Isotope Shifts and Charge Radius of Halo Nuclei

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<u>Collaborators</u>

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Main Theme:

• Derive nuclear charge radii by combining atomic theory with high precision spectroscopy (especially ⁶He and ¹¹Li halo nuclei).

What's New?

- 1. Essentially exact solutions to the quantum mechanical three- and fourbody problems.
- 2. Recent advances in calculating QED corrections especially the Bethe logarithm.
- 3. Single atom spectroscopy.

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Nucleon-Nucleon Interaction at Low Energy



- Fundamental theory QCD not calculable in low-energy regime (nucleus structure)
- Modern nuclear calculation uses "effective potential" between nucleons

Effective Model & Quantum Monte Carlo Calculation

S. Pieper and R. Wiringa. Ann. Rev. Nucl. Part. Sci. 51, 53 (2001)

Two-body potential
Argonne V18 $H = \sum_{i} K_{i} + \sum_{i < j} v_{ij}^{\gamma} + v_{ij}^{\pi} + v_{ij}^{R}$ $K_{i} = \sum_{i} K_{i} + \sum_{i < j} v_{ij}^{\gamma} + v_{ij}^{\pi} + v_{ij}^{R}$

Coupling parameters fit to NN scattering data

Problem: binding energy of most light nuclei too small

Three-body potential *Illinois-2*

$$V_{ijk} = V_{ijk}^{2\pi} + V_{ijk}^{3\pi} + V_{ijk}^{R}$$

$$\begin{vmatrix} \pi \\ \pi \\ a \end{vmatrix} = \int_{\pi}^{\pi} \int_{\pi$$

Coupling parameters fit to energy levels of light nuclei

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)

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

Group	Measurements
Amsterdam (Eikema et al.)	He 1s ^{2 1} S – 1s2p ¹ P
NIST (Bergeson et al.)	He 1s ^{2 1} S – 1s2s ¹ S
Harvard (Gabrielse)	He 1s2s ³ S – 1s2p ³ P
N. Texas (Shiner et al.)	He 1s2s ³ S – 1s2p ³ P
Florence (Inguscio et al.)	He 1s2s ³ S – 1s2p ³ P
York (Storry & Hessels)	He 1s2p ³ P fine structure
Argonne (ZT. Lu et al.)	He 1s3p ³ P fine structure
Paris (Biraben et al.)	He 1s2s ³ S – 1s3d ³ D
NIST (Sansonetti & Gillaspy)	He 1s2s ¹ S – 1snp ¹ P
Argonne (ZT. Lu et al.)	6 He I.S. completed June/04
Yale (Lichten et al.)	He 1s2s ¹ S – 1snd ¹ D
Colorado State (Lundeen et al.)	He 10 ^{1,3} L – 10 ^{1,3} (L+1)
York (Rothery & Hessels)	He 10 1,3 L – 10 1,3 (L+1)
Strathclyde (Riis et al.)	Li ⁺ 1s2s ³ S – 1s2p ³ P
York (Clarke & van Wijngaarden)	Li ⁺ 1s2s ³ S – 1s2p ³ P
U. West. Ont (Holt & Rosner)	Be ⁺⁺ 1s2s ³ S – 1s2p ³ P
Argonne (Berry et al.)	B ³⁺ 1s2s ³ S – 1s2p ³ P
Florida State (Myers et al.)	N ⁵⁺ 1s2s ³ S – 1s2p ³ P
Florida State (Myers/Silver)	F^{7+} 1s2p 3 P fine structure
Florida State (Myers/Tarbutt)	${\rm Mg}^{10+}$ 1s2p ${\rm ^{3}P}$ fine structure

High precision measurements for helium and He-like ions.

Group	Measurements
NIST (Radziemski et al. [1])	many transitions
York (Van Wijngaarden et al. [2])	2 ² S – 2 ² P I.S.
GSI (Bushaw et al. [3])	2 ² S – 3 ² S I.S.
GSI (Ewald et al. [4])	⁸ Li, ⁹ Li I.S.
TRIUMF/GSI (Nörtershäuser et al.)	¹¹ Li I.S. completed.
Windsor/UNB (Yan, Drake [5])	theory

High precision measurements for lithium.

