Properties of Halo Nuclei from Precision Atomic Physics

Gordon W.F. Drake
University of Windsor,

Zong-Chao Yan
University of New Brunswick

Collaborators

Zheng Zhong (Ph.D. student)
Qixue Wu (Ph.D. student)
Atef Titi (Ph.D. student)
Eva Schulhof (M.Sc. student)

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Main Theme:

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

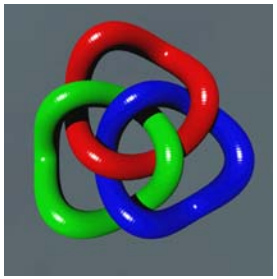
What's New?

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

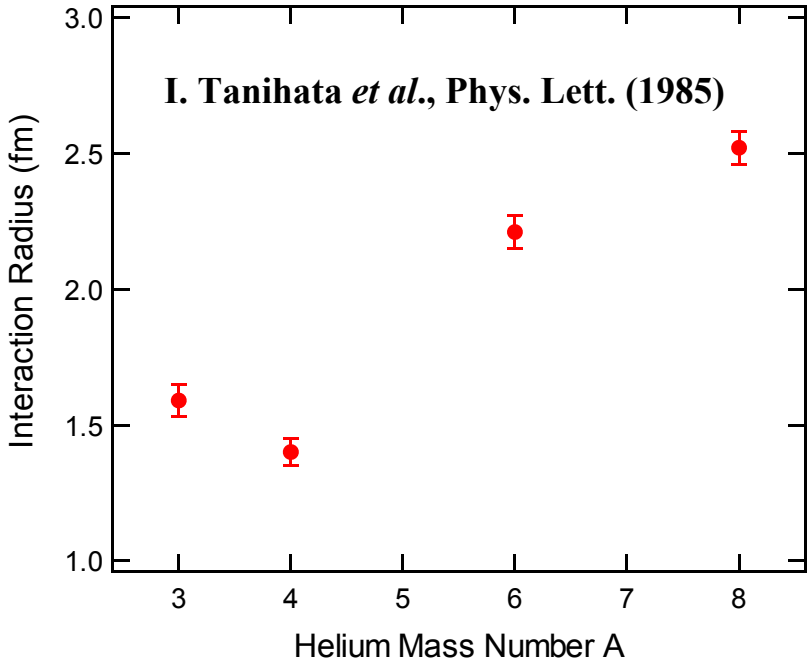
June 2008.

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)

HIGH PRECISION SPECTROSCOPY

THEORY

– Hyperfine structure
– N.R. energies and relativistic corrections
– QED effects

Fine Structure Isotope Shift (SIS)

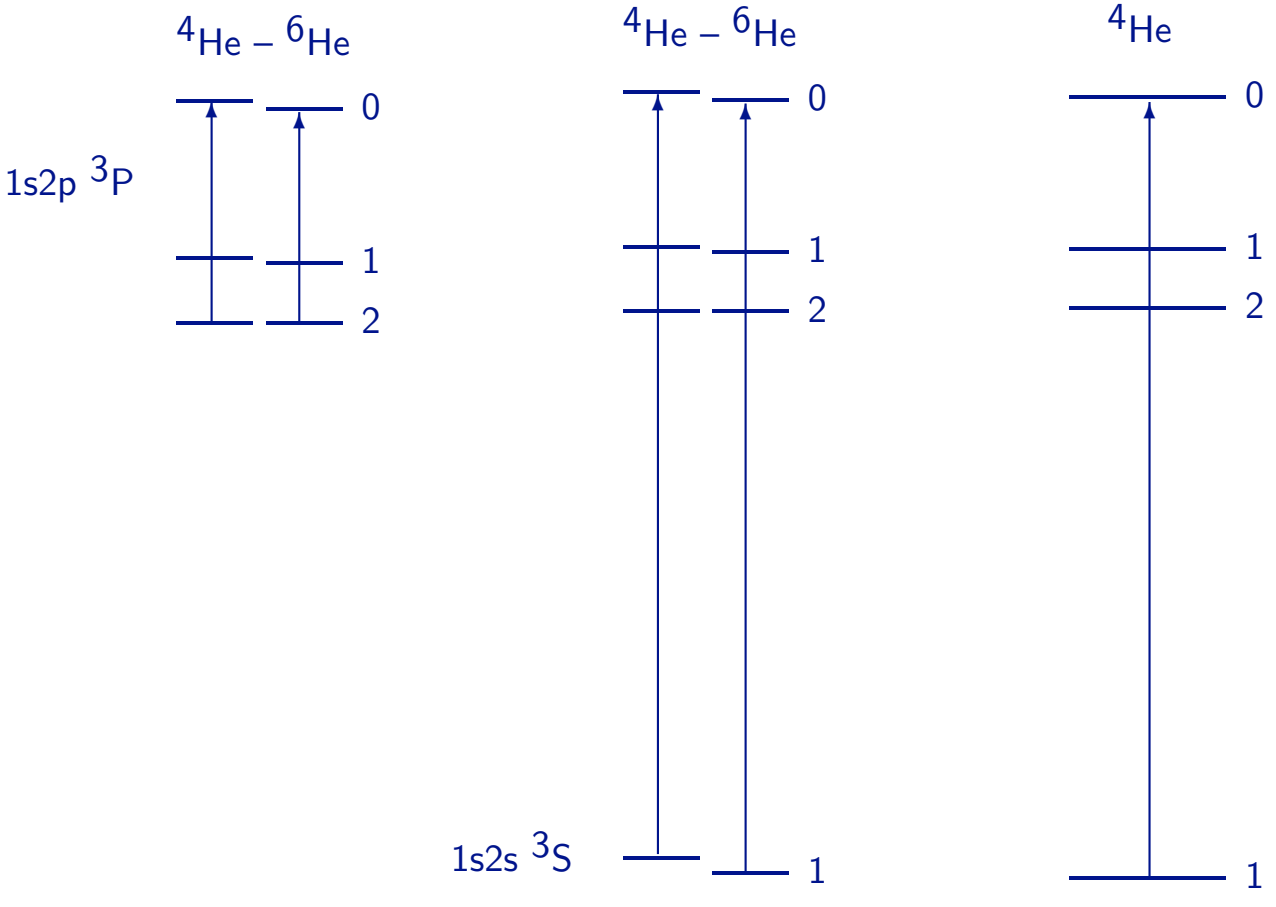
$\Rightarrow$ internal check of theory and experiment

Transition Isotope Shift

$\Rightarrow$ nuclear radius

Total Transition Frequency

$\Rightarrow$ QED shift

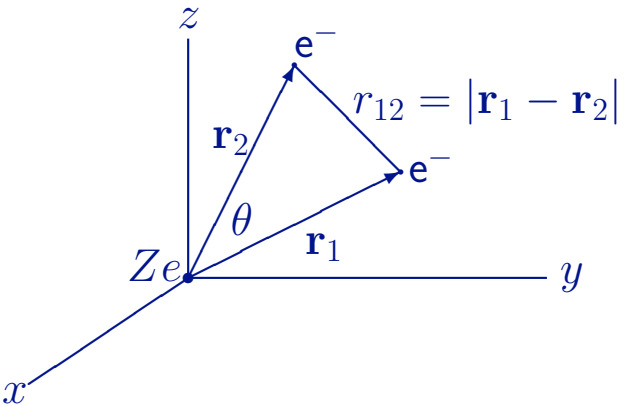


Flow diagram for types of measurements.

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	$Z^2(\mu/M)^2$
Relativistic corrections	$Z^4\alpha^2$
Relativistic recoil	$Z^4\alpha^2\mu/M$
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	$Z^4\langle R_N/a_0\rangle^2$
Nuclear polarization	$Z^3 e^2 \alpha_{\mathrm{d,nuc}}/(\alpha a_0)$

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

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

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

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	

[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).
[5] A. Bürgers, D. Wintgen, J.-M. Rost, J. Phys. B: At. Mol. Opt. Phys. **28**, 3163 (1995).
[6] J.D. Baker, D.E. Freund, R.N. Hill, J.D. Morgan III, Phys. Rev. A **41**, 1247 (1990).

Variational Basis Set for Lithium

Solve for Ψ_0 and Ψ_1 by expanding in Hylleraas coordinates

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

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

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

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

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

Variational upper bounds for nonrelativistic eigenvalues.

State	N_{terms}	E_∞ ($2R_\infty$)	E_M ($2R_M$)
Li($1s^2 2s\ ^2$S)	6413	–7.478 060 323 869	–7.478 036 728 322
	9577	–7.478 060 323 892	–7.478 036 728 344
	9576	–7.478 060 323 890[a]	
Li($1s^2 3s\ ^2$S)	6413	–7.354 098 421 392	–7.354 075 591 755
	9577	–7.354 098 421 425	–7.354 075 591 788
Li($1s^2 2p\ ^2$P)	5762	–7.410 156 532 488	–7.410 137 246 549
	9038	–7.410 156 532 593	–7.410 137 246 663
Be^+($1s^2 2s\ ^2$S)	6413	–14.324 763 176 735	–14.324 735 613 884
	9577	–14.324 763 176 767	–14.324 735 613 915
Be^+($1s^2 3s\ ^2$S)	6413	–13.922 789 268 430	–13.922 763 157 509
	9577	–13.922 789 268 518	–13.922 763 157 598
Be^+($1s^2 2p\ ^2$P)	5762	–14.179 333 293 227	–14.179 323 188 964
	9038	–14.179 333 293 333	–14.179 323 189 509

[a] M. Puchalski and K. Pachucki, Phys. Rev. A **73**, 022503 (2006).

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)

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

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

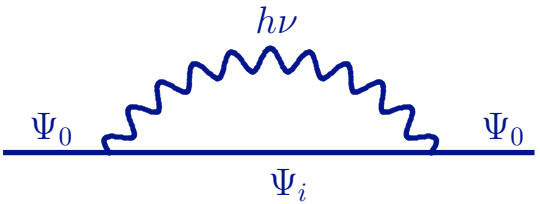
Two-Electron QED Shift

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

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

where $\beta(1s n\ell)$ is the two-electron Bethe logarithm defned by

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



The sum in the denominator can be completed by closure:

$$\mathcal{D} = \langle \Psi_0 | \mathbf{p}(H - E_0)\mathbf{p} | \Psi_0 \rangle = 2\pi Z |\Psi_0(0)|^2$$

where $\mathbf{p} = \mathbf{p}_1 + \mathbf{p}_2$.

Schwartz (1961) transformed the numerator to read

$$\mathcal{N} = \lim_{K\to\infty} \left(-K\langle \Psi_0 | \mathbf{p}\cdot\mathbf{p} | \Psi_0 \rangle + \mathcal{D}\ln(K) + \int_0^K k\, dk \langle \Psi_0 | \mathbf{p}(H - E_0 + k)^{-1}\mathbf{p} | \Psi_0 \rangle \right)$$

Expensive in computer time and slowly convergent. Recent work by

J. D. Baker,R. C. Rorrrey, M. Jerziorska, and J. D. Morgan III (unpublished),
V. I. Korobov and S. V. Korobov, Phys. Rev. A **59**, 3394 (1999).

Alternative method: demonstration for hydrogen

Define a variational basis set with multiple distance scales according to:

$$\chi_{i,j} = r^i \exp(-\alpha_j r) \cos(\theta),$$

with

$$\begin{aligned} j &= 0, 1, \ldots, \Omega - 1 \\ i &= 0, 1, \ldots, \Omega - j - 1 \end{aligned}$$

and

$$\alpha_j = \alpha_0 \times g^j, \quad g \simeq 10$$

The number of elements is $N = \Omega(\Omega + 1)/2$.

Diagonalize the Hamiltonian in this basis set to generate a set of pseudostates.

