$
$$\chi_2 = 2\alpha(1)\alpha(2)\beta(3) - [\alpha(1)\beta(2) + \beta(1)\alpha(2)]\alpha(3)$$

The complete wave function is

$$\psi = \mathcal{A}(\phi_1\chi_1 + \phi_2\chi_2)$$

where $\mathcal{A}$ is the total antisymmetrizer

$$\mathcal{A} = e - (12) - (13) - (23) + (123) + (132)$$

Question: Do we need both χ_1 and χ_2?

Larsson's Argument

Sven Larsson, Phys. Rev **169**, 59 (1968).

Suppose that a function $\psi_1 = \mathcal{A}\{\phi \cdot (\alpha\beta - \beta\alpha)\alpha\}$ is contained in the basis set. Now we can generate new functions by permuting the labels in ϕ. The key point is that this is equivalent to permuting the spin labels after antisymmetrization, multiplied by the original ϕ. For example

$$\psi' = \mathcal{A}\{(13)\phi \cdot (\alpha\beta - \beta\alpha)\alpha\} = -\mathcal{A}\{\phi \cdot (\alpha\beta\alpha - \alpha\alpha\beta)\}$$

and

$$\psi'' = \mathcal{A}\{(23)\phi \cdot (\alpha\beta - \beta\alpha)\alpha\} = -\mathcal{A}\{\phi \cdot (\alpha\alpha\beta - \beta\alpha\alpha)\}$$

Since there are only two doublet spin functions, ψ_1, ψ', and ψ'' are not all linearly independent. Choose ψ_1 and ψ_{12}, where

$$\begin{aligned} \psi_{12} = \psi' - \psi'' &= \mathcal{A}\{[(13) - (23)]\phi \cdot (\alpha\beta\alpha - \beta\alpha\alpha)\} \\ &= \mathcal{A}\{\phi \cdot (2\alpha\alpha\beta - \beta\alpha\alpha - \alpha\beta\alpha)\} \end{aligned}$$

Note that if ϕ has exact (12) symmetry, then

$$[(13) - (23)]\phi \equiv 0$$

For example, if

$$\phi(r_1, r_2, r_3) = \phi_{1s}(r_1)\,\phi_{1s}(r_2)\,\phi_{2s}(r_3)$$

then $[(13) - (23)]\phi \equiv 0$.

Convergence study for the nonrelativistic energy of Li in the ground state.

Ω	N	$E(\Omega)$	$R(\Omega)$
		with only χ_1	
12	9056	−7.478 060 323 909 450	5.986
13	13248	−7.478 060 323 909 950	8.174
14	18935	−7.478 060 323 910 102	3.290
15	26520	−7.478 060 323 910 134	4.679
∞		−7.478 060 323 910 143(9)	
		with only χ_2	
12	9056	−7.478 060 323 891 747	4.994
13	13248	−7.478 060 323 902 848	6.009
14	18935	−7.478 060 323 908 907	1.832
15	26520	−7.478 060 323 909 791	6.851
∞		−7.478 060 323 909 94(15)	
		with both χ_1 and χ_2	
12	12168	−7.478 060 323 910 044	7.582
13	18108	−7.478 060 323 910 128	6.213
14	24552	−7.478 060 323 910 145	4.956
15	34020	−7.478 060 323 910 147	8.327
∞		−7.478 060 323 910 147(1)	
Sims *et al.*	16764	−7.478 060 323 452	
Stanke *et al.*	10000	−7.478 060 323 81	
Yan *et al.*	9577	−7.478 060 323 892 4	
Puchalski *et al.*	30632	−7.478 060 323 910 097	
Puchalski *et al.*	∞	−7.478 060 323 910 2(2)	

Relativistic Corrections

Relativistic corrections of $O(\alpha^2)$ and anomalous magnetic moment corrections of $O(\alpha^3)$ are (in atomic units)

$$\Delta E_{\rm rel} \;=\; \langle\Psi|H_{\rm rel}|\Psi\rangle_J\,, \tag{3}$$

where Ψ is a nonrelativistic wave function and $H_{\rm rel}$ is the Breit interaction defined by

$$\begin{aligned} H_{\rm rel} \;=\; & B_1 + B_2 + B_4 + B_{\rm so} + B_{\rm soo} + B_{\rm ss} + \frac{m}{M}(\tilde\Delta_2 + \tilde\Delta_{\rm so}) \\ & + \gamma\left(2B_{\rm so} + \frac{4}{3}B_{\rm soo} + \frac{2}{3}B_{3e}^{(1)} + 2B_5\right) + \gamma\,\frac{m}{M}\tilde\Delta_{\rm so}\,. \end{aligned}$$

where $\gamma = \alpha/(2\pi)$ and

$$B_1 = \frac{\alpha^2}{8}(p_1^4 + p_2^4)$$

$$B_2 = -\frac{\alpha^2}{2}\left(\frac{1}{r_{12}}\mathbf{p}_1\cdot\mathbf{p}_2 + \frac{1}{r_{12}^3}\mathbf{r}_{12}\cdot(\mathbf{r}_{12}\cdot\mathbf{p}_1)\mathbf{p}_2\right)$$

$$B_4 = \alpha^2\pi\left(\frac{Z}{2}\delta(\mathbf{r}_1) + \frac{Z}{2}\delta(\mathbf{r}_2) - \delta(\mathbf{r}_{12})\right)$$

$$H_{\rm rel} = B_1 + B_2 + B_4 + B_{\rm so} + B_{\rm soo} + B_{\rm ss} + \frac{m}{M}(\tilde{\Delta}_2 + \tilde{\Delta}_{\rm so}) + \gamma\left(2B_{\rm so} + \frac{4}{3}B_{\rm soo} + \frac{2}{3}B_{3e}^{(1)} + 2B_5\right) + \gamma\,\frac{m}{M}\tilde{\Delta}_{\rm so}\,.$$