 L. J. Radziemski, R. Engleman, Jr., and J. W. Brault, Phys. Rev. A 52, 4462 (1995).
 J. Walls, R, Ashby J.J. Clarke, B. Lu, and W.A. van Wijngaarden, Eur. Phys. J D 22 159 (2003).

[3] B. A. Bushaw, W. Nörtershäuser, G. Ewalt, A. Dax, and G. W. F. Drake, Phys. Rev. Lett. **91**, 043004 (2003).

[4] G. Ewald, W. Nördershäuser, A. Dax, S. Göte, R. Kirchner, H.-J. Kluge, Th. Kühl, R. Sanchez, A. Wojtaszek, B.A. Bushaw, G.W.F. Drake, Z.-C. Yan, and C. Zimmermann, Phys. Rev. Lett. **93**, 113002 (2004) (2004).

[5] Z.-C. Yan and G.W.F. Drake, Phys. Rev. Lett. 91, 113004 (2003).

transp05.tex, Feb., 2005

Comparison of nuclear charge radius determinations for ³He.



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Comparison of nuclear charge radius determinations for ⁶Li.



The inner error bars exclude the ± 0.03 fm uncertainty due to the reference radius $r_{\rm c}(^{7}{\rm Li}) = 2.39(3)$ fm.

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Contributions to the energy and their orders of magnitude in terms of Z, $\mu/M = 1.370745624 \times 10^{-4}$, and $\alpha^2 = 0.5325136197 \times 10^{-4}$.

Contribution	Magnitude
Nonrelativistic energy	Z^2
Mass polarization	$Z^2 \mu/M$
Second-order mass polarization	$Z^2(\mu/M)^2$
Relativistic corrections	$Z^4 lpha^2$
Relativistic recoil	$Z^4 lpha^2 \mu/M$
Anomalous magnetic moment	$Z^4 lpha^3$
Hyperfine structure	$Z^3 g_I \mu_0^2$
Lamb shift	$Z^4 \alpha^3 \ln \alpha + \cdots$
Finite nuclear size	$Z^4 \langle R_N/a_0 \rangle^2$

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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

$$\Psi(\mathbf{r}_{1}, \mathbf{r}_{2}) = \sum_{i,j,k} a_{ijk} r_{1}^{i} r_{2}^{j} r_{12}^{k} e^{-\alpha r_{1} - \beta r_{2}} \mathcal{Y}_{l_{1} l_{2} L}^{M}(\mathbf{\hat{r}_{1}}, \mathbf{\hat{r}_{2}})$$

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

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Diagonalize H in the

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

basis set to satisfy the variational condition

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

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.

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Mass Scaling

$$m, e$$

 \mathbf{X}_1
 \mathbf{X}_2
 \mathbf{X}_1
 \mathbf{X}_2
 \mathbf{X}_1
 \mathbf{X}_2
 $\mathbf{$

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

and ignore centre-of-mass motion. Then

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

Rescale distances and energies according to

$$oldsymbol{
ho} = \mathbf{r}/a_{\mu}$$

 $\mathcal{E} = E/(e^2/a_{\mu})$

where $a_{\mu} = \frac{\hbar^2}{\mu e^2}$ is the reduced mass Bohr radius, and $\frac{e^2}{a_{\mu}} = 2R_{\mu} = 2\frac{\mu}{m}R_{\infty} = 2\left(1 - \frac{\mu}{M}\right)R_{\infty}$.

The Schrödinger equation is then (in mass-scaled atomic units)

$$\left\{-\frac{1}{2}\nabla_{\rho_{1}}^{2}-\frac{1}{2}\nabla_{\rho_{2}}^{2}-\frac{\mu}{M}\nabla_{\rho_{1}}\cdot\nabla_{\rho_{2}}-\frac{Z}{\rho_{1}}-\frac{Z}{\rho_{2}}+\frac{1}{|\rho_{1}-\rho_{2}|}\right\}\Psi=\mathcal{E}\Psi$$