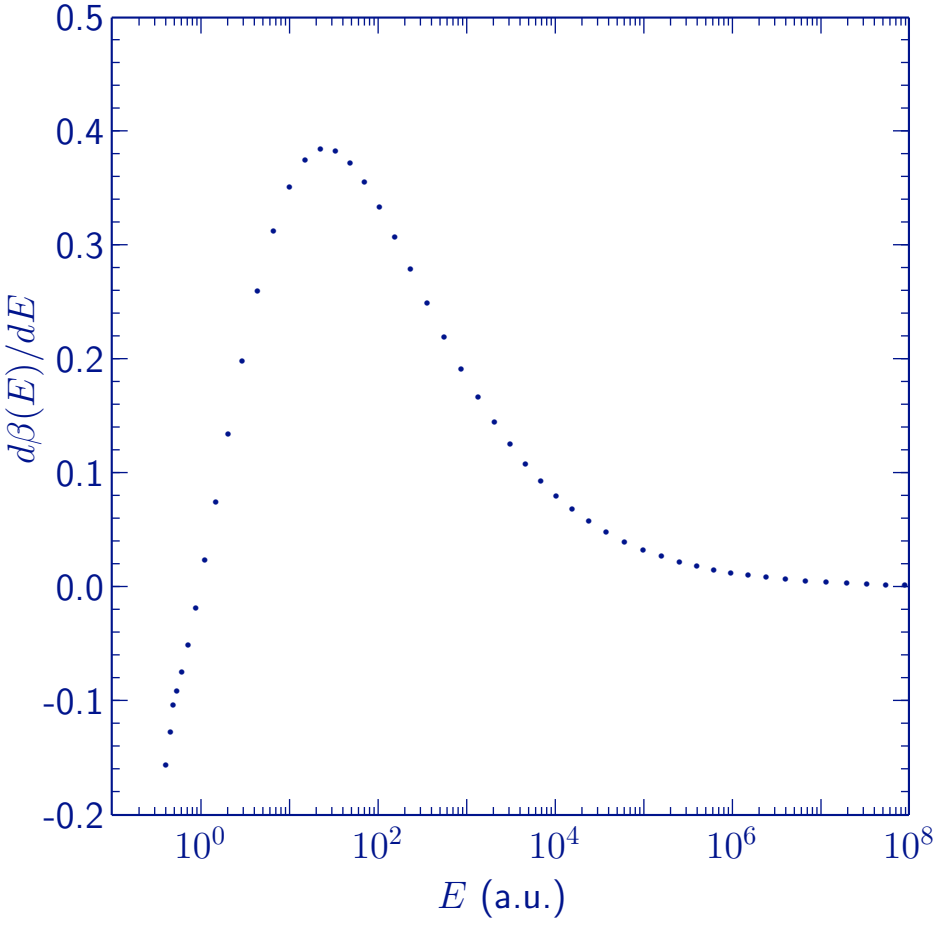
The sequence of basis sets is:

$$\Omega = 1;\ N = 1:$$
$$e^{-\alpha r}$$

$$\Omega = 2;\ N = 3:$$
$$e^{-10\alpha r}$$
$$e^{-\alpha r},\quad re^{-\alpha r}$$

$$\Omega = 3;\ N = 6:$$
$$e^{-100\alpha r}$$
$$e^{-10\alpha r},\quad re^{-10\alpha r},$$
$$e^{-\alpha r},\quad re^{-\alpha r},\quad r^2e^{-\alpha r}$$

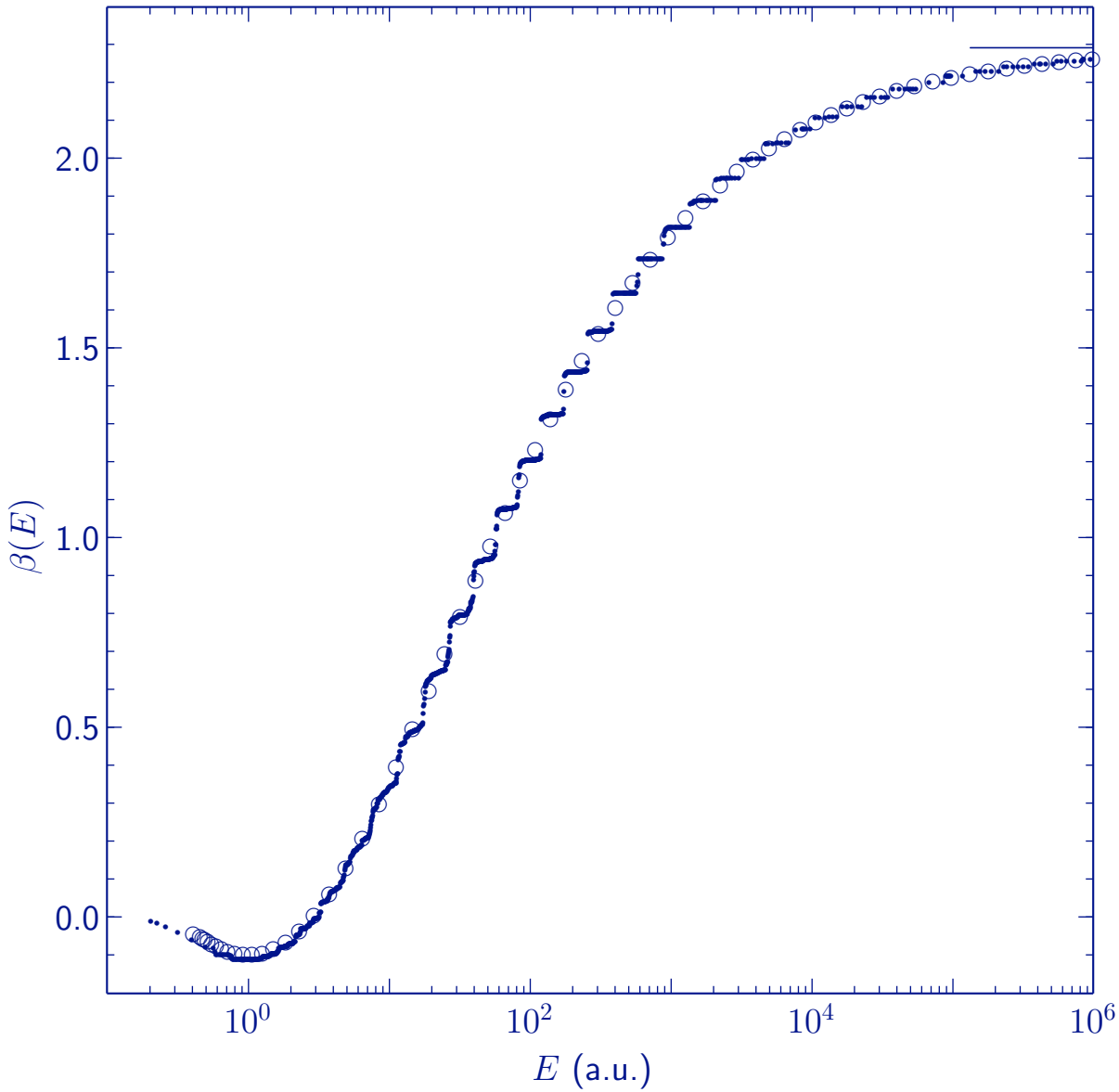
$$\Omega = 4:\ N = 10$$
$$e^{-1000\alpha r}$$
$$e^{-100\alpha r},\quad re^{-100\alpha r},$$
$$e^{-10\alpha r},\quad re^{-10\alpha r},\quad r^2e^{-10\alpha r}$$
$$e^{-\alpha r},\quad re^{-\alpha r},\quad r^2e^{-\alpha r},\quad r^3e^{-\alpha r}$$



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

Convergence of the Bethe logarithm for hydrogen.

Ω	N	$\beta(1s)$	Differences	Ratios
2	3	2.04133473671235643207		
3	6	2.25562501021050378880	0.21429027349814735672	
4	10	2.28660583806175080919	0.03098082785124702039	6.917
5	15	2.29046731873800820861	0.00386148067625739942	8.023
6	21	2.29092465658916831858	0.00045733785116010997	8.443
7	28	2.29097528980426278650	0.00005063321509446792	9.032
8	36	2.29098074679466355929	0.00000545699040077279	9.279
9	45	2.29098131145011677157	0.00000056465545321228	9.664
10	55	2.29098136890590489232	0.00000005745578812075	9.828
11	66	2.29098137458983244603	0.00000000568392755370	10.108
12	78	2.29098137514650642811	0.00000000055667398208	10.211
13	91	2.29098137519991895769	0.00000000005341252957	10.422
14	105	2.29098137520502205119	0.00000000000510309350	10.467
15	120	2.29098137520550236046	0.00000000000048030928	10.625
16	136	2.29098137520554763881	0.00000000000004527834	10.608
17	153	2.29098137520555186303	0.00000000000000422422	10.719
18	171	2.29098137520555226032	0.00000000000000039729	10.633
19	190	2.29098137520555229746	0.00000000000000003714	10.697
20	210	2.29098137520555230096	0.00000000000000000351	10.594
Extrap.		2.29098137520555230133		



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	2.983 865 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).

ASYMPTOTIC EXPANSIONS

Core Polarization Model (Drachman)

– neglect exchange.

– Rydberg electron moves in the field generated by the polarizable core.

$$V(x) = -\frac{Z-1}{x} + \Delta V(x)$$

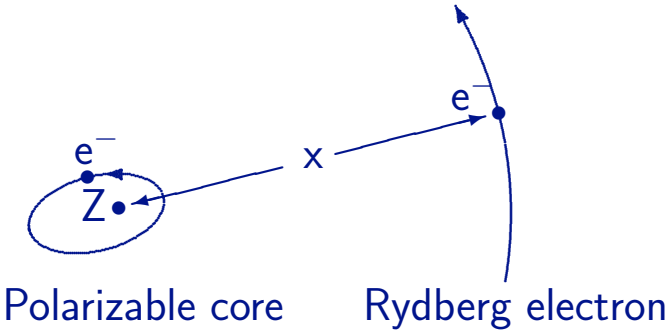


Illustration of the physical basis for the asymptotic expansion method in which the Rydberg electron moves in the field generated by the polarized core.

$$\Delta V(x) = -\frac{c_4}{x^4} - \frac{c_6}{x^6} - \frac{c_7}{x^7} - \frac{c_8}{x^8} - \frac{c_9}{x^9} - \frac{c_{10}}{x^{10}} + \cdots$$

For example, $c_4 = \frac{1}{2}\alpha_1$.

Then

$$\Delta E_{nL} = -\frac{(Z-1)^2}{2n^2} + \langle \chi_0 \mid \Delta V(x) \mid \chi_0 \rangle + \langle \chi_0 \mid \Delta V(x) \mid \chi_1 \rangle$$

where $\mid \chi_1 \rangle$ = first-order perturbation correction to $\mid \chi_0 \rangle$ due to $\Delta V(x)$; i.e.

$$[h_0(x) - e_0] \mid \chi_1 \rangle + \Delta V(x) \mid \chi_0 \rangle = \mid \chi_0 \rangle \langle \mid \Delta V(x) \mid \chi_0 \rangle$$

Asymptotic expansion for the energy of the 1s10k state of helium.

Quantity	Value
$-Z^2/2$	–2.000 000 000 000 000 00
$-1/(2n^2)$	–0.005 000 000 000 000 00
$c_4\langle r^{-4}\rangle$	–0.000 000 007 393 341 95
$c_6\langle r^{-6}\rangle$	0.000 000 000 004 980 47
$c_7\langle r^{-7}\rangle$	0.000 000 000 000 278 95
$c_8\langle r^{-8}\rangle$	–0.000 000 000 000 224 33
$c_9\langle r^{-9}\rangle$	–0.000 000 000 000 002 25
$c_10\langle r^{-10}\rangle$	0.000 000 000 000 003 73
Second order	–0.000 000 000 000 070 91
Total	–2.005 000 007 388 376 30(74)
Variational	–2.005 000 007 388 375 8769(0)
Difference	–0.000 000 000 000 000 42(74)
	$\simeq 3$ Hz

Two-electron Bethe logs for high angular momentum

$$\beta(1snl) = \beta(1s) + \left(\frac{Z-1}{Z}\right)^4 \frac{\beta(nl)}{n^3} + \frac{0.316205}{Z^6}\langle x^{-4}\rangle + \Delta\beta(1snl)$$

Residual two-electron Bethe logs $n^3\Delta\beta(1snl)$.

State	$n^3\Delta\beta(1snl)$	Least squares fit	Difference
$3\,^1$D	–0.000 001 08(4)		
$3\,^3$D	0.000 181 74(5)		
$4\,^1$D	–0.000 018 4(3)		
$4\,^3$D	0.000 231 18(7)		
$5\,^1$D	–0.000 026 84(9)		
$5\,^3$D	0.000 249 73(12) [a]		
$4\,^1$F	0.000 006 58(2)	0.000 006 60	–0.000 000 02(2)
$4\,^3$F	0.000 007 63(2)	0.000 007 64	–0.000 000 01(2)
$5\,^1$F	0.000 008 70(3)	0.000 008 69	0.000 000 01(3)
$5\,^3$F	0.000 010 42(3)	0.000 010 41	0.000 000 01(3)
$6\,^1$F	0.000 009 8(1)	0.000 009 83	0.000 000 0(1)
$6\,^3$F	0.000 011 9(3)	0.000 011 98	–0.000 000 1(3)
$5\,^1$G	0.000 000 770(3)	0.000 000 770	0.000 000 000(3)
$5\,^3$G	0.000 000 771(3)	0.000 000 771	0.000 000 000(3)
$6\,^1$G	0.000 001 043(3)	0.000 001 042	0.000 000 001(3)
$6\,^3$G	0.000 001 050(8)	0.000 001 047	0.000 000 003(8)
$6\,^1$H	0.000 000 127(2)	0.000 000 127	0.000 000 000(2)
$6\,^3$H	0.000 000 127(2)	0.000 000 127	0.000 000 000(2)

[a] Corresponds to an energy uncertainty of ±14 Hz.

A least-squares fit gives

$$\Delta\beta(1snl\ ^1\mathrm{L}) = 95.6(0.9)\langle x^{-6}\rangle - 841(19)\langle x^{-7}\rangle + 1394(50)\langle x^{-8}\rangle$$

$$\Delta\beta(1snl\ ^3\mathrm{L}) = 95.0(0.9)\langle x^{-6}\rangle - 840(23)\langle x^{-7}\rangle + 1581(60)\langle x^{-8}\rangle$$

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 $\Delta\beta_{\rm MP}$.

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

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

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.