Spin-dependent terms

$$B_{\rm so} = \frac{Z\alpha^2}{4}\left[\frac{1}{r_1^3}(\mathbf{r}_1 \times \mathbf{p}_1)\cdot\boldsymbol{\sigma}_1 + \frac{1}{r_2^3}(\mathbf{r}_2 \times \mathbf{p}_2)\cdot\boldsymbol{\sigma}_2\right]$$

$$B_{\rm soo} = \frac{\alpha^2}{4}\left[\frac{1}{r_{12}^3}\mathbf{r}_{12}\times\mathbf{p}_2\cdot(2\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2) - \frac{1}{r_{12}^3}\mathbf{r}_{12}\times\mathbf{p}_1\cdot(2\boldsymbol{\sigma}_2 + \boldsymbol{\sigma}_1)\right]$$

$$B_{\rm ss} = \frac{\alpha^2}{4}\left[-\frac{8}{3}\pi\delta(\mathbf{r}_{12}) + \frac{1}{r_{12}^3}\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2 - \frac{3}{r_{12}^3}(\boldsymbol{\sigma}_1\cdot\mathbf{r}_{12})(\boldsymbol{\sigma}_2\cdot\mathbf{r}_{12})\right]$$

Relativistic recoil terms (A.P. Stone, 1961)

$$\tilde{\Delta}_2 = -\frac{Z\alpha^2}{2}\left\{\frac{1}{r_1}(\mathbf{p}_1 + \mathbf{p}_2)\cdot\mathbf{p}_1 + \frac{1}{r_1^3}br_1\cdot[\mathbf{r}_1\cdot(\mathbf{p}_1 + \mathbf{p}_2)]\mathbf{p}_1 + \frac{1}{r_2}(\mathbf{p}_1 + \mathbf{p}_2)\cdot\mathbf{p}_2 + \frac{1}{r_2^3}br_2\cdot[\mathbf{r}_2\cdot(\mathbf{p}_1 + \mathbf{p}_2)]\mathbf{p}_2\right\}$$

$$\tilde{\Delta}_{\rm so} = \frac{Z\alpha^2}{2}\left(\frac{1}{r_1^3}\mathbf{r}_1\times\mathbf{p}_2\cdot\boldsymbol{\sigma}_1 + \frac{1}{r_2^3}\mathbf{r}_2\times\mathbf{p}_1\cdot\boldsymbol{\sigma}_2\right)$$

QED Corrections

the QED shift for a $1s^2nL\, n\,^2L$ state of lithium then has the form

$$E_{\rm QED} = E_{\rm L,1} + E_{\rm M,1} + E_{\rm R,1} + E_{\rm L,2}$$

where the main one-electron part is (in atomic units)

$$E_{\rm L,1} \; = \; \frac{4Z\alpha^3\langle\delta(\mathbf{r}_i)\rangle^{(0)}}{3}\left\{\ln(Z\alpha)^{-2} - \beta(n\,^2L) + \frac{19}{30} + \cdots\right\}$$

the mass scaling and mass polarization corrections are

$$E_{\rm M,1} = \frac{\mu\langle\delta(\mathbf{r}_i)\rangle^{(1)}}{M\langle\delta(\mathbf{r}_i)\rangle^{(0)}}E_{\rm L,1} + \frac{4Z\alpha^3\mu\langle\delta(\mathbf{r}_i)\rangle^{(0)}}{3M}\left[1 - \Delta\beta_{\rm MP}(n\,^2L)\right]$$

and the recoil corrections (including radiative recoil) are given by

$$E_{\rm R,1} \; = \; \frac{4Z^2\mu\alpha^3\langle\delta(\mathbf{r}_i)\rangle^{(0)}}{3M}\left[\frac{1}{4}\ln(Z\alpha)^{-2} - 2\beta(n\,^2L) - \frac{1}{12} - \frac{7}{4}a(n\,^2L)\right]$$

where $\beta(n\,^2L) = \ln(k_0/Z^2R_\infty)$ is the two-electron Bethe logarithm.

Two-Electron QED Shift

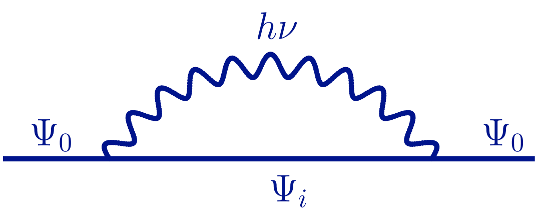
The lowest order helium Lamb shift is given exactly by the Kabir-Salpeter formula (in atomic units)

$$E_{L,1} = \frac{4}{3} Z\alpha^3 |\Psi_0(0)|^2 \left[\ln \alpha^{-2} - \beta(1sn\ell) + \frac{19}{30}\right]$$

where $\beta(1sn\ell)$ is the two-electron Bethe logarithm defined by

$$\beta(1sn\ell) = \frac{\mathcal{N}}{\mathcal{D}} = \frac{\sum_i |\langle \Psi_0 | \mathbf{p}_1 + \mathbf{p}_2 | i \rangle|^2 (E_i - E_0) \ln |E_i - E_0|}{\sum_i |\langle \Psi_0 | \mathbf{p}_1 + \mathbf{p}_2 | i \rangle|^2 (E_i - E_0)}$$

and for hydrogenic ions, $|\Psi_0(0)|^2 \longrightarrow \dfrac{Z^3}{\pi n^3}$.