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Expand

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

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

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

The "normal" isotope shift is

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

The first-order "specific" isotope shift is

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

The second-order "specific" isotope shift is

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

New Variational Techniques

I. Double the basis set

If
$$\phi_{i,j,k}(\alpha,\beta) = r_1^i r_2^j r_{12}^k e^{-\alpha r_1 - \beta r_2}$$

then $\tilde{\phi}_{i,j,k} = a_1 \phi_{i,j,k}(\alpha_1,\beta_1) + a_2 \phi_{i,j,k}(\alpha_2,\beta_2)$
asymptotic inner correlation

II. Include the screened hydrogenic function

$$\phi_{\mathsf{SH}} = \psi_{1s}(Z)\psi_{nL}(Z-1)$$

explicitly in the basis set.

III. Optimize the nonlinear parameters

$$\frac{\partial E}{\partial \alpha_t} = -2\langle \Psi_{\mathsf{tr}} \mid H - E \mid r_1 \Psi(\mathbf{r}_1, \mathbf{r}_2; \alpha_t) \pm r_2 \Psi(\mathbf{r}_2, \mathbf{r}_1; \alpha_t) \rangle$$

$$\frac{\partial E}{\partial \beta_t} = -2\langle \Psi_{\mathsf{tr}} \mid H - E \mid r_2 \Psi(\mathbf{r}_1, \mathbf{r}_2; \alpha_t) \pm r_1 \Psi(\mathbf{r}_2, \mathbf{r}_1; \alpha_t) \rangle$$

for t = 1, 2, with $\langle \Psi_{tr} | \Psi_{tr} \rangle = 1$. $\Psi(\mathbf{r}_1, \mathbf{r}_2; \alpha_t) = \text{terms in } \Psi_{tr}$ which depend explicitly on α_t .

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	-2.903724377033543320480	
10	443	-2.903724377034047783838	7.90
11	549	-2.903724377034104634696	8.87
12	676	-2.903724377034116928328	4.62
13	814	-2.903724377034119224401	5.35
14	976	-2.903724377034119539797	7.28
15	1150	-2.903724377034119585888	6.84
16	1351	-2.903724377034119596137	4.50
17	1565	-2.903724377034119597856	5.96
18	1809	-2.903724377034119598206	4.90
19	2067	-2.903724377034119598286	4.44
20	2358	-2.903724377034119598305	4.02
Extrapolation	∞	-2.903724377034119598311(1)	
Korobov [2]	5200	-2.903724377034119598311158	7
Korobov extrap.	∞	-2.903724377034119598311159	4(4)
Schwartz [3]	10259	-2.903724377034119598311159	245 194 404 4400
Schwartz extrap.	∞	-2.903724377034119598311159	245 194 404 446
Goldman [4]	8066	-2.90372437703411959382	
Bürgers et al. [5]	24 497	-2.903724377034119589(5)	
Baker et al. [6]	476	-2.9037243770341184	

[1] G.W.F. Drake, M.M. Cassar, and R.A. Nistor, Phys. Rev. A 65, 054501 (2002).

[2] V.I. Korobov, Phys. Rev. A 66, 024501 (2002).

[3] C. Schwartz, http://xxx.aps.org/abs/physics/0208004

[4] S.P. Goldman, Phys. Rev. A 57, R677 (1998).

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[6] J.D. Baker, D.E. Freund, R.N. Hill, J.D. Morgan III, Phys. Rev. A 41, 1247 (1990). transp24.tex, Nov./00

Variational Basis Set for Lithium

Solve for Ψ_0 and Ψ_1 by expanding in Hylleraas coordinates

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

where $\mathcal{Y}_{(\ell_1\ell_2)\ell_{12},\ell_3}^{LM}$ 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

$$j_1 + j_2 + j_3 + j_{12} + j_{23} + j_{31} \leq \Omega, \qquad (2)$$

and study the eigenvalues as Ω is progressively increased. The explicit mass-dependence of E is

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

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Relativistic Corrections

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

$$\Delta E_{\rm rel} = \langle \Psi | H_{\rm rel} | \Psi \rangle_J , \qquad (3)$$