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

Contribution	$2\,^3S_1$	$3\,^3P_2$	$2\,^3S_1 - 3\,^3P_2$
$E_{\rm nr}$	52 947.324(19)	17 549.785(6)	35 397.539(16)
μ/M	2 248.202(1)	–5 549.112(2)	7 797.314(2)
$(\mu/M)^2$	–3.964	–4.847	0.883
$\alpha^2\mu/M$	1.435	0.724	0.711
$E^{\rm a}_{\rm nuc}$	–1.264	0.110	–1.374
$\alpha^3\mu/M$, 1-e	–0.285	–0.037	–0.248
$\alpha^3\mu/M$, 2-e	0.005	0.001	0.004
Total	55 191.453(19)	11 996.625(4)	43 194.828(16)
Experiment[b]			43 194.772(56)
Difference			0.046(56)

[a]Assumed nuclear radius is $r_{\rm nuc}(^6{\rm He}) = 2.04$ fm.

In general, ${\rm IS}(2S-3P) = 43\,196.202(16) + 1.008[r^2_{\rm nuc}(^4{\rm He}) - r^2_{\rm nuc}(^6{\rm He})]$.

Adjusted nuclear radius is $r_{\rm nuc}(^6{\rm He}) = 2.054(14)$ fm.

[b]Z.-T. Lu, Argonne collaboration.

Nuclear Charge Radius of ^{8}He

P. Mueller,[1,*] I. A. Sulai,[1,2] A. C. C. Villari,[3] J. A. Alcántara-Núñez,[3] R. Alves-Condé,[3] K. Bailey,[1] G. W. F. Drake,[4] M. Dubois,[3] C. Eléon,[3] G. Gaubert,[3] R. J. Holt,[1] R. V. F. Janssens,[1] N. Lecesne,[3] Z.-T. Lu,[1,2] T. P. O'Connor,[1] M.-G. Saint-Laurent,[3] J.-C. Thomas,[3] and L.-B. Wang[5]

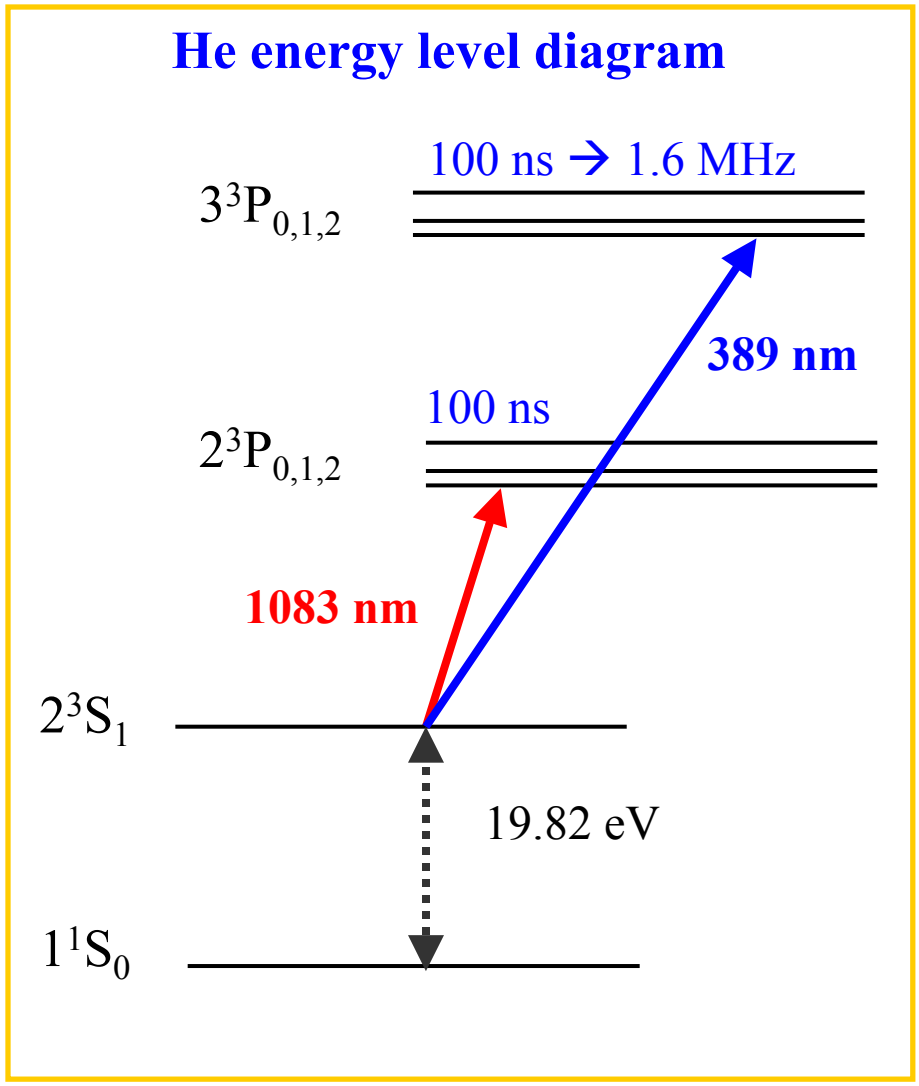
[1]*Physics Division, Argonne National Laboratory, Argonne, Illinois 60439, USA*
[2]*Department of Physics and Enrico Fermi Institute, University of Chicago, Chicago, Illinois 60637, USA*
[3]*GANIL (IN2P3/CNRS-DSM/CEA), B.P. 55027 F-14076 Caen Cedex 5, France*
[4]*Physics Department, University of Windsor, Windsor, Ontario, Canada N9B 3P4*
[5]*Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA*

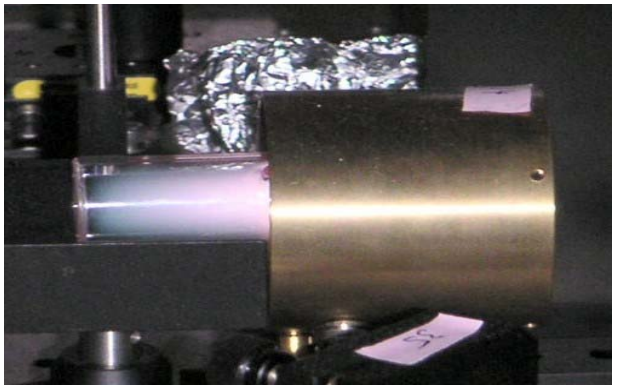
(Received 21 November 2007; published 21 December 2007)

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.

DOI: 10.1103/PhysRevLett.99.252501 PACS numbers: 21.10.Ft, 21.60.−n, 27.20.+n, 31.30.Gs

Atomic Energy Levels of Helium





A helium glow discharge

Laser Spectroscopic Determination of the Nuclear Charge Radius of ^{6}He

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

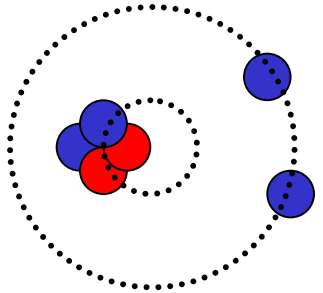
- Test the Standard Nuclear Structure Model;
- Study nucleon interactions in neutron-rich matter.

Method: Atomic isotope shift

^{6}He – ^{4}He isotope shift at 2 $^3S_1$ – 3 $^3P_2$, 389 nm

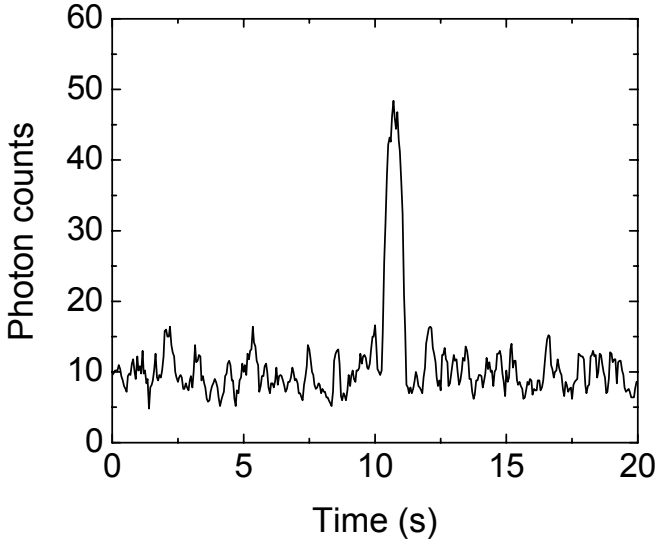
IS (MHz) = 43,196.202(20) + 1.008 x [$\langle r^2 \rangle_{4He}$ - $\langle r^2 \rangle_{6He}$]

-- G.W.F. Drake, Nucl. Phys. A737c, 25 (2004)

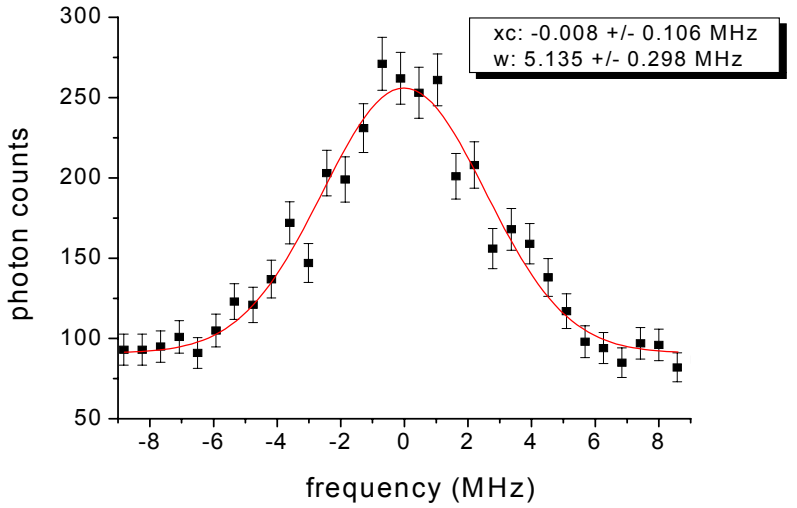


^{6}He: ^{4}He + 2n

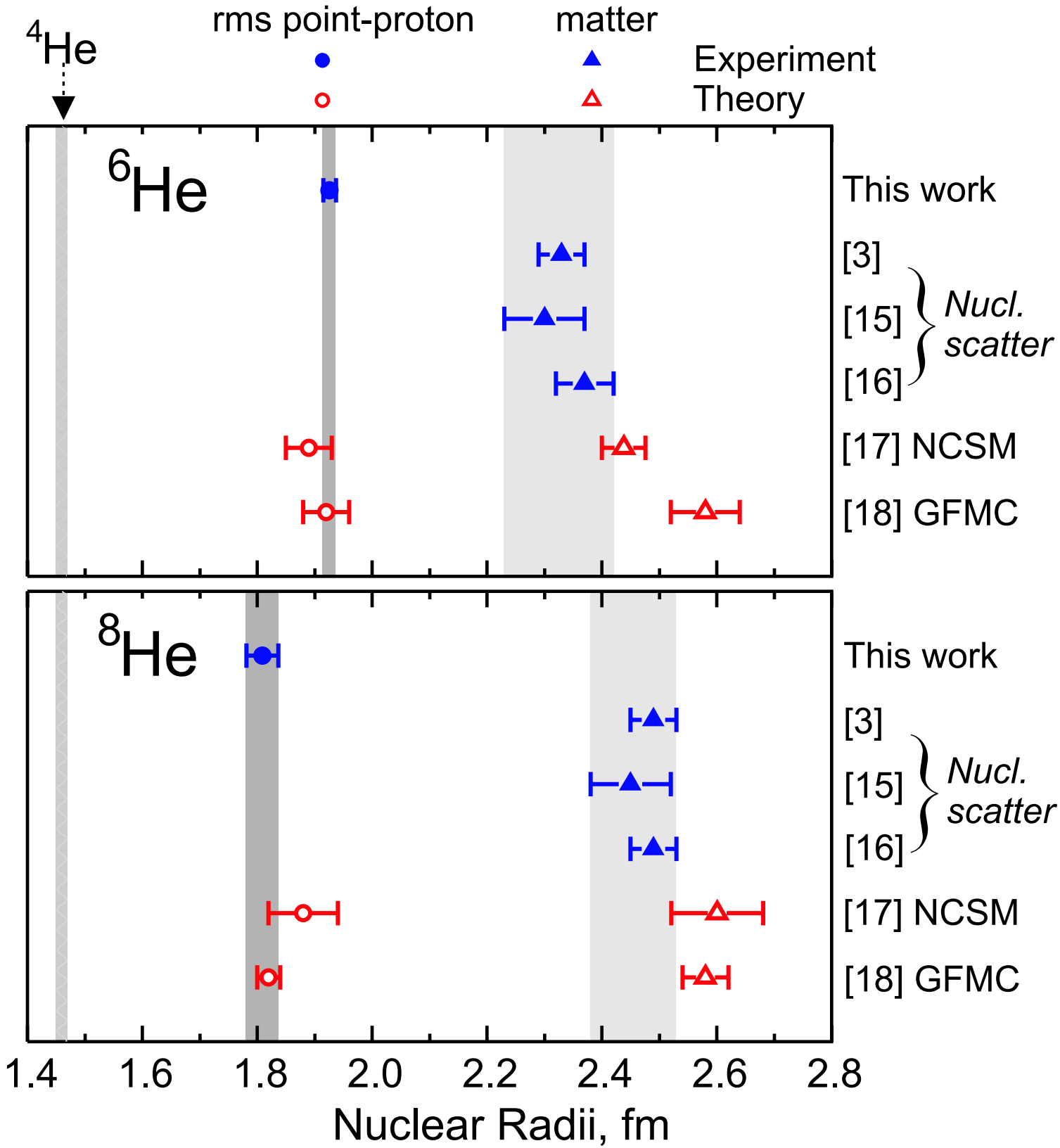
Its charge radius expands due to the motion of the ^{4}He core



Fluorescence signal of one trapped ^{6}He atom



Spectrum of 150 ^{6}He atoms in one hour


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

Comparison between theory and experiment for the total transition frequencies of ^{7}Li and $^9Be^+$. Units are cm^{-1}.