Bethe logarithms for He-like atoms.

State	$Z=2$	$Z=3$	$Z=4$	$Z=5$	$Z=6$
$1\,^1$S	2.983 865 9(1)	2.982 624 558(1)	2.982 503 05(4)	2.982 591 383(7)	2.982 716 949
$2\,^1$S	2.980 118 275(4)	2.976 363 09(2)	2.973 976 98(4)	2.972 388 16(3)	2.971 266 29(
$2\,^3$S	2.977 742 36(1)	2.973 851 679(2)	2.971 735 560(4)	2.970 424 952(5)	2.969 537 065
$2\,^1$P	2.983 803 49(3)	2.983 186 10(2)	2.982 698 29(1)	2.982 340 18(7)	2.982 072 79(
$2\,^3$P	2.983 690 84(2)	2.982 958 68(7)	2.982 443 5(1)	2.982 089 5(1)	2.981 835 91(
$3\,^1$S	2.982 870 512(3)	2.981 436 5(3)	2.980 455 81(7)	2.979 778 086(4)	2.979 289 8(9
$3\,^3$S	2.982 372 554(8)	2.980 849 595(7)	2.979 904 876(3)	2.979 282 037	2.978 844 34(
$3\,^1$P	2.984 001 37(2)	2.983 768 943(8)	2.983 584 906(6)	2.983 449 763(6)	2.983 348 89(
$3\,^3$P	2.983 939 8(3)	2.983 666 36(4)	2.983 479 30(2)	2.983 350 844(8)	2.983 258 40(
$4\,^1$S	2.983 596 31(1)	2.982 944 6(3)	2.982 486 3(1)	2.982 166 154(3)	2.981 932 94(
$4\,^3$S	2.983 429 12(5)	2.982 740 35(4)	2.982 291 37(7)	2.981 988 21(2)	2.981 772 015
$4\,^1$P	2.984 068 766(9)	2.983 961 0(2)	2.983 875 8(1)	2.983 813 2(1)	2.983 766 6(2
$4\,^3$P	2.984 039 84(5)	2.983 913 45(9)	2.983 828 9(1)	2.983 770 1(2)	2.983 727 5(2
$5\,^1$S	2.983 857 4(1)	2.983 513 01(2)	2.983 267 901(6)	2.983 094 85(5)	2.982 968 66(
$5\,^3$S	2.983 784 02(8)	2.983 422 50(2)	2.983 180 677(6)	2.983 015 17(3)	2.982 896 13(
$5\,^1$P	2.984 096 174(9)	2.984 038 03(5)	2.983 992 23(1)	2.983 958 67(5)	2.983 933 65(
$5\,^3$P	2.984 080 3(2)	2.984 014 4(4)	2.983 968 9(4)	2.983 937 2(4)	2.983 914 07(

For He$^+$, $\beta(1s) = 2.984\,128\,555\,765$

G.W.F. Drake and S.P. Goldman, Can. J. Phys. **77**, 835 (1999).

Comparison of Bethe Logarithms $\ln(k_0)$ in units of $\ln(Z^2 R_\infty)$.

Atom	$1s^2 2s$	$1s^2 3s$	$1s^2 2p$	$1s^2$	$1s$
Li	2.981 06(1)	2.982 36(6)	2.982 57(6)	2.982 624	2.984 128
Be^+	2.979 26(2)	2.981 62(1)	2.982 27(6)	2.982 503	2.984 128

Comparison of Bethe Logarithm finite mass coefficient $\Delta\beta_{\mathrm{MP}}$.

Atom	$1s^2 2s$	$1s^2 3s$	$1s^2 2p$	$1s^2$	$1s$
Li	0.113 05(5)	0.110 5(3)	0.111 2(5)	0.1096	0.0
Be^+	0.125 58(4)	0.117 1(1)	0.121 7(6)	0.1169	0.0

$$\ln(k_0/Z^2 R_M) = \beta_\infty + (\mu/M)\Delta\beta_{\mathrm{MP}}$$

where β_∞ is the Bethe logarithm for infinite nuclear mass.

The Electron-Electron Term

The electron-electron part is (Araki and Sucher)

$$\Delta E_{L,2} \;=\; \alpha^3\Big(\frac{14}{3}\ln\alpha + \frac{164}{15}\Big)\langle\delta(\mathbf{r}_{ij})\rangle - \frac{14}{3}\alpha^3 Q\,, \tag{6}$$

where the Q term is defined by

$$Q \;=\; (1/4\pi)\lim_{\epsilon\to 0}\langle r_{ij}^{-3}(\epsilon) + 4\pi(\gamma + \ln\epsilon)\delta(\mathbf{r}_{ij})\rangle\,. \tag{7}$$

γ is Euler's constant, ϵ is the radius of a sphere about $r_{ij} = 0$ excluded from the integration.

Finite Nuclear Size Correction

In lowest order

$$\Delta E_{\rm nuc} = \frac{2\pi Z r_{\rm rms}^2}{3}\langle\delta(\mathbf{r}_i)\rangle\,, \tag{8}$$

where $r_{\rm rms} = R_{\rm rms}/a_{\rm Bohr}$, $R_{\rm rms}$ is the root-mean-square radius of the nuclear charge distribution, and $a_{\rm Bohr}$ is the Bohr radius.