 \mathbf{m}

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

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

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

$$B_{1} = \frac{\alpha^{2}}{8}(p_{1}^{4} + p_{2}^{4})$$
$$B_{2} = -\frac{\alpha^{2}}{2}\left(\frac{1}{r_{12}}\mathbf{p}_{1} \cdot \mathbf{p}_{2} + \frac{1}{r_{12}^{3}}\mathbf{r}_{12} \cdot (\mathbf{r}_{12} \cdot \mathbf{p}_{1})\mathbf{p}_{2}\right)$$
$$B_{4} = \alpha^{2}\pi\left(\frac{Z}{2}\delta(\mathbf{r}_{1}) + \frac{Z}{2}\delta(\mathbf{r}_{2}) - \delta(\mathbf{r}_{12})\right)$$

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

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)

$$\begin{split} \tilde{\Delta}_{2} &= -\frac{Z\alpha^{2}}{2} \left\{ \frac{1}{r_{1}} (\mathbf{p}_{1} + \mathbf{p}_{2}) \cdot \mathbf{p}_{1} + \frac{1}{r_{1}^{3}} br_{1} \cdot [\mathbf{r}_{1} \cdot (\mathbf{p}_{1} + \mathbf{p}_{2})] \mathbf{p}_{1} \\ &+ \frac{1}{r_{2}} (\mathbf{p}_{1} + \mathbf{p}_{2}) \cdot \mathbf{p}_{2} + \frac{1}{r_{2}^{3}} br_{2} \cdot [\mathbf{r}_{2} \cdot (\mathbf{p}_{1} + \mathbf{p}_{2})] \mathbf{p}_{2} \right\} \\ &\tilde{\Delta}_{so} = \frac{Z\alpha^{2}}{2} \left(\frac{1}{r_{1}^{3}} \mathbf{r}_{1} \times \mathbf{p}_{2} \cdot \boldsymbol{\sigma}_{1} + \frac{1}{r_{2}^{3}} \mathbf{r}_{2} \times \mathbf{p}_{1} \cdot \boldsymbol{\sigma}_{2} \right) \end{split}$$

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Two-Electron QED Shift

The lowest order helium Lamb shift is given 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

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



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Differential contributions to the Bethe logarithm for the ground state of hydrogen. Each point represents the contribution from one pseudostate.



Partial Bethe logarithm sums for the ground state of helium, summed over pseudostates up to energy E. Each solid point represents the contribution from one pseudostate. The open circles are the corresponding partial sums for hydrogen.

Bethe logarithms for He-like atoms.

State	Z = 2	Z = 3	Z = 4	Z = 5	Z = 6
1 ¹ S	2.9838659(1)	2.982624558(1)	2.982 503 05(4)	2.982 591 383(7)	2.982716949
2 ¹ S	2.980 118 275(4)	2.976 363 09(2)	2.973 976 98(4)	2.97238816(3)	2.971 266 29(
2 ³ S	2.977 742 36(1)	2.973851679(2)	2.971735560(4)	2.970 424 952(5)	2.969 537 065
2 ¹ P	2.983 803 49(3)	2.983 186 10(2)	2.98269829(1)	2.98234018(7)	2.98207279(
2 ³ P	2.983 690 84(2)	2.98295868(7)	2.982 443 5(1)	2.9820895(1)	2.981 835 91(
3 ¹ S	2.982 870 512(3)	2.981 436 5(3)	2.980 455 81(7)	2.979778086(4)	2.979 289 8(9
3 ³ S	2.982 372 554(8)	2.980 849 595(7)	2. 979 904 876(3)	2.979282037	2.978 844 34(
3 ¹ P	2. 984 001 37(2)	2.983768943(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)	2.982166154(3)	2.981 932 94(
4 ³ S	2.983 429 12(5)	2.98274035(4)	2.982 291 37(7)	2.981 988 21(2)	2.981772015
4 ¹ P	2.984 068 766(9)	2.9839610(2)	2.983 875 8(1)	2.983 813 2(1)	2.9837666(2
4 ³ P	2.98403984(5)	2.983 913 45(9)	2.983 828 9(1)	2.9837701(2)	2.9837275(2
5 ¹ S	2.983 857 4(1)	2.98351301(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)	2.98301517(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)	2.9839689(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).