Atom/Ion	$2\ ^2P_{1/2} - 2\ ^2S_{1/2}$	$2\ ^2P_{3/2} - 2\ ^2S_{1/2}$	$3\ ^2S_{1/2} - 2\ ^2S_{1/2}$	$2\ ^2S_{1/2}$ I.P.
^{7}Li (this work)	14 903.647 9(10)	14 903.983 2(10)	27 206.093 0(10)	43 487.158 3(10)
^{7}Li (expt.)	14 903.648 130(14)[a]	14 903.983 648(14)[a]	27 206.094 20(10)[b]	43 487.159 40(18)[c]
Difference	–0.000 2(10)	–0.000 4(10)	–0.001 2(10)	–0.001 1(10)
$^9Be^+$ (this work)	31 928.738(5)	31 935.310(5)	88 231.920(6)	146 882.923(5)
$^9Be^+$ (expt.)	31 928.744[d]	31 935.320[d]	88 231.915[d]	146 882.86[d]
		31 935.310(47)[e]		
Difference	–0.006(5)	–0.010(5)	0.005(6)	0.063(5)
		0.000(47)		

[a] Sansonetti *et al.*
[b] Bushaw *et al.*
[c] Bushaw *et al.*
[d] Ralchenko *et al.*
[e] Nakamura *et al.*

The ToPLiS Collaboration

EXPERIMENT

GSI

A. Dax, **G. Ewald**, S. Götte, **R. Kirchner**, H.-J. Kluge
Th. Kühl, **R. Sanchez**, A. Wojtaszek

Universität Tübingen

W. Nörtershäuser, C. Zimmermann

Pacific Northwest National Lab

B. A. Bushaw

TRIUMF

D. Albers, J. Behr, P. Bricault, J. Dilling, M. Dombsky,
J. Lassen, P. Levy, M. Pearson, E. Prime, V. Rijkov

THEORY

University of Windsor, Canada

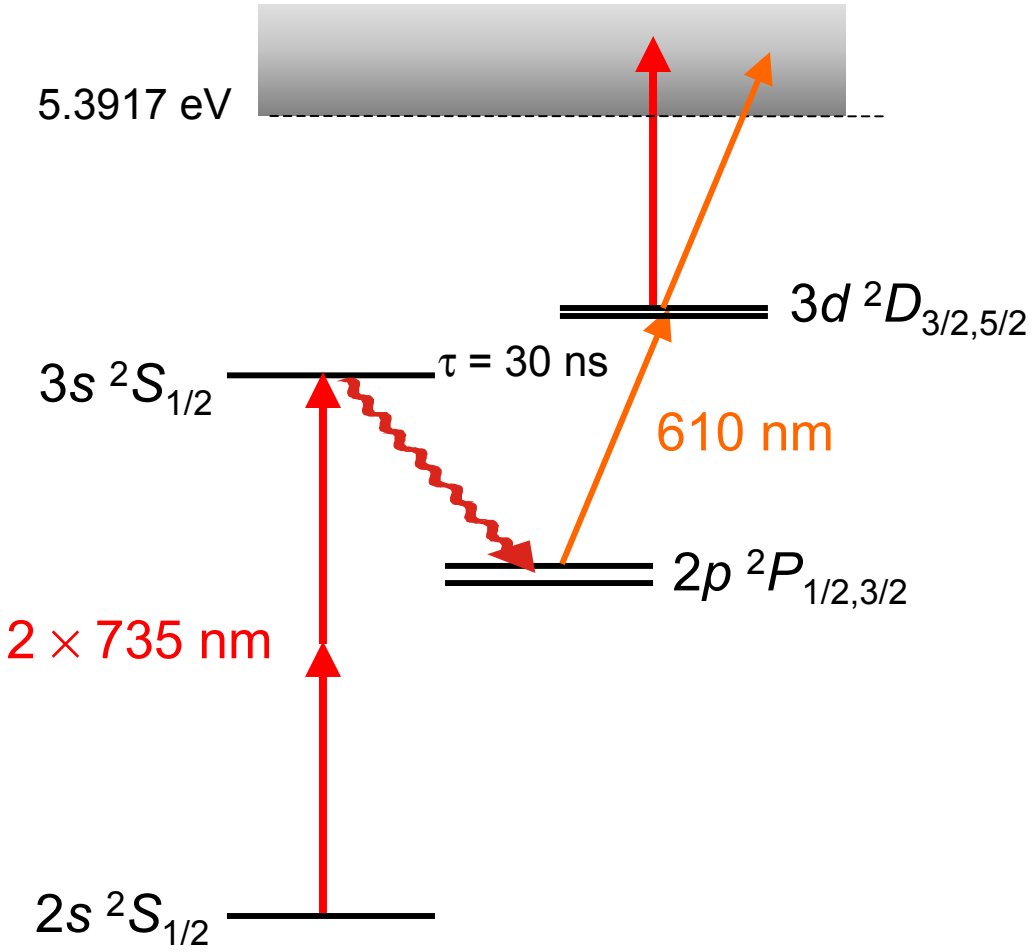
G. W. F. Drake

University of New Brunswick, Canada

Z.-C. Yan

Resonance Ionization of Lithium

"Doubly-Resonant-4-Photon Ionization"



2s – 3s transition

→ Narrow line

2-photon spectroscopy

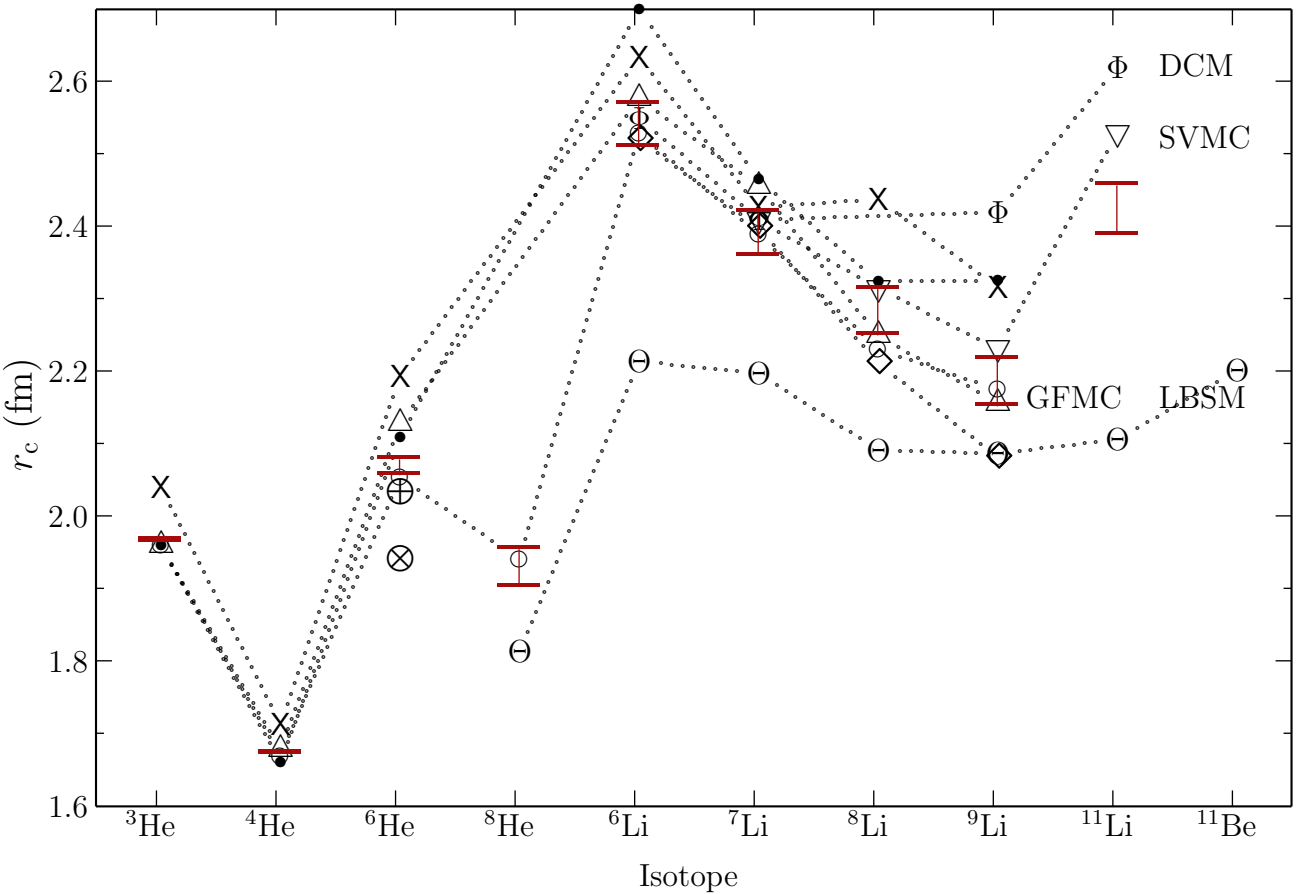
→ Doppler cancellation

Spontaneous decay

→ Decoupling of precise spectroscopy and efficient ionization

2p – *3d* transition

→ Resonance enhancement for efficient ionization



LBSM – Large Basis Shell Model (Navrátil et al., 2003).
SVMC – Stochastic Variational MultiCluster (Suzuki et al., 2002).
DCM – Dynamic Correlation Model (Tomaselli et al., 2002).
GFMC – Green's Function Monte Carlo (Wiringa & Peiper, 2007).

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 helium and lithium.
- 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 $\pm$0.002 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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Contributions to the ^{7}Li–^{6}Li isotope shifts for the $1s^2 2p\,{}^2\mathrm{P}_J$–$1s^2 2s\,{}^2\mathrm{S}$ transitions and comparison with experiment. Units are MHz.

Contribution	$2\,{}^2\mathrm{P}_{1/2}$–$2\,{}^2\mathrm{S}$	$2\,{}^2\mathrm{P}_{3/2}$–$2\,{}^2\mathrm{S}$
	Theory	
μ/M	10 533.508(5)[a]	10 533.508(5)[a]
$(\mu/M)^2$	0.061	0.061
$\alpha^2\,\mu/M$	–1.4855(13)	–1.0904(13)
$\alpha^3\,\mu/M$, anom. magnetic	–0.000 17	0.000 09
$\alpha^3\,\mu/M$, one-electron	0.0184	0.0184
$\alpha^3\,\mu/M$, two-electron	0.009(2)	0.009(2)
$r^2_{\rm rms}$	0.194±0.271	0.194±0.271
$r^2_{\rm rms}\,\mu/M$	–0.000 73(11)	–0.000 73(11)
Total	10 534.052(6)	10 534.448(6)
RCI-MBPT[b]	10608(300)	10607(300)
	Experiment	
Sansonetti *et al.*[c]	10 532.9(6)	10 533.3(5)
Windholz *et al.*[d]	10 534.3(3)	10 539.9(1.2)
Scherf *et al.*[e]	10 533.13(15)	10 534.93(15)
Walls *et al.*[f]	10 534.26(13)	
Noble *et al.*[g]	10 534.039(70)	

[a]The additional uncertainty from the atomic mass determinations is ±0.008 MHz.

[b]V.A. Korol and M.G. Kozlov, Phys. Rev. A **76**, 022103 (2007).

[c]C. J. Sansonetti et al., Phys. Rev. A **52**, 2682 (1995).

[d]L. Windholz and C. Umfer, Z. Phys. D **29**, 121 (1994).

[e]W. Scherf, O. Khait, H. Jäger, and L. Windholz, Z. Phys. D **36**, 31, (1996).

[f]J. Walls et al., Eur. Phys. J. **D 22** 159 (2003).

[g]G.A. Noble, B.E. Schultz, H. Ming, W.A. van Wijngaarden, Phys. Rev. A **74**, 012502 (2006).

Contributions to the ^{7}Li–^{6}Li isotope shifts for the $1s^2 2p\ ^2\mathrm{P}_J$–$1s^2 2s\ ^2\mathrm{S}$ transitions and comparison with experiment. Units are MHz.