The dominating nuclear excitations are $E1$ transitions by the electric dipole coupling $-\vec{d}\cdot\vec{E}$ [20]. The energy shift due to the two-photon exchange in the temporal gauge is

$$E_{\rm pol} = ie^2\psi^2(0)\int\frac{d\omega}{2\pi}\int\frac{d^3k}{(2\pi)^3}\omega^2\frac{(\delta^{ik}-\frac{k^ik^k}{\omega^2})}{\omega^2-k^2}\frac{(\delta^{jl}-\frac{k^jk^l}{\omega^2})}{\omega^2-k^2}\times{\rm Tr}\left[\left(\gamma^j\frac{1}{\not p-\not k-m}\gamma^i+\gamma^i\frac{1}{\not p+\not k-m}\gamma^j\right)\frac{(\gamma^0+I)}{4}\right]\times\langle\phi_N|d^k\frac{1}{E_N-H_N-\omega}d^l|\phi_N\rangle, \tag{14}$$

where $\psi^2(0) = (m\alpha)^3\langle\sum_a\delta^3(r_a)\rangle$, $p = (m, \vec{0})$, and we used plane wave approximation for the electrons, since the characteristic photon momentum k is much larger than the inverse Bohr radius. After performing k integration and replacing $\omega = iw$, one obtains

$$E_{\rm pol} = -m\alpha^4\left\langle\sum_a\delta^3(r_a)\right\rangle(m^3\tilde{\alpha}_{\rm pol}), \tag{15}$$

where $\tilde{\alpha}_{\rm pol}$ is a kind of electric polarizability of the nucleus, which is given by the following double integral:

$$\tilde{\alpha}_{\rm pol} = \frac{16\alpha}{3}\int_{E_T}^{\infty}dE\frac{1}{e^2}|\langle\phi_N|\vec{d}|E\rangle|^2$$

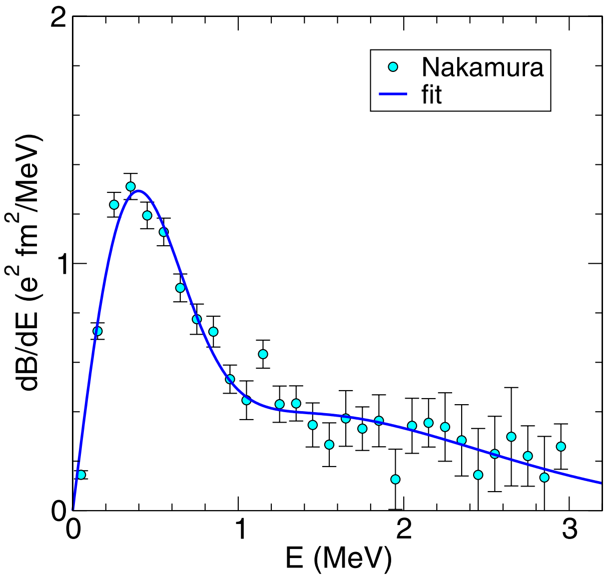
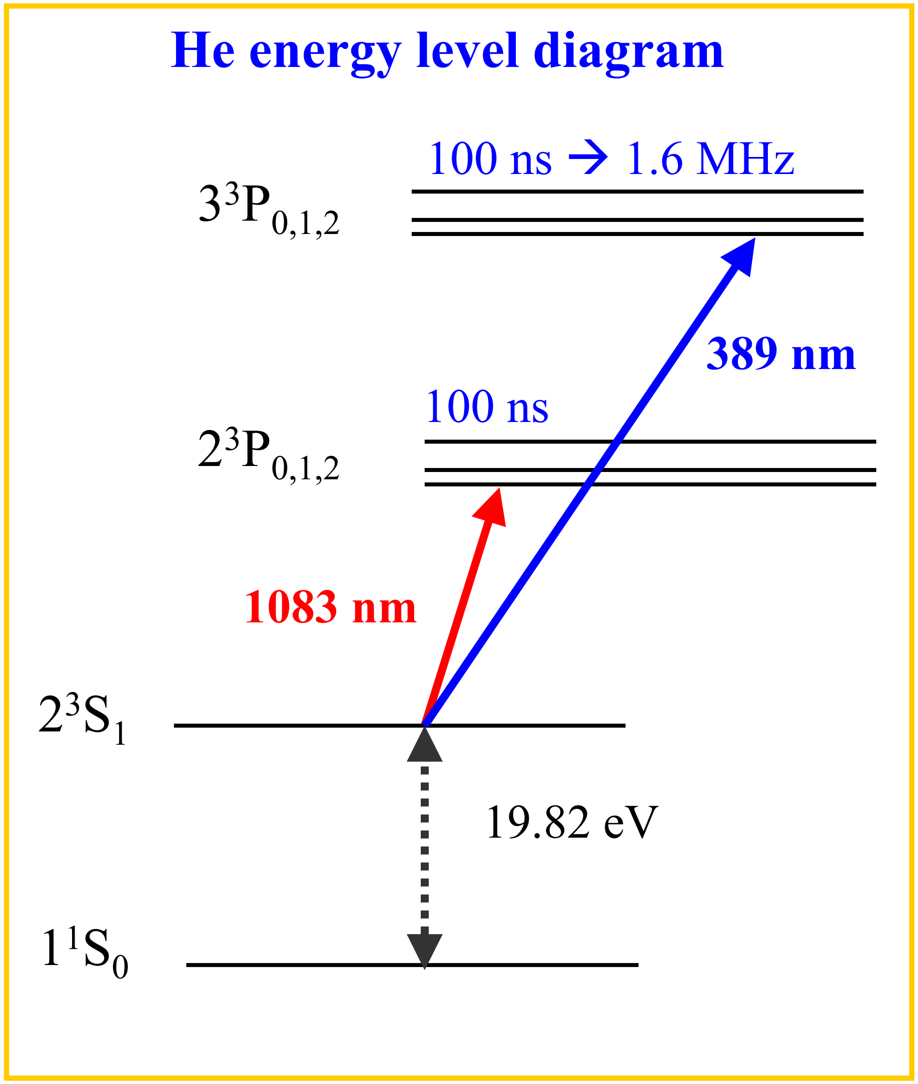
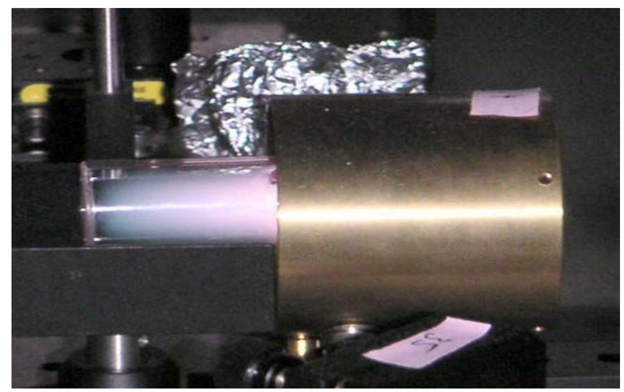