semin12.tex, March 99

Bethe logarithms for lithium

N	$eta(2\ ^2\mathrm{S})$	Difference	Ratio
87	2.846 5271		
207	2.964 2629	0.117 7357	
459	2.978 9857	0.014 7228	8.00
937	2.9807196	0.0017339	8.49
1763	2.980 9043	0.000 1847	9.39
Extrp.	2.98093(3)		
$Li^{+}(1s^{2} {}^{1}S)$	2.982624555(4)		
N	$\beta(3\ ^2\mathrm{S})$	Difference	Ratio
N 87	β(3 ² S) 2.746 4739	Difference	Ratio
N 87 207	β(3 ² S) 2.746 4739 2.939 4848	Difference 0.193 0108	Ratio
N 87 207 459	$eta(3\ ^2\mathrm{S})$ 2.746 4739 2.939 4848 2.975 0774	Difference 0.193 0108 0.035 5926	Ratio 5.42
N 87 207 459 937	$\begin{array}{c} \beta(3\ ^2\mathrm{S}) \\ 2.746\ 4739 \\ 2.939\ 4848 \\ 2.975\ 0774 \\ 2.981\ 2660 \end{array}$	Difference 0.193 0108 0.035 5926 0.006 1886	Ratio 5.42 5.75
N 87 207 459 937 1763	$\begin{array}{c} \beta(3\ ^2\mathrm{S}) \\ 2.746\ 4739 \\ 2.939\ 4848 \\ 2.975\ 0774 \\ 2.981\ 2660 \\ 2.982\ 2261 \end{array}$	Difference 0.193 0108 0.035 5926 0.006 1886 0.000 9601	Ratio 5.42 5.75 6.45
N 87 207 459 937 1763 Extrp.	$\beta(3 \ ^2S)$ 2.746 4739 2.939 4848 2.975 0774 2.981 2660 2.982 2261 2.982 4(2)	Difference 0.193 0108 0.035 5926 0.006 1886 0.000 9601	Ratio 5.42 5.75 6.45

Z.-C. Yan and G. W. F. Drake, "Bethe logarithm and QED shift for lithium", Phys. Rev. Lett. **91**, 113004 (2003).

Bethe logarithms for lithium – finite mass correction

N	$\Delta\beta_M(2^2\mathrm{S})$	Difference	Ratio
87	0.123748		
207	0.119291	0.004 457	
459	0.115 390	0.003 901	1.14
937	0.114 140	0.001 250	3.12
1763	0.113845	0.000 295	4.24
Extrap	0.1135(3)		
$Li^+(1s^2 \ ^1\mathrm{S})$	0.1096		
N	$\Delta\beta_M(3\ ^2{ m S})$	Difference	Ratio
<u> </u>	$\Delta \beta_M (3 \ ^2{ m S})$ 0.098298281	Difference	Ratio
N 87 207	$\begin{array}{c} \Delta\beta_M(3\ ^2\mathrm{S}) \\ \hline 0.098298281 \\ 0.104933801 \end{array}$	Difference	Ratio
N 87 207 459	$\begin{array}{c} \Delta\beta_M(3\ ^2\mathrm{S}) \\ 0.098298281 \\ 0.104933801 \\ 0.110410361 \end{array}$	Difference	Ratio
N 87 207 459 937	$\begin{array}{c} \Delta\beta_M(3\ ^2\mathrm{S}) \\ 0.098298281 \\ 0.104933801 \\ 0.110410361 \\ 0.112767733 \end{array}$	Difference	Ratio
N 87 207 459 937 1763	$\begin{array}{c} \Delta\beta_M(3\ ^2\mathrm{S}) \\ 0.098298281 \\ 0.104933801 \\ 0.110410361 \\ 0.112767733 \\ 0.110416727 \end{array}$	Difference	Ratio
N 87 207 459 937 1763 Extrap	$\begin{array}{c} \Delta\beta_M(3\ ^2\mathrm{S}) \\ 0.098298281 \\ 0.104933801 \\ 0.110410361 \\ 0.112767733 \\ 0.110416727 \\ 0.112(1) \end{array}$	Difference	Ratio

Z.-C. Yan and G. W. F. Drake, "Bethe logarithm and QED shift for lithium", Phys. Rev. Lett. 91, 113004 (2003).