Contribution	$2\,^2\mathrm{P}_{1/2}$–$2\,^2\mathrm{S}$	$2\,^2\mathrm{P}_{3/2}$–$2\,^2\mathrm{S}$
	Theory	
μ/M	10 533.508(5)[a]	10 533.508(5)[a]
$(\mu/M)^2$	0.061	0.061
$\alpha^2\,\mu/M$	–1.4855(13)	–1.0904(13)
$\alpha^3\,\mu/M$, anom. magnetic	–0.000 17	0.000 09
$\alpha^3\,\mu/M$, one-electron	0.0184	0.0184
$\alpha^3\,\mu/M$, two-electron	0.009(2)	0.009(2)
r^2_{rms}	0.194±0.271	0.194±0.271
$r^2_{\mathrm{rms}}\,\mu/M$	–0.000 73(11)	–0.000 73(11)
Total	10 534.052(6)	10 534.448(6)
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	Experiment	
Sansonetti *et al.*[c]	10 532.9(6)	10 533.3(5)
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Noble *et al.*[g]	10 534.039(70)	

[a]The additional uncertainty from the atomic mass determinations is ±0.008 MHz.

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[d]L. Windholz and C. Umfer, Z. Phys. D **29**, 121 (1994).

[e]W. Scherf, O. Khait, H. Jäger, and L. Windholz, Z. Phys. D **36**, 31, (1996).

[f]J. Walls et al., Eur. Phys. J. **D 22** 159 (2003).

[g]G.A. Noble, B.E. Schultz, H. Ming, W.A. van Wijngaarden, Phys. Rev. A **74**, 012502 (2006).

Spin-independent Relativistic Corrections of $O(\alpha^4)$ a.u.

$$\Delta E_{\rm B}^{(4)} = \alpha^4 \langle H_{\rm e-n}(1) + H_{\rm e-n}(2) + H_V \rangle + \sum_I \alpha^4 \left\langle B_I \frac{1}{(E-H)'} B_I \right\rangle$$

where

$$H_{\rm e-n}(i) = \frac{p_i^6}{16} - \frac{1}{8}\left[\mathbf{p}_i, \frac{Z}{r_i}\right]^2 - \frac{5}{128}\left[p_i^2, \left[p_i^2, \frac{Z}{r_i}\right]\right] - \frac{3}{32} p_i^2 \left[\mathbf{p}_i, \left[\mathbf{p}_i, \frac{Z}{r_i}\right]\right]$$

and

$B_I =$ Breit interaction terms.

K. Pachucki, Phys. Rev. Lett. **84**, 4561 (2000).
V. I. Korobov, Phys. Rev. A **66**, 024501 (2002).

M. H. Chen, K. T. Cheng, and W. R. Johnson, Phys. Rev. A 47, 3692 (1993).

For the $O(\alpha^4)$ contributions to the fine structure splittings in He-like ions:

$$\nu_{02}^{(4)} = (Z\alpha)^4[-\frac{5}{256}Z^2 + 0.144\,772\,9Z + c_{02} + \cdots] ,$$

$$\nu_{12}^{\prime(4)} = (Z\alpha)^4[-\frac{5}{384}Z^2 + 0.058\,776\,8Z + c_{12} + \cdots] ,$$

Method	c_{02}	c_{12}
Nonrelativistic (Drake)	–0.4645(20)	–0.13(10)
Relativistic CI (CCJ)	–0.51	–0.154

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

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

The "normal" isotope shift is

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

The first-order "specific" isotope shift is

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

The second-order "specific" isotope shift is

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

Two contexts

I. For total transition frequencies

$$\Delta E = E_i - E_f$$

and the dominant source of uncertainty is the higher-order QED term $\alpha^4 \mathcal{E}^{(0)}_{\rm ho} \simeq 10^{-8}$, where here and throughout the superscript denotes the power of λ.

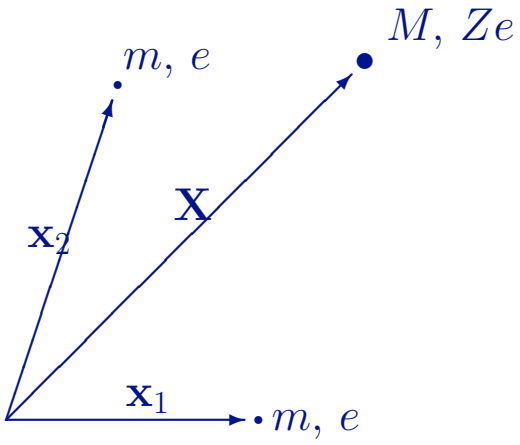
II. For isotope shifts

terms independent of λ cancel (except for the last $\bar{r}^2_{\rm c}$ term), and the term $\alpha^4 \lambda \mathcal{E}^{(1)}_{\rm ho} \simeq 10^{-12}$ contributes only at the level of a few kHz. The isotope shift between isotopes A and B in the same atomic state is then

$$\begin{aligned}
&\Delta E(B-A) = \\
&\lambda_- \left[\mathcal{E}^{(1)}_{\rm NR} - \mathcal{E}^{(0)}_{\rm NR} + \lambda_+ \left(\mathcal{E}^{(2)}_{\rm NR} - \mathcal{E}^{(1)}_{\rm NR}\right) + \alpha^2 \left(\mathcal{E}^{(1)}_{\rm rel} - \mathcal{E}^{(0)}_{\rm rel}\right)\right. \\
&\left. + \alpha^3 \left(\mathcal{E}^{(1)}_{\rm QED} - \mathcal{E}^{(0)}_{\rm QED}\right) + \alpha^4 \left(\mathcal{E}^{(1)}_{\rm ho} - \mathcal{E}^{(0)}_{\rm ho}\right)\right] \\
&+ \left(\bar{r}^2_{{\rm c},B} - \bar{r}^2_{{\rm c},A}\right) \mathcal{E}^{(0)}_{\rm nuc}
\end{aligned} \tag{1}$$

where $\lambda_\pm = (\mu/M)_B \pm (\mu/M)_A$.

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

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

New Variational Techniques

I. Double the basis set

$$\begin{aligned} \text{If} \quad \phi_{i,j,k}(\alpha,\beta) &= r_1^i r_2^j r_{12}^k e^{-\alpha r_1 - \beta r_2} \\ \text{then} \quad \tilde{\phi}_{i,j,k} &= a_1 \phi_{i,j,k}(\alpha_1,\beta_1) + a_2 \phi_{i,j,k}(\alpha_2,\beta_2) \end{aligned}$$

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

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

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

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.

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

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

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

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

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

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

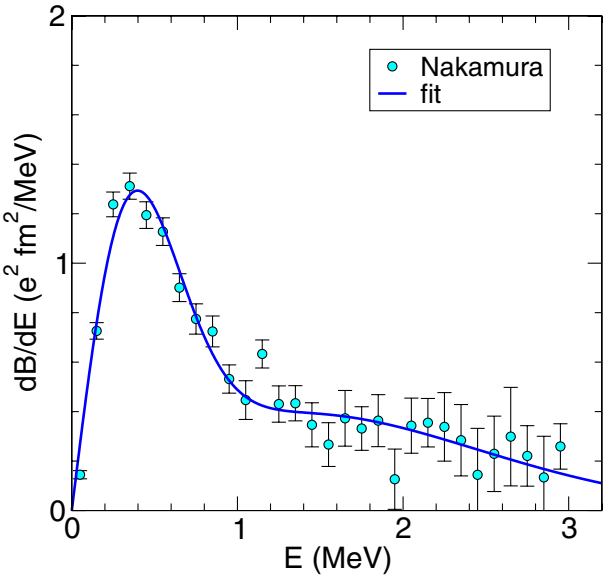


FIG. 1 (color online). Electric dipole line strength by Nakamura *et al.* [20] adapted to the new value of E_T from Ref. [7].

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

Calculated isotope shift parameter $\Delta E^{(0)}_{B-A}$ for various transitions in Li and Be^+. Units are MHz.

Isotopes	$2\,^2P_{1/2}$–$2\,^2S_{1/2}$	$2\,^2P_{3/2}$–$2\,^2S_{1/2}$	$3\,^2S_{1/2}$–$2\,^2S_{1/2}$
^{7}Li–^{6}Li	–10 532.111(6)	–10 532.506(6)	–11 452.821(2)
^{7}Li–^{8}Li	7 940.627(5)	7 940.925(5)	8 634.989(2)
^{7}Li–^{9}Li	14 098.840(8)	14 099.369(8)	15 331.799(3)
^{7}Li–^{11}Li[a]	23 082.642(11)	23 083.493(11)	25 101.470(5)
^{9}Be–^{7}Be	–49 225.765(19)	-49 231.814(19)	-48 514.03(2)
^{9}Be–^{10}Be	17 310.44(6)	17 312.57(6)	17 060.56(6)
^{9}Be–^{11}Be	31 560.01(6)	31 563.89(6)	31 104.60(6)

[a]Includes nuclear polarization corrections of 62 kHz for the $3\,^2P_J$-$2\,^2S_{1/2}$ transitions, and 39 kHz for the $3\,^2S_{1/2}$–$2\,^2S_{1/2}$ transition.

$$\begin{aligned}\Delta E(B-A) &= \lambda_-\left[\mathcal{E}^{(1)}_{\rm tot}-\mathcal{E}^{(0)}_{\rm tot}+\lambda_+\left(\mathcal{E}^{(2)}_{\rm tot}-\mathcal{E}^{(1)}_{\rm tot}\right)\right]+C\left(\bar{r}^2_{{\rm c},B}-\bar{r}^2_{{\rm c},A}\right)\\ &= \Delta E^{(0)}_{(B-A)}+C\left(\bar{r}^2_{{\rm c},B}-\bar{r}^2_{{\rm c},A}\right)\end{aligned}$$

and for Be^+:
$C(2\,^2P-2\,^2S) = 16.912$ MHz/fm^2
$C(3\,^2S-2\,^2S) = 10.376$ MHz/fm^2

Contributions to the ^{7}Li–^{6}Li isotope shift for the $1s^2 3s\ ^2\mathrm{S}$–$1s^2 2s\ ^2\mathrm{S}$ transition. Units are MHz.

Contribution	$3\ ^2\mathrm{S}$–$2\ ^2\mathrm{S}$
μ/M	11 454.6557[a]
$(\mu/M)^2$	–1.7940
$\alpha^2\,\mu/M$	0.0156(3)
$\alpha^3\,\mu/M$, one-electron	–0.067(2)
$\alpha^3\,\mu/M$, two-electron	0.010(2)
$r^2_{\rm rms}$	1.238±0.39
$r^2_{\rm rms}\,\mu/M$	–0.000 7(1)
Total	11 454.058(2)±0.39
King[b]	11 446.1
Vadla *et al.*[c] (experiment)	11 434(20)
Bushaw *et al.*[d] (experiment)	11 453.734(30)

[a]The additional uncertainty from the atomic mass determinations is ±0.008 MHz.

[b]F. W. King, Phys. Rev. A **40**, 1735 (1989); **43**, 3285 (1991).

[c]C. Vadla, A. Obrebski, and K. Niemax, Opt. Commun. **63**, 288 (1987).

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

Total coefficients for various transitions in Li and Be^+. Units are a.u.

Atom/ion transition	$\mathcal{E}^{(0)}_{\rm tot}$	$\mathcal{E}^{(1)}_{\rm tot}$	$\mathcal{E}^{(2)}_{\rm tot}$
Li($2\,^2P_{1/2} - 2\,^2S_{1/2}$)	0.067 915 6344(29)	–0.122 990 87(7)	–0.004 236(3)
Li($2\,^2P_{3/2} - 2\,^2S_{1/2}$)	0.067 917 1624(29)	–0.122 995 47(7)	–0.004 236(3)
Li($3\,^2S_{1/2} - 2\,^2S_{1/2}$)	0.123 970 5407(35)	–0.133 764 36(3)	0.123 6596(6)
Li($2\,^2S_{1/2}$) I.P.	0.198 158 5744(26)	–0.211 012 55(3)	0.235 2863(6)
Be^+($2\,^2P_{1/2} - 2\,^2S_{1/2}$)	0.145 504 341(25)	–0.432 048 23(7)	–0.094 75(14)
Be^+($2\,^2P_{3/2} - 2\,^2S_{1/2}$)	0.145 534 287(25)	–0.432 101 32(7)	–0.094 75(14)
Be^+($3\,^2S_{1/2} - 2\,^2S_{1/2}$)	0.402 040 134(26)	–0.425 861 69(7)	0.339 98300(2)
Be^+($2\,^2S_{1/2}$) I.P.	0.669 290 555(24)	–0.701 626 33(7)	0.721 96394(1)

$$\Delta E(B-A) = \lambda_- \left[\mathcal{E}^{(1)}_{\rm tot} - \mathcal{E}^{(0)}_{\rm tot} + \lambda_+ \left(\mathcal{E}^{(2)}_{\rm tot} - \mathcal{E}^{(1)}_{\rm tot}\right)\right] + \left(\bar{r}^2_{{\rm c},B} - \bar{r}^2_{{\rm c},A}\right) \mathcal{E}^{(0)}_{\rm nuc}$$

where $\lambda_\pm = (\mu/M)_B \pm (\mu/M)_A$, and

$$\mathcal{E}^{(k)}_{\rm tot} = \mathcal{E}^{(k)}_{\rm NR} + \alpha^2 \mathcal{E}^{(k)}_{\rm rel} + \alpha^3 \mathcal{E}^{(k)}_{\rm QED} + \alpha^4 \mathcal{E}^{(k)}_{\rm ho} \qquad \text{for each } k = 0,\ 1,\ 2.$$

Calculated isotope shift parameter $\Delta\nu^{(0)}_{B-A}$ for various transitions in Li and Be^+. Units are MHz.