FIG. 1 (color online). Electric dipole line strength by Nakamura *et al.* [20] adapted to the new value of E_T from Ref. [7].

$$\tilde{\alpha}_{\rm pol} = 60.9(6.1)\ {\rm fm}^3 = 1.06(0.11)\times10^{-6}m^{-3} \tag{18}$$

Atomic Energy Levels of Helium





A helium glow discharge

Contributions to the ^{6}He - ^{4}He isotope shift (MHz).

Contribution	$2\ ^3\mathrm{S}_1$	$3\ ^3\mathrm{P}_2$	$2\ ^3\mathrm{S}_1 - 3\ ^3\mathrm{P}_2$
E_{nr} [a]	52 947.286(1)	17 549.773(1)	35 397.539(16)
μ/M	2 248.200	–5 549.108	7 797.314(2)
$(\mu/M)^2$	–3.964	–4.847	0.883
$\alpha^2\mu/M$	1.435	0.724	0.711
E_{nuc}	0.000	0.000	0.000
$\alpha^3\mu/M$, 1-e	–0.285	–0.037	–0.248
$\alpha^3\mu/M$, 2-e	0.005	0.001	0.004
Nuclear pol.			0.014(3)
Total	55 192.677(1)	11 996.506(1)	43 196.185(3)
Experiment[b]			43 194.751(10)
Difference			1.434(10)

[a]Using $m(^6\mathrm{He}) = 6.018\,885\,883(57)$ u from Brodeur et al. (2012).
Assumed nuclear radius for $r_{\mathrm{nuc}}(\,^4\mathrm{He}) = 1.681(4)$ fm.

In general, $\mathrm{IS}(2S - 3P) = 43\,196.185(3) + 1.008[r^2_{\mathrm{nuc}}(\,^4\mathrm{He}) - r^2_{\mathrm{nuc}}(\,^6\mathrm{He})]$.

Adjusted nuclear radius is $r_{\mathrm{nuc}}(\,^6\mathrm{He}) = 2.061(8)$ fm.

[b]P. Mueller and Argonne collaboration.

PRL **99,** 252501 (2007) PHYSICAL REVIEW LETTERS week ending 21 DECEMBER 2007

Nuclear Charge Radius of ^{8}He

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The root-mean-square (rms) nuclear charge radius of ^{8}He, the most neutron-rich of all particle-stable nuclei, has been determined for the first time to be 1.93(3) fm. In addition, the rms charge radius of ^{6}He was measured to be 2.068(11) fm, in excellent agreement with a previous result. The significant reduction in charge radius from ^{6}He to ^{8}He is an indication of the change in the correlations of the excess neutrons and is consistent with the ^{8}He neutron halo structure. The experiment was based on laser spectroscopy of individual helium atoms cooled and confined in a magneto-optical trap. Charge radii were extracted from the measured isotope shifts with the help of precision atomic theory calculations.