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The Electron-Electron Term

The electron-electron part is (Araki and Sucher)

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

where the Q term is defined by

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

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Term	$3 {}^{2}S_{1/2} - 2 {}^{2}S_{1/2}$	$2 {}^2\mathrm{S}_{1/2}$ I.P.
Nonrelativistic	27 206.492 856(4)	43 488.220 2449(16)
Nonrel., μ/M	-2.29585430(16)	-3.621707668(4)
Nonrel., $(\mu/M)^2$	0.000 165 962	0.000 315 803
Relativistic, $lpha^2$	2.0890(4)	2.811 33(2)
Rel. recoil, $lpha^2 \mu/M$	-0.00004(1)	-0.000011(9)
QED(e ⁻ -nucl.), $lpha^3$	-0.1986(3)	-0.25832(3)
QED(e $^-$ –e $^-$), $lpha^3$	0.010747	0.013884
QED higher order, $\alpha^4 \cdots$	-0.0054(4)	-0.007 0(4)
Nuclear size, R^2	-0.000298(8)	-0.000389(10)
Total	27 206.092 6(9)	43 487.158 3(6)
Expt.	27 206.095 2(10) ^a	43 487.150(5) ^c
	27 206.094 20(9) ^b	43 487.159 34(17) ^d
Diff.	-0.0016(9)	-0.0010(5)

Contributions to the ⁷Li $1s^23s$ ²S $-1s^22s$ ²S transition energy and $1s^22s$ ²S ionization potential (I.P.), in units of cm⁻¹.

^aL. J. Radziemski, R. Engleman, Jr., and J. W. Brault, Phys. Rev. A 52, 4462 (1995).
^bB. A. Bushaw, W. Nörtershäuser, G. Ewalt, A. Dax, and G. W. F. Drake, Phys. Rev. Lett. 91, 043004 (2003).

^cC. E. Moore, NSRDS-NBS Vol. 14 (U.S. Department of Commerce, Washington, DC, 1970.

^dBruce Bushaw, preliminary value.

Laser Spectroscopic Determination of the Nuclear Charge Radius of ⁶He

L.-B. Wang, P. Mueller, K. Bailey, J.P. Greene, D. Henderson, R.J. Holt, R.V.F. Janssens, C.L. Jiang, Z.-T. Lu, T.P. O'Connor, R.C. Pardo, K.E. Rehm, J.P. Schiffer, X.D. Tang *Argonne National Lab.* G.W.F. Drake *University of Windsor*

Motivation

- Test the Standard Nuclear Structure Model;
- Study nucleon interactions in neutron-rich matter.

Method: Atomic isotope shift

⁶He – ⁴He isotope shift at 2 ${}^{3}S_{1}$ – 3 ${}^{3}P_{2}$, 389 nm *IS (MHz)* = 43,196.202(20) + 1.008 x [$\langle r^{2} \rangle_{4He}$ - $\langle r^{2} \rangle_{6He}$] -- G.W.F. Drake, Nucl. Phys. A737c, 25 (2004)



⁶He: ⁴He + 2n Its charge radius expands due to the motion of the ⁴He core





Spectrum of 150 ⁶He atoms in one hour

Experimental Setup - Schematic



Atomic Energy Levels of Helium





A helium glow discharge



Contribution	2 $^{3}S_{1}$	$3 {}^{3}\mathrm{P}_{2}$	$2 {}^{3}S_{1} - 3 {}^{3}P_{2}$
$E_{ m nr}$	52947.324(19)	17 549.785(6)	35 397.539(16)
μ/M	2248.202(1)	-5 549.112(2)	7797.314(2)
$(\mu/M)^2$	-3.964	-4.847	0.883
$lpha^2 \mu/M$	1.435	0.724	0.711
$E_{ m nuc}^{ m a}$	-1.264	0.110	-1.374
$lpha^3 \mu/M$, 1-e	-0.285	-0.037	-0.248
$lpha^3 \mu/M$, 2-e	0.005	0.001	0.004
Total	55 191.453(19)	11 996.625(4)	43 194.828(16)
$Experiment^{\mathrm{b}}$			43 194.772(56)
Difference			0.046(56)

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

^aAssumed nuclear radius is $r_{\rm nuc}({}^{6}{\rm He}) = 2.04$ fm.