Isotopes	$2\,^2P_{1/2}$–$2\,^2S_{1/2}$	$2\,^2P_{3/2}$–$2\,^2S_{1/2}$	$3\,^2S_{1/2}$–$2\,^2S_{1/2}$
^{7}Li–^{6}Li	–10 532.111(6)	–10 532.506(6)	–11 452.821(2)
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^{9}Be–^{11}Be	31 560.01(6)	31 563.89(6)	31 104.60(6)

[a]Includes nuclear polarization corrections of 62 kHz for the $3\,^2P_J$-$2\,^2S_{1/2}$ transitions, and 39 kHz for the $3\,^2S_{1/2}$–$2\,^2S_{1/2}$ transition.

Determination of the Nuclear Radius for Isotopes of Lithium

$$R^2_{\rm rms}(\,^A{\rm Li}) = R^2_{\rm rms}(\,^6{\rm Li}) + \frac{E^A_{\rm meas} - E^A_0}{C} \tag{1}$$

where $E^A_{\rm meas}$ is the measured isotope shift for ^{A}Li relative to ^{6}Li, and E^A_0 contains all the calculated contributions to the isotope shift with the exception of the shift due to finite nuclear size.

Values of E^A_0 to determine $R^2_{\rm rms}$ from the measured isotope shift in various transitions. Units are MHz.

Isotopes	$E^A_0(2\,^2P_{1/2} - 2\,^2S)$	$E^A_0(2\,^2P_{3/2} - 2\,^2S)$	$E^A_0(3\,^2S - 2\,^2S)$
^{7}Li–^{6}Li	10 532.19(7)	10 532.58(7)	11 453.00(6)
^{8}Li–^{6}Li	18 472.86(12)	18 473.55(12)	20 088.10(10)
^{9}Li–^{6}Li	24 631.11(16)	24 632.03(16)	26 785.01(13)
^{10}Li–^{6}Li	29 575.46(20)	29 576.56(20)	32 161.92(17)
^{11}Li–^{6}Li	33 615.19(24)	33 616.45(24)	36 555.11(21)

$C = -2.4565$ MHz/fm^2 for the $2\,^2{\rm P}_J - 2\,^2{\rm S}_{1/2}$ I.S.
$C = -1.5661$ MHz/fm^2 for $3\,^2{\rm S}_{1/2} - 2\,^2{\rm S}_{1/2}$ I.S.

Comparison between theory and experiment for the fine structure splittings and ^{7}Li–^{6}Li splitting isotope shift (SIS). Units are MHz.

Reference	^{7}Li $2\,^2P_{3/2} - 2\,^2P_{1/2}$	^{6}Li $2\,^2P_{3/2} - 2\,^2P_{1/2}$	SIS
Present work	10 051.333±3[a]	10 050.937±3[a]	0.395
Brog *et al.* [b]	10 053.24(22)	10 052.76(22)	0.48(31)
Scherf *et al.* [c]	10 053.4(2)	10 051.62(20)	1.78(28)
Walls *et al.* [d]	10 052.37(11)	10 053.044(91)	–0.67(14)
Orth *et al.* [e]	10 053.184(58)		
Noble *et al.* [f]	10 053.119(58)	10 052.964(50)	0.155(76)
Das *et al.* [g]	10 052.862(67)	10 051.999(46)	–0.863(79)
Recommended value	10 053.2(1)	10 052.8(1)	

[a] Includes uncertainty of ±3 MHz due to mass-independent higher-order terms not yet calculated.

[b] K.C. Brog, Phys. Rev. **153**, 91 (1967).

[c] W. Scherf, O. Khait, H. Jager, and L. Windholz, Z. Phys. D **36**, 31 (1996).

[d] J. Walls, R. Ashby, J. J. Clarke, B. Lu, and W. A. van Wijngaarden, Eur. Phys. J **D 22** 159 (2003).

[e] H. Orth, H. Ackermann, and E.W. Otten, Z. Phys. A **273**, 221 (1975).

[f] G.A. Noble, B.E. Schultz, H. Ming, W.A. van Wijngaarden, Phys. Rev. A **74**, 012502 (2006).

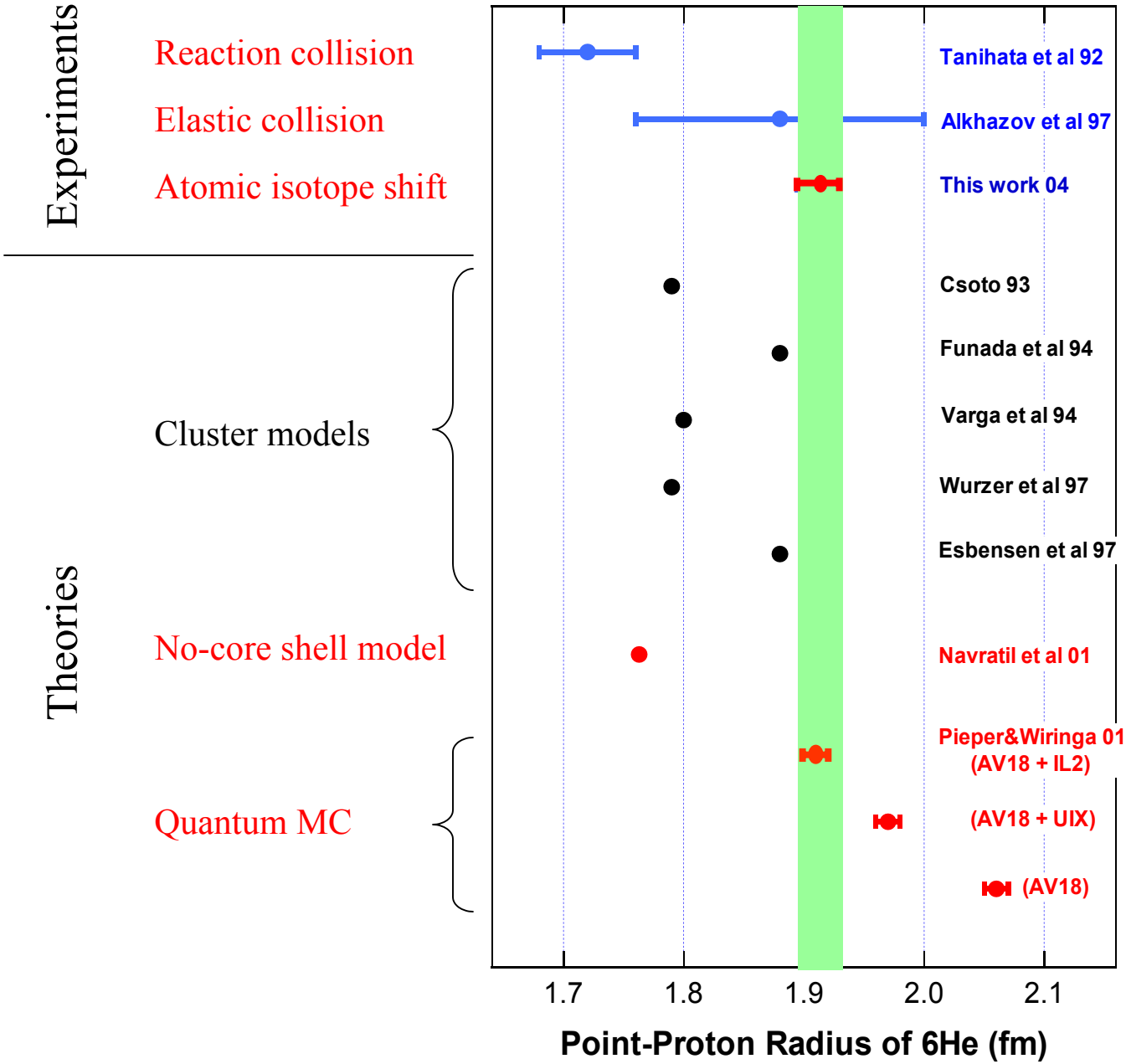
[g] D. Das and V. Natarajan, Phys. Rev. A **75**, 052508 (2007).

Contributions to the $^{9}Be^{+}$–$^{11}Be^{+}$ isotope shifts for the $1s^2 2p\,^2\mathrm{P}_J$–$1s^2 2s\,^2\mathrm{S}$ transitions. Units are MHz.

Contribution	$2\,^2\mathrm{P}_{1/2}$–$2\,^2\mathrm{S}$	$2\,^2\mathrm{P}_{3/2}$–$2\,^2\mathrm{S}$
	Theory	
μ/M	31 568.486(8)(56)[a]	31 568.486(8)(56)[a]
$(\mu/M)^2$	0.764(1)	0.764(1)
$\alpha^2\,\mu/M$	–10.041(2)	–6.165(1)
$\alpha^3\,\mu/M$, anom. magnetic	–0.002	0.001
$\alpha^3\,\mu/M$, one-electron	0.773(7)	0.773(7)
$\alpha^3\,\mu/M$, two-electron	0.030(5)	0.030(5)
r_{rms}^2	1.147±2.3	1.147±2.3
Total	31 561.154(57)	31 565.033(57)

The SIS is 3.879 MHz.

A Proving Ground for Nuclear Structure Theories



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Conclusions

- Sufficiently accurate theory is in place to measure nuclear radii from high precision spectroscopy on two- and three-electron atoms.
- New QED theory is now available for for the spin-independent terms of order α^4 Ryd. These can be tested at present levels of experimental accuracy.
- A new measurement of the fine structure constant can be obtained from helium fine structure, but a substantial discrepancy between theory and experiment remains for the $J = 1 \longrightarrow 2$ interval.

Main Theme:

- Obtain essentially exact solutions up to order α^3 Ry for the entire singly excited spectrum of helium and lithium – new results for Be^+.

What's New?

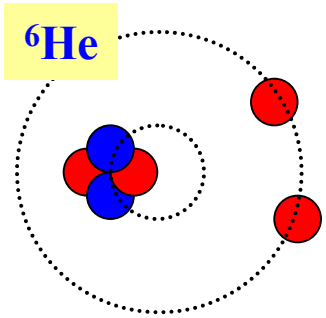
1. Essentially exact solutions to the quantum mechanical three- and four-body problems.
2. Recent advances in calculating QED corrections – especially the Bethe logarithm.
3. Single atom spectroscopy.

March 2008.

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

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D. Shiner et al., Phys. Rev. Lett. **74**, 3553 (1995).

Proposed experiment: lithium "halo" isotopes

Summary of the nuclear spin (S), lifetime ($T_{1/2}$), atomic mass (M_A), magnetic dipole and electric quadrupole nuclear moments (μ_I and Q), hyperfine structure splitting (HFS, in the $2S$ state), rms mass radius $R^{(m)}_{\rm rms}$, and charge radius $R^{(e)}_{\rm rms}$ for the isotopes of lithium.

Quantity	^{7}Li	^{8}Li	^{9}Li	^{11}Li
S	3/2	2	3/2	3/2
$T_{1/2}$ (ms)	∞	838(6)	178.3(4)	8.59(14)
M_A (u)	7.016 0040(5)	8.022 4867(5)	9.026 7891(21)	11.043 796(29)
μ_I (nm)	3.256 4268(17)	1.653 560(18)	3.439 1(6)	3.667 8(25)
Q (mbarn)	–40.0(3)	31.1(5)	–27.4(1.0)	–31.2(4.5)
HFS (MHz)	803.504 0866(10)	382.543(7)	856(16)	920(39)
$R^{(m)}_{\rm rms}$ (fm)	2.35(3)	2.38(2)	2.32(2)	3.10(17)
$R^{(e)}_{\rm rms}$ (fm)	2.39(3)	2.25(1)[a]	2.17(1)[a]	?

[a]Quantum Monte Carlo calculation by Steven C. Pieper and Robert B. Wiringa, ANL.

Experiment: Use two-photon spectroscopy to measure the isotope shift in the 2S – 3S transition for ^{11}Li to an accuracy of $\pm$200 kHz. Compare with high precision theory to determine the nuclear charge radius to an accuracy of $\pm$0.03 fm.

Comparison Result for Li^+

From the isotope shift in the $1s2s\ ^3S_1 - 1s2p\ ^3P_J$ transitions of Li^+,

$$R_{\rm rms}(^6{\rm Li}) - R_{\rm rms}(^7{\rm Li}) = 0.15 \pm 0.01\ {\rm fm}$$

From nuclear scattering data

$$\begin{aligned} R_{\rm rms}(^6{\rm Li}) &= 2.55 \pm 0.04\ {\rm fm} \\ R_{\rm rms}(^7{\rm Li}) &= 2.39 \pm 0.03\ {\rm fm} \\ {\rm difference} &= 0.16 \pm 0.05\ {\rm fm} \end{aligned}$$

E. Riis, A. G. Sinclair, O. Poulsen, G. W. F. Drake, W. R. C. Rowley and A. P. Levick, Phys. Rev. A **49**, 207 (1994).

Comparison between theory and experiment for the ^{7}Li transition frequencies and ionization potential. Units are cm^{-1}.