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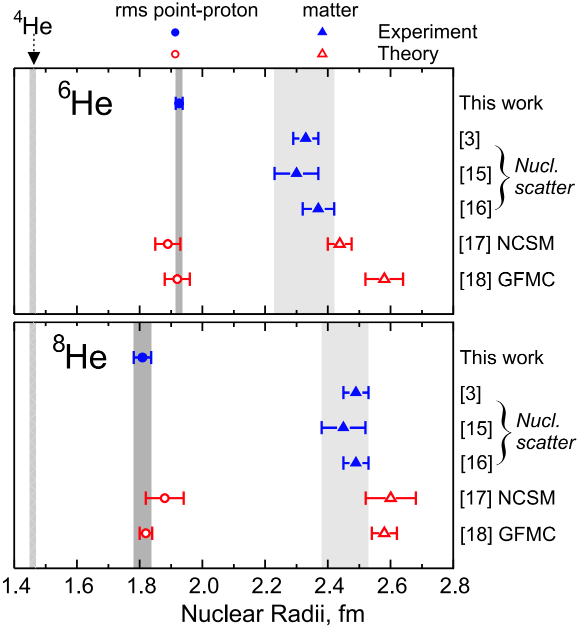


rms point-proton
matter
Experiment
Theory
^{4}He
^{6}He
This work
[3]
[15]
[16]
Nucl. scatter
[17] NCSM
[18] GFMC
^{8}He
This work
[3]
[15]
[16]
Nucl. scatter
[17] NCSM
[18] GFMC
1.4
1.6
1.8
2.0
2.2
2.4
2.6
2.8
Nuclear Radii, fm

TABLE I: Comparison between theory and experiment for the total transition frequencies of ^{7}Li. Units are cm^{-1}.

Atom	$2\,^2P_{1/2} - 2\,^2S_{1/2}$	$2\,^2P_{3/2} - 2\,^2S_{1/2}$	$3\,^2S_{1/2} - 2\,^2S_{1/2}$
^{7}Li (theory)	14 903.648 5(10)[a]	14 903.983 8(10)[a]	27 206.093 9(10)[a]
^{7}Li (expt.)	14 903.648 130(14)[b]	14 903.983 648(14)[b]	27 206.094 20(10)[c]
Difference	0.000 4(10)	0.000 2(10)	−0.000 3(10)

[a]Yan, Nörtershäuser, and Drake [1]
[b]Sansonetti *et al.* [2]
[c]Bushaw *et al.* [3]
[d]Bushaw *et al.* [4]

$$10^{-6}\ \mathbf{cm}^{-1} = 4 \times 10^{-12}\ \textbf{atomic units of energy.}$$

[1] Z.-C. Yan, W. Nörtershäuser, and G.W.F. Drake, [Phys. Rev. Lett. **100**, 243002 (2008).
[2] C.J. Sansonetti, B. Richou, R. Engleman, Jr., and L.J. Radziemski, Phys. Rev. A **52**, 2682 (1995).
[3] B. A. Bushaw, W. Nörtershäuser, G. Ewald, A. Dax, and G.W.F. Drake, Phys. Rev. Lett. **91**, 043004 (2003).
[4] B.A. Bushaw, W. Nörtershäuser, G.W.F. Drake, and H.-J. Kluge, Phys. Rev. A **75**, 052503 (2007).

Contributions to the isotope shift of ^{A}Li (A =7, 8, 9, 11) relative to ^{6}Li in the $2s\ ^2\mathrm{S}_{1/2} \rightarrow 3s\ ^2\mathrm{S}_{1/2}$ transition. Contributions of the mass dependent-terms are calculated using the masses listed in the first row. The mass of the reference isotope ^{6}Li is 6.015122794(16) amu . All other values are in MHz. Both sets of theoretical results are given in cases where they differ (see text).

Term	^{7}Li	^{8}Li	^{9}Li	^{11}Li
M (amu)	7.0160034256(45)	8.02248624(12)	9.02679020(21)	11.04372361(69)
μ/M [a]	11 454.655 2(1)[c]	20 090.837 3(6)[c]	26 788.479 2(10)[c]	36 559.175 4(25)[c]
	11 454.655 2(2)[d]	20 090.837 3(9)[d]	26 788.479 2(13)[d]	36 559.175 4(27)[d]
$(\mu/M)^2$	–1.794 0	–2.964 4	–3.764 2	–4.761 9
$\alpha^2\mu/M$	0.017 2[c]	0.030 2[c]	0.040 2[c]	0.055 0[c]
	0.016 8(1)[d]	0.029 5(2)[d]	0.039 3(3)[d]	0.053 7(4)[d]
$\alpha^3\mu/M$	–0.048 5	–0.085 1	–0.113 5	–0.154 8
$\alpha^4\mu/M$	–0.009 2(23)[c]	–0.016 1(40)[c]	–0.021 5(63)[c]	–0.029 4(73)[c]
	–0.008 4(28)[d]	–0.014 7(41)[d]	–0.019 6(66)[d]	–0.026 8(90)[d]
ν_{pol}				0.039(4)
Total	11 452.820 7(23)[c]	20 087.801 9(40)[c]	26 784.620 2(64)[c]	36 554.323(9)[c]
	11 452.821 1(28)[d]	20 087.802 6(50)[d]	26 784.621 3(67)[d]	36 554.325(9)[d]
$C_{A,A'}$ [b]	–1.571 9(16)	–1.571 9(16)	–1.572 0(16)	–1.570 3(16)

[a] Uncertainties for this line are dominated by the nuclear mass uncertainty.