In general, $IS(2S - 3P) = 43\,196.202(16) + 1.008[r_{nuc}^2({}^{4}He) - r_{nuc}^2({}^{6}He)].$ Adjusted nuclear radius is $r_{nuc}({}^{6}He) = 2.054(14)$ fm.

^bZ.-T. Lu, Argonne collaboration.

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Final Results for the ⁶He Isotope Shift

Using the accurately measured transition frequency in 4 He as a reference, the transition frequency in 6 He can be accurately calculated to be

$$\nu(2 \,{}^{3}S_{1} - 2 \,{}^{3}P_{2}) = 276\,766\,663.53(2) - 1.2104\bar{r}_{^{6}He}^{2} \text{ MHz}$$
(9)

where $\bar{r}_{^{6}\mathrm{He}}$ is the rms nuclear radius of $^{6}\mathrm{He}$, in units of fm, and the $^{6}\mathrm{He}$ – $^{4}\mathrm{He}$ isotope shift is

$$\delta\nu(2\,^{3}\mathrm{S}_{1} - 2\,^{3}\mathrm{P}_{2}) = 34\,473.625(13) + 1.2104(\bar{r}_{^{4}\mathrm{He}}^{2} - \bar{r}_{^{6}\mathrm{He}}^{2}) \,\mathrm{MHz}\,.$$
(10)

$$\delta\nu(2\,^{3}S_{1} - 3\,^{3}P_{2}) = 43\,196.202(16) + 1.008(\bar{r}_{^{4}He}^{2} - \bar{r}_{^{6}He}^{2}) \text{ MHz}.$$
(11)

The uncertainty of ± 16 kHz is due entirely to the uncertainty in the measured atomic mass of ⁶He (6.018 888(1) u), and not to the atomic structure calculations themselves. From Eq. (11) it follows that a measurement of the isotope shift to an accuracy of 100 kHz is sufficient to determine the nuclear radius of ⁶He (relative to ⁴He) to an accuracy of 1%. The result provides a direct test of the theoretical value $\bar{r}_{^6\text{He}} = 2.04$ fm recently obtained by Monte Carlo techniques by

S.C. Pieper, and R.B. Wiringa. Ann. Rev. Nucl. Part. Science **51**, 53 (2001); S.C. Pieper, K. Varga, and R.B. Wiringa, Phys. Rev. C **66**, 044310 (2002).

<u>Argonne Collaboration</u> L.-B. Wang, P. Mueller, K. Bailey, G.W.F. Drake, J. Greene, D. Henderson, R.J. Holt, R.V.F. Janssens, C.L. Jiang, Z.-T. Lu, T.P. O'Conner, R.C. Pardo, K.E. Rehm, J.P. Schiffer, and X.-D. Tang.

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A Proving Ground for Nuclear Structure Theories

The ToPLiS Collaboration



FS SS Ť

Two-Photon Lithium Spectroscopy

Resonance Ionization of Lithium



- 2s 3s transition
- \rightarrow Narrow line

2-photon spectroscopy

 \rightarrow Doppler cancellation

Spontaneous decay

 → Decoupling of precise spectroscopy and efficient ionization

2p - 3d transition

→ Resonance enhancement for efficient ionization



Experimental Arrangement









Contributions to the ⁷Li–⁶Li isotope shifts for the $1s^22p\,^2P_J$ – $1s^22s\,^2S$ transitions and comparison with experiment. Units are MHz.