Transition	Theory	Experiment	Difference
$2\,^2\mathrm{P}_{1/2} - 2\,^2\mathrm{S}_{1/2}$	14 903.6541(10)	14 903.648130(14)[a]	–0.0060(10) *
$2\,^2\mathrm{P}_{3/2} - 2\,^2\mathrm{S}_{1/2}$	14 903.9893(10)	14 903.983648(14)[a]	–0.0057(10) *
$3\,^2\mathrm{S}_{1/2} - 2\,^2\mathrm{S}_{1/2}$	27 206.0926(9)	27 206.0952(10)[b]	–0.0025(25)
		27 206.09420(10)[c]	–0.0016(9)
		27 206.09412(13)[d]	–0.0015(9)
$2\,^2\mathrm{S}_{1/2}$ I.P.	43 487.1583(6)	43 487.150(5)[e]	0.0083(50)
		43 487.159 34(17)[f]	–0.0010(6)

[a] C. J. Sansonetti, B. Richou, R. Engleman, Jr., and L. J. Radziemski, Phys. Rev. A **52**, 2682 (1995).

[b] L. J. Radziemski, R. Engleman, Jr., and J. W. Brault, Phys. Rev. A **52**, 4462 (1995).

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

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[e] C. E. Moore, NSRDS-NBS Vol. 14 (U.S. Department of Commerce, Washington, DC, 1970)

[f] B.A. Bushaw, preliminary value

* no Bethe log calculation for $2\,^2\mathrm{P}$ states.

Partial contributions to the Bethe log for the $1s5g\ ^1\mathrm{G}$ state of He.

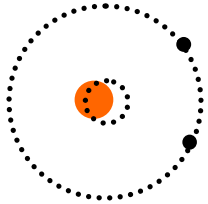
Ω	N	Partial Bethe log	Difference	Ratio
		$5\ ^1\mathrm{G} - n\ ^1\mathrm{F}$ (25.9%)		
4	222	4.369 008 3539		
5	353	4.370 451 7910	0.001 443 4372	
6	522	4.370 605 2673	0.000 153 4763	9.405
7	688	4.370 622 6186	0.000 017 3513	8.845
8	878	4.370 624 3521	0.000 001 7335	10.009
9	1105	4.370 624 5545	0.000 000 2023	8.568
10	1399	4.370 624 5749	0.000 000 0204	9.916
11	1716	4.370 624 5772	0.000 000 0023	8.836
Extrap.		4.370 624 5775	0.000 000 0003	
		$5\ ^1\mathrm{G} - n\ ^1\mathrm{G^o}$ (33.3%)		
4	169	4.370 262 9044		
5	265	4.370 397 1135	0.000 134 2091	
6	385	4.370 411 1743	0.000 014 0608	9.545
7	530	4.370 412 7458	0.000 001 5715	8.947
8	699	4.370 412 9039	0.000 000 1582	9.935
9	894	4.370 412 9227	0.000 000 0187	8.443
10	1126	4.370 412 9247	0.000 000 0020	9.353
12	1384	4.370 412 9249	0.000 000 0003	7.664
Extrap.		4.370 412 9250	0.000 000 0001	
		$5\ ^1\mathrm{G} - n\ ^1\mathrm{H}$ (40.7%)		
4	260	4.370 124 5941		
5	403	4.370 283 7562	0.000 159 1621	
6	585	4.370 299 9202	0.000 016 1640	9.847
7	806	4.370 301 7021	0.000 001 7818	9.071
8	1066	4.370 301 8745	0.000 000 1725	10.332
9	1372	4.370 301 8944	0.000 000 0199	8.669
10	1742	4.370 301 8965	0.000 000 0020	9.705
Extrap.		4.370 301 8967	0.000 000 0002	

Atomic Isotope Shift

Isotope Shift $\delta\nu = \delta\nu_{MS} + \delta\nu_{FS}$

Mass shift:

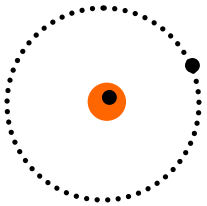
due to nucleus recoil



$$\delta\nu_{MS} \propto \frac{A - A'}{AA'}$$

Field shift:

due to nucleus size



$$\delta\nu_{FS} \propto Z \times \Delta[\Psi(0)]^2 \times \delta\langle r^2\rangle$$

$$IS(2^3S_1 - 2^3P_2) = 34473.625(20) + 1.210(\langle r^2\rangle_{He4} - \langle r^2\rangle_{He6})\ MHz$$

$$IS(2^3S_1 - 3^3P_2) = 43196.202(20) + 1.008(\langle r^2\rangle_{He4} - \langle r^2\rangle_{He6})\ MHz$$

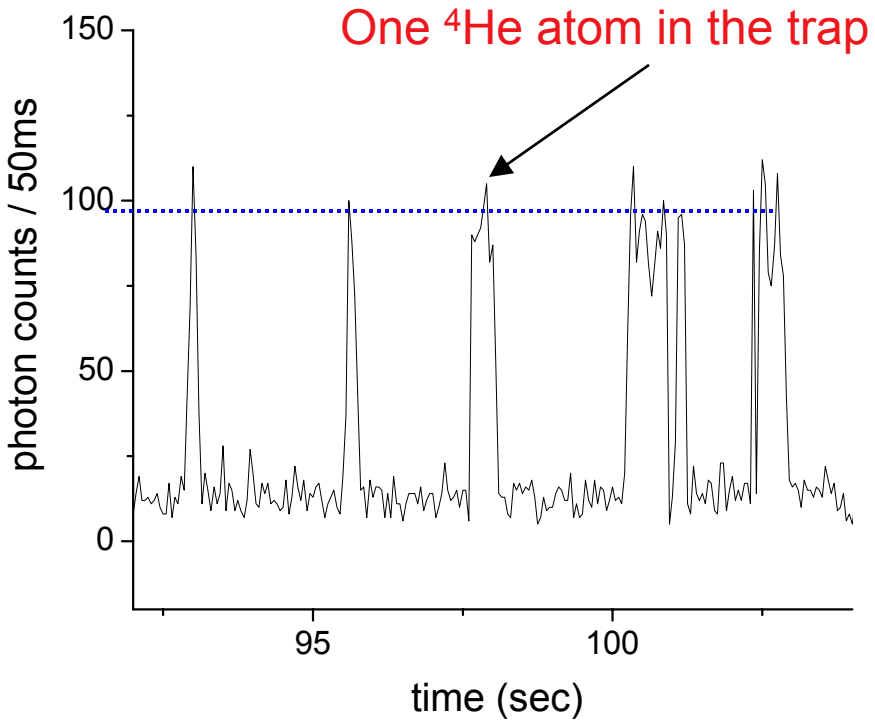
*G. Drake, Univ. of Windsor, private communication

100 kHz error in frequency ←→ 1% error in radius

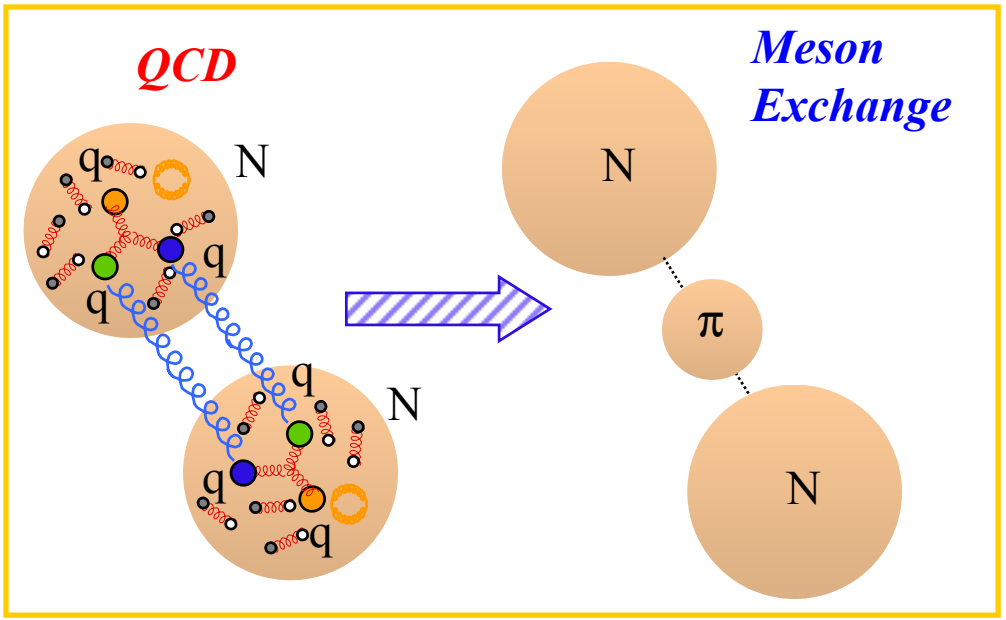
Single Atom Detection

- Capture efficiency ~ 10^{-8}

  Single atom detection necessary!
- Single-atom signal ~ 1.5 kHz
- Single-atom S/N ~ 10 in 100 ms
- ^{6}He capture rate ~ 100 per hour



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

Isotope Shifts and Charge Radius of Halo Nuclei

Gordon W.F. Drake

University of Windsor and GSI

Collaborators

Zong-Chao Yan (UNB)
Mark Cassar (PDF)
Zheng Zhong (Ph.D. student)
Qixue Wu (Ph.D. student)
Atef Titi (Ph.D. student)
Razvan Nistor (M.Sc. completed)
Levent Inci (M.Sc. completed)

Financial Support: NSERC and SHARCnet

Imperial College, February 27, 2006.

semin00.tex

Main Theme:

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

What's New?

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

Helium: Slaying the Dragon of Atomic Physics

Variational energies for the $n = 10$ singlet and triplet states of helium.

State	Singlet	Triplet
10 S	–2.005 142 991 747 919(79)	–2.005 310 794 915 611 3(11)
10 P	–2.004 987 983 802 217 9(26)	–2.005 068 805 497 706 7(30)
10 D	–2.005 002 071 654 256 81(75)	–2.005 002 818 080 228 84(53)
10 F	–2.005 000 417 564 668 80(11)	–2.005 000 421 686 604 88(26)
10 G	–2.005 000 112 764 318 746(22)	–2.005 000 112 777 003 317(21)
10 H	–2.005 000 039 214 394 532(17)	–2.005 000 039 214 417 416(17)
10 I	–2.005 000 016 086 516 1947(3)	–2.005 000 016 086 516 2194(3)
10 K	–2.005 000 007 388 375 8769(0)	–2.005 000 007 388 375 8769(0)

$$\begin{aligned} E &= -2 - \frac{1}{2n^2} + \cdots \\ &= -2.005 \cdots \end{aligned}$$

Effective Model & Quantum Monte Carlo Calculation

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

Two-body potential

Argonne V18

$$H = \sum_i K_i + \sum_{i<j} v_{ij}^{\gamma} + v_{ij}^{\pi} + v_{ij}^{R}$$

EM 1-π short-range

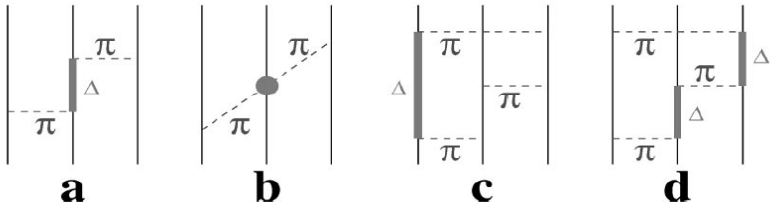
Coupling parameters fit to NN scattering data

Problem: binding energy of most light nuclei too small

Three-body potential

Illinois-2

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



Coupling parameters fit to energy levels of light nuclei

High precision measurements for lithium.