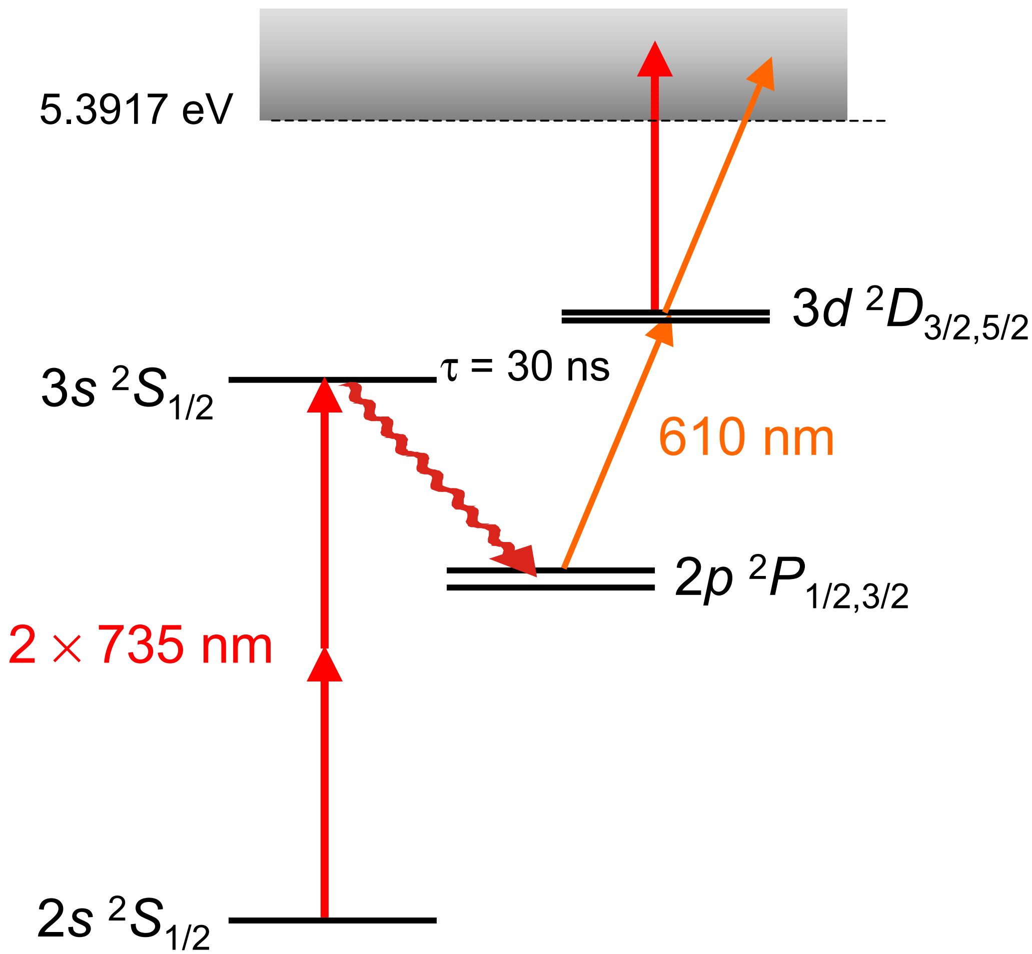
[b] 25% Error bar of the relativistic correction is assumed due to the estimation of the relativistic correction to the wave function at the origin on the basis of a known result for hydrogenic systems.

[c] Calculation by Puchalski and Pachucki.

[d] Calculation by Yan and Drake.

Resonance Ionization of Lithium

"Doubly-Resonant-4-Photon Ionization"



2s – 3s transition

→ Narrow line

2-photon spectroscopy

→ Doppler cancellation

Spontaneous decay

→ Decoupling of precise spectroscopy and efficient ionization

2p – *3d* transition

→ Resonance enhancement for efficient ionization

PHYSICAL REVIEW A **83**, 012516 (2011)

Isotope-shift measurements of stable and short-lived lithium isotopes for nuclear-charge-radii determination

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Changes in the mean square nuclear charge radii along the lithium isotopic chain were determined using a combination of precise isotope shift measurements and theoretical atomic structure calculations. Nuclear charge radii of light elements are of high interest due to the appearance of the nuclear halo phenomenon in this region of the nuclear chart. During the past years we have developed a laser spectroscopic approach to determine the charge radii of lithium isotopes which combines high sensitivity, speed, and accuracy to measure the extremely small field shift of an 8-ms-lifetime isotope with production rates on the order of only 10 000 atoms/s. The method was applied to all bound isotopes of lithium including the two-neutron halo isotope ^{11}Li at the on-line isotope separators at GSI, Darmstadt, Germany, and at TRIUMF, Vancouver, Canada. We describe the laser spectroscopic method in detail, present updated and improved values from theory and experiment, and discuss the results.

DOI: 10.1103/PhysRevA.83.012516 PACS number(s): 32.10.Fn, 21.10.Gv, 21.10.Ft, 27.20.+n