Contribution	$2 {}^2\!P_{1/2}$ – $2 {}^2\!S$	$2 {}^2P_{3/2}$ – $2 {}^2S$
	Theory	
μ/M	10 533.501 92(60) ^a	$10533.50192(60)^{\mathrm{a}}$
$(\mu/M)^2$	0.057 3(20)	0.057 3(20)
$lpha^2\mu/M$	-1.397(66)	-1.004(66)
$lpha^3\mu/M$, anom. magnetic	-0.000 175 3(84)	0.0000875(84)
$lpha^3\mu/M$, one-electron	0.0045(10)	0.0045(10)
$lpha^3\mu/M$, two-electron	0.0105(20)	0.0105(20)
$r_{ m rms}^2$	1.94(61)	1.94(61)
$r_{ m rms}^2\mu/M$	-0.00073(11)	-0.00073(11)
Total	10534.12(7)±0.61	$10534.51(7){\pm}0.61$
	Experiment	
Sansonetti $et \ al.^{\mathrm{b}}$	10532.9(6)	10533.3(5)
Windholz <i>et al.</i> ^c	10534.3(3)	10539.9(1.2)
Scherf <i>et al.</i> ^d	10533.13(15)	10534.93(15)
Walls $et al.^{e}$	10534.26(13)	

^aThe additional uncertainty from the atomic mass determinations is ± 0.008 MHz.

- ^bC. J. Sansonetti, B. Richou, R. Engleman, Jr., and L. J. Radziemski, Phys. Rev. A 52, 2682 (1995).
- ^cL. Windholz and C. Umfer, Z. Phys. D 29, 121 (1994).
- ^dW. Scherf, O. Khait, H. Jäger, and L. Windholz, Z. Phys. D 36, 31, (1996).
- ^eJ. Walls, R. Ashby, J. J. Clarke, B. Lu, and W. A. van Wijngaarden, Eur. Phys. J D **22** 159 (2003).

Contributions to the $^7{\rm Li-^6Li}$ isotope shift for the $1s^23s\,^2\!S-\!1s^22s\,^2\!S$ transition. Units are MHz.

Contribution	$3^{2}S-2^{2}S$
μ/M	11 454.668 801(29) ^a
$(\mu/M)^2$	-1.7938640(41)
$lpha^2 \mu/M$	0.190(55)
$lpha^3\mu/M$, one-electron	-0.0642(3)
$lpha^3\mu/M$, two-electron	0.0112(2)
$r_{ m rms}^2$	$1.24{\pm}0.39$
$r_{ m rms}^2\mu/M$	-0.000677(98)
Total	$11454.25(5)\pm0.39$
$King^\mathrm{b}$	11 446.1
Vadla $et \ al.^{c}$ (experiment)	11 434(20)
Bushaw <i>et al.</i> ^d (experiment)	11 453.734(30)

^aThe additional uncertainty from the atomic mass determinations is ±0.008 MHz.
^bF. W. King, Phys. Rev. A 40, 1735 (1989); 43, 3285 (1991).
^cC. Vadla, A. Obrebski, and K. Niemax, Opt. Commun. 63, 288 (1987).
^dB. A. Bushaw, W. Nörtershäuser, G. Ewalt, A. Dax, and G. W. F. Drake, Phys. Rev. Lett. 91, 043004 (2003).

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Comparison of nuclear structure theories with experiment for the rms nuclear charge radius r_c . The dotted lines connect sequences of calculations for different nuclei, and the error bars denote the experimental values, relative to the ⁴He and ⁷Li reference nuclei. The points are grouped as (\otimes) variational microcluster calculations and a no-core shell model ; (\oplus) effective three-body cluster models ; (Θ) large-basis shell model ; (∇) stochastic variational multicluster ; (Φ) dynamic correlation model . The remaining points are quantum Monte Carlo calculations with various effective potentials as follows: (X) AV8'; (•) AV18/UIX; (•) AV18/IL2; (\triangle) AV18/IL3; (\diamond) AV18/IL4 (for



Charge Radii of Lithium Isotopes



Conclusions

- The finite basis set method with multiple distance scales provides an effective and efficient method of calculating Bethe logarithms, thereby enabling calculations up to order α^3 Ry for lithium.
- The objective of calculating isotope shifts to better than \pm 100 kHz has been achieved for two- and three-electron atoms, thus allowing measurements of the nuclear charge radius to ± 0.02 fm.
- The results provide a significant test of theoretical models for the nucleon-nucleon potential, and hence for the properties of nuclear matter in general.

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