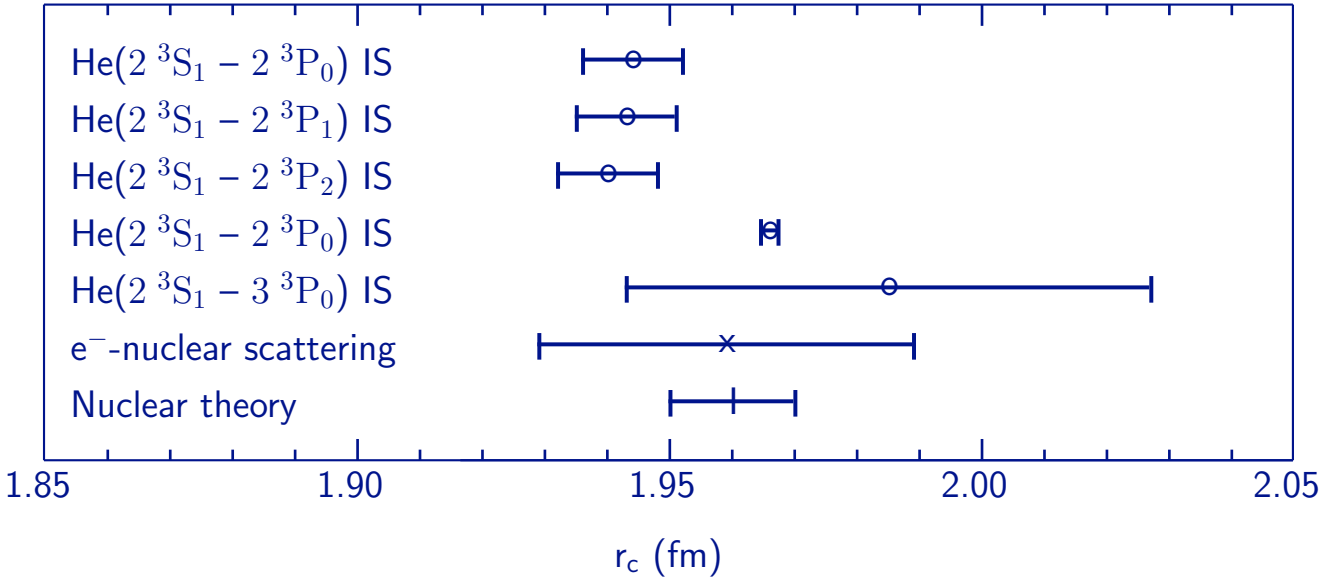
Group	Measurements
NIST (Radziemski et al. [1])	many transitions
York (Van Wijngaarden et al. [2])	2 ^{2}S – 2 ^{2}P I.S.
GSI (Bushaw et al. [3])	2 ^{2}S – 3 ^{2}S I.S.
GSI (Ewald et al. [4])	^{8}Li, ^{9}Li I.S.
TRIUMF/GSI (Sánchez et al. [5])	^{11}Li I.S.
Windsor/UNB (Yan, Drake [6])	theory

[1] L. J. Radziemski, R. Engleman, Jr., and J. W. Brault, Phys. Rev. A **52**, 4462 (1995).
[2] 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. Sánchez, A. Wojtaszek, B.A. Bushaw, G.W.F. Drake, Z.-C. Yan, and C. Zimmermann, Phys. Rev. Lett. **93**, 113002 (2004) (2004).
[5] R. Sánchez et al. Phys. Rev. Lett. **96**, 033022 (2006).
[6] Z.-C. Yan and G.W.F. Drake, Phys. Rev. Lett. **91**, 113004 (2003).

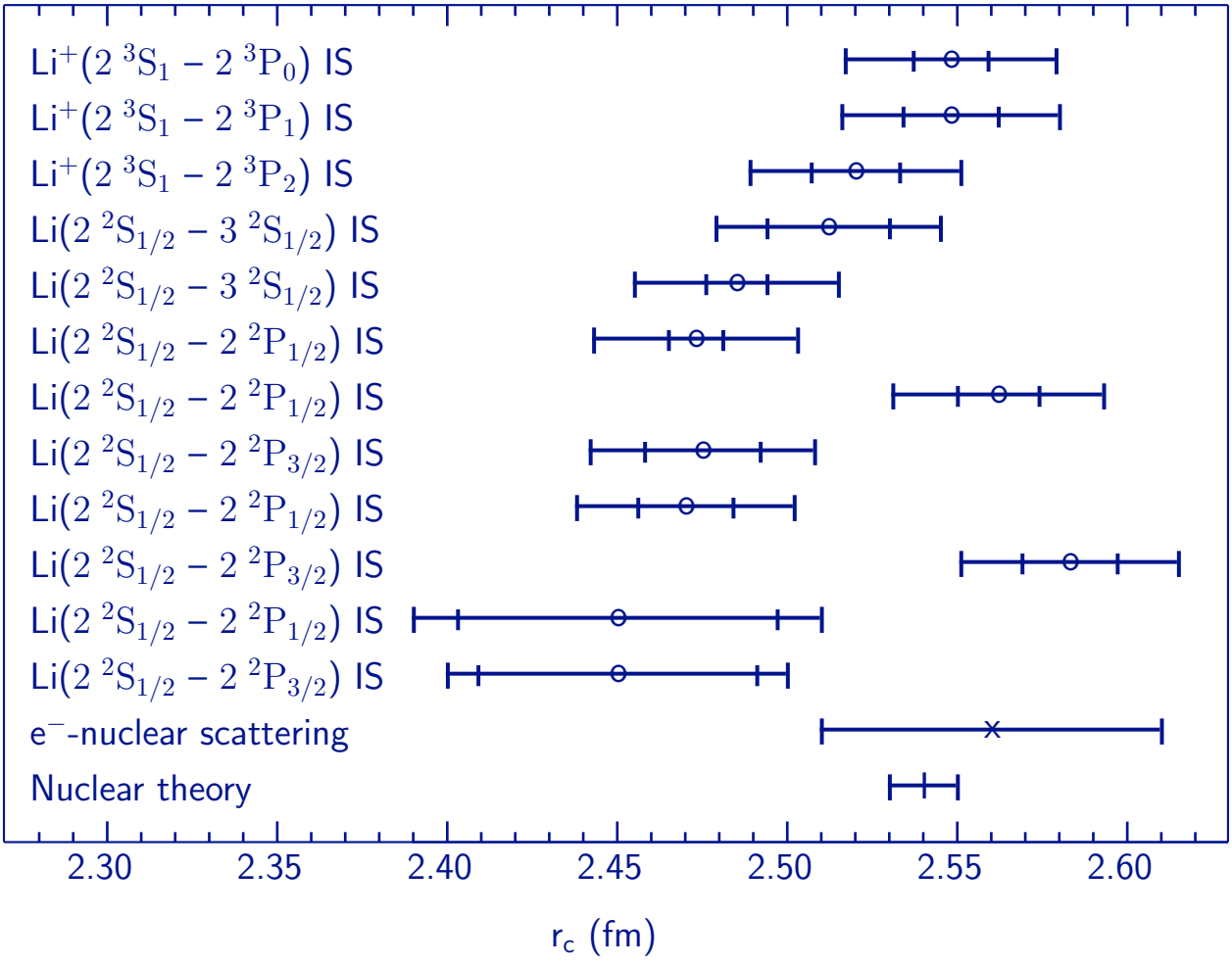
Comparison of values for the rms nuclear charge radius R of ^{3}He obtained by various methods. (IS: isotope shift)

Method	R (fm)	Year	Author
e^- scattering	1.87(5)	1965	Collard *et al.*
e^- scattering	1.88(5)	1970	McCarthy *et al.*
e^- scattering	1.844(45)	1977	McCarthy *et al.*
e^- scattering	1.89(5)	1977	Szalata *et al.*
e^- scattering	1.935(30)	1983	Dunn *et al.*
e^- scattering	1.877(30)	1984	Retzlaff *et al.*
e^- scattering	1.976(15)	1985	Ottermann *et al.*
e^- scattering	1.959(30)[a]	1994	Amroun *et al.*
Theory	1.92	1983	Hadjimichael *et al.*
Theory	1.92	1986	Schiavilla *et al.*
Theory	1.93	1986	Chen *et al.*
Theory	1.95	1987	Strueve *et al.*
Theory	1.92	1988	Kim *et al.*
Theory	1.958(6)	1993	Wu *et al.*
Theory	1.954(7)	1993	Friar *et al.*
Theory	1.96(1)	2001	Piper and Wiringa
Atomic IS	1.951(10)[b]	1993	Drake
Atomic IS	1.9659(14)	1994	Shiner *et al.*
Atomic IS	1.985(42)	1994	Marin *et al.*

Comparison of nuclear charge radius determinations for ^{3}He.



Comparison of nuclear charge radius determinations for ^{6}Li.



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

Strategy

1. Calculate nonrelativistic eigenvalues for helium-like and lithium-like ions to spectroscopic accuracy.
2. Include finite nuclear mass (mass polarization) effects up to second order by perturbation theory.
3. Include relativistic and QED corrections by perturbation theory.
4. Compare the results for transition frequencies with high precision measurements.
5. Use the residual discrepancy between theory and experiment to measure the nuclear charge radius of exotic "halo" isotopes of lithium such as ^{11}Li.

Question: Why not use hydrogenic ions where the theory is much simpler?

Answer: Line widths are narrower in the corresponding helium-like or lithium-like ion by a factor of 100 or more, and these charge states are easier to produce.

Bethe logarithms for lithium

N	$\beta(2\ ^2\mathrm{S})$	Difference	Ratio
87	2.846 5271		
207	2.964 2629	0.117 7357	
459	2.978 9857	0.014 7228	8.00
937	2.980 7196	0.001 7339	8.49
1763	2.980 9043	0.000 1847	9.39
Extrp.	2.980 93(3)		
$Li^+(1s^2\ ^1\mathrm{S})$	2.982 624 555(4)		

N	$\beta(3\ ^2\mathrm{S})$	Difference	Ratio
87	2.746 4739		
207	2.939 4848	0.193 0108	
459	2.975 0774	0.035 5926	5.42
937	2.981 2660	0.006 1886	5.75
1763	2.982 2261	0.000 9601	6.45
Extrp.	2.982 4(2)		
$Li^+(1s^2\ ^1\mathrm{S})$	2.982 624 555(4)		

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	0.123 748		
207	0.119 291	0.004 457	
459	0.115 390	0.003 901	1.14
937	0.114 140	0.001 250	3.12
1763	0.113 845	0.000 295	4.24
Extrap	0.113 5(3)		
$\mathrm{Li}^+(1s^2\ ^1\mathrm{S})$	0.1096		

N	$\Delta\beta_M(3\ ^2\mathrm{S})$	Difference	Ratio
87	0.098298281		
207	0.104933801		
459	0.110410361		
937	0.112767733		
1763	0.110416727		
Extrap	0.112(1)		
$\mathrm{Li}^+(1s^2\ ^1\mathrm{S})$	0.1096		

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

Final Results for the ^{6}He 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

$$\nu(2\,^3\mathrm{S}_1 - 2\,^3\mathrm{P}_2) = 276\,766\,663.53(2) - 1.2104\bar{r}^2_{^6\mathrm{He}}\ \ \mathrm{MHz} \tag{9}$$

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

$$\delta\nu(2\,^3\mathrm{S}_1 - 2\,^3\mathrm{P}_2) = 34\,473.625(13) + 1.2104(\bar{r}^2_{^4\mathrm{He}} - \bar{r}^2_{^6\mathrm{He}})\ \ \mathrm{MHz}\,. \tag{10}$$

$$\delta\nu(2\,^3\mathrm{S}_1 - 3\,^3\mathrm{P}_2) = 43\,196.202(16) + 1.008(\bar{r}^2_{^4\mathrm{He}} - \bar{r}^2_{^6\mathrm{He}})\ \ \mathrm{MHz}\,. \tag{11}$$

The uncertainty of $\pm$16 kHz is due entirely to the uncertainty in the measured atomic mass of ^{6}He (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 ^{6}He (relative to ^{4}He) to an accuracy of 1%. The result provides a direct test of the theoretical value $\bar{r}_{^6\mathrm{He}} = 2.04$ 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).

Argonne Collaboration 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.

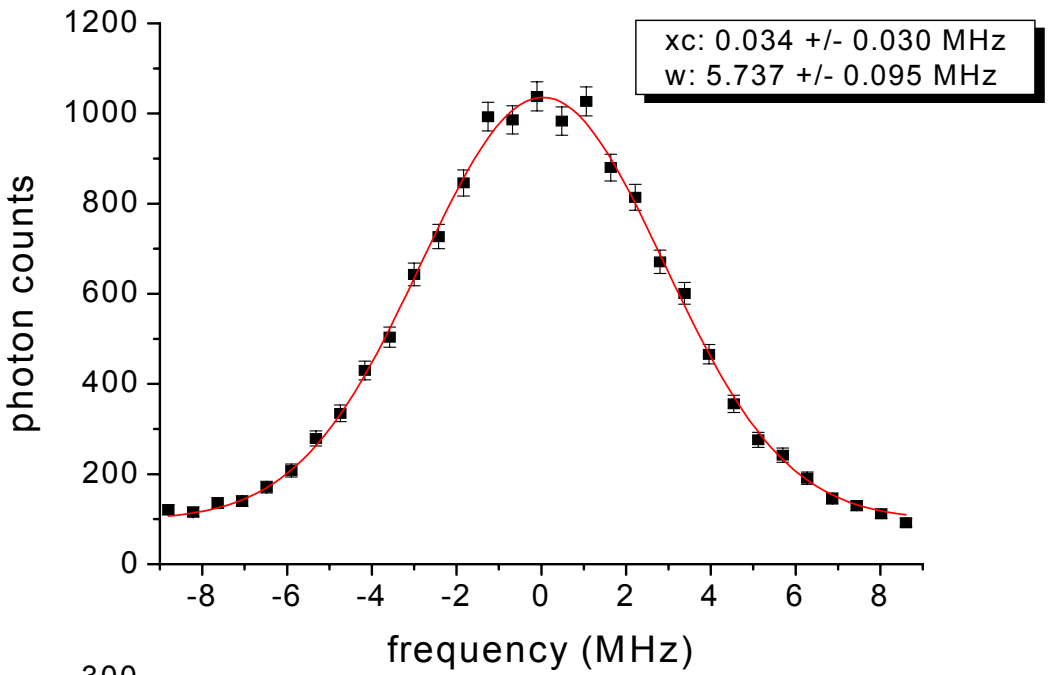
Single Atom Spectroscopy