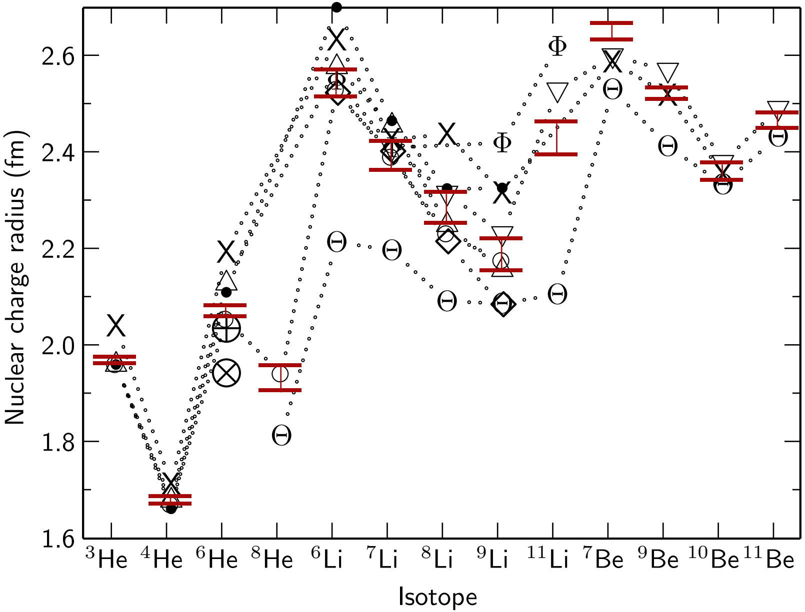

Fig. 4. Comparison of various nuclear structure theories with experiment for the rms nuclear charge radius r_c. The points are grouped as ($\bigotimes$) variational microcluster calculations[41–43] and a no-core shell model;[44,45] ($\bigoplus$) effective three-body cluster models;[46,47] (Θ) large-basis shell model;[48] ($\bigtriangledown$) stochastic variational multicluster;[49] (Φ) dynamic correlation model.[50] The remaining points are quantum Monte Carlo calculations[51,52] with various effective potentials as follows: (X) AV8'; ($\bullet$) AV18/UIX; ($\bigcirc$) AV18/IL2; ($\triangle$) AV18/IL3; ($\diamond$) AV18/IL4 (for Li only).

Conclusions

- The combination of high-precision theory and experiment continues to provide opportunities to create new measurement tools, and to probe fundamental physics, especially at the interface between atomic and nuclear physics. There has been tremendous progress over the past 20 years.

- The objective of calculating isotope shifts to better than $\pm$ 10 kHz has been achieved for two- and three-electron atoms, thus allowing measurements of the nuclear charge radius to ± 0.002 fm.

- A measurement of the isotope shift for muonic helium in comparison with electronic helium would provide an important supplement to the measured discrepancy in the proton charge radius. (104 references to Randolf Pohl's paper in $Nature$, July 2010).

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See posters 1b (p. 60) on the splitting isotope shift in lithium, and 13b (p. 92) for isotope shifts in high-Z Li-like ions.

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TABLE I. Contributions to the energies of the $n=2$ states of He^+. Each entry includes reduced mass corrections. The values of the fundamental constants are $R_\infty=10\,973\,731.568\,516(84)$ m^{-1}, $\alpha^{-1}=137.035\,999\,58(52)$, and $M/m=7294.299\,508(16)$ for the α particle to electron mass ratio. Units are MHz.

Contribution (αmc^2)	$2\,^2S_{1/2}$	$2\,^2P_{1/2}$	$2\,^2P_{3/2}$
$(Z\alpha)^4 \ln(Z\alpha)^{-2}$	18 340.595	0.000	0.000
$(Z\alpha)^4$	−4 725.621	−206.095	200.725
$\alpha(Z\alpha)^4$	2.037	0.414	−0.207
$\alpha^2(Z\alpha)^4$	0.004	−0.003	0.002
$(Z\alpha)^4$ muonic pol.	−0.010	0.000	0.000
$(Z\alpha)^4$ hadronic pol.	−0.006	0.000	0.000
$(Z\alpha)^5$	228.402	0.000	0.000
$\alpha(Z\alpha)^5$ (one loop)	0.061	0.000	0.000
$\alpha(Z\alpha)^5$ (two-loop VP)	0.088	0.000	0.000
$\alpha(Z\alpha)^5$ (two-loop SE)	−1.339	0.000	0.000
$(Z\alpha)^6 \ln^2(Z\alpha)^{-2}$	−7.396	0.000	0.000
$(Z\alpha)^6 \ln(Z\alpha)^{-2}$	−0.391	1.677	0.944
$(Z\alpha)^6 G_{SE}(Z\alpha)$	−10.620(9)	−0.330(3)	−0.165(3)
$(Z\alpha)^6 G_{VP}(Z\alpha)$	−0.276	−0.022	−0.005
$(Z\alpha)^6 G_{WK}(Z\alpha)$	0.019	0.000	0.000
$\alpha(Z\alpha)^6 \ln^3(Z\alpha)^{-2}$	−0.144	0.000	0.000
$\alpha(Z\alpha)^6 \ln^2(Z\alpha)^{-2}$	0.010(130)[a]	0.006	0.006
$\alpha(Z\alpha)^6 \ln(Z\alpha)^{-2}$	−0.003	0.000(3)[a]	0.000(3)[a]
Terms of order $\alpha(Z\alpha)^7$	0.000(15)[a]	0.000(15)[a]	0.000(15)[a]
$(Z\alpha)^5 m/M$	2.547	−0.138	−0.138
$(Z\alpha)^6 m/M$	−0.015	0.007	0.007
$(Z\alpha)^7 \ln^2(Z\alpha) m/M$	−0.001	0.000	0.000
$\alpha(Z\alpha)^5 m/M$	−0.035	0.000	0.000
$Z(Z\alpha)^5(m/M)^2$	0.002	0.000	0.000
$\alpha(Z\alpha)^6 m/M$	0.002	0.000	0.000
Finite nuclear size	8.786(10)	0.000	0.000
Subtotal	13 836.697(130)	−204.485(15)	201.170(15)
Dirac fine structure	0.000	0.000	175 187.848
Total	13 836.697(130)	−204.485(15)	175 389.018(15)
$E(2\,^2S_{1/2})-E(2\,^2P_{1/2})$	14 041.18(13)		
$E(2\,^2P_{3/2})-E(2\,^2P_{1/2})$	175 593.50(2)		

[a]Uncertainties due to uncalculated terms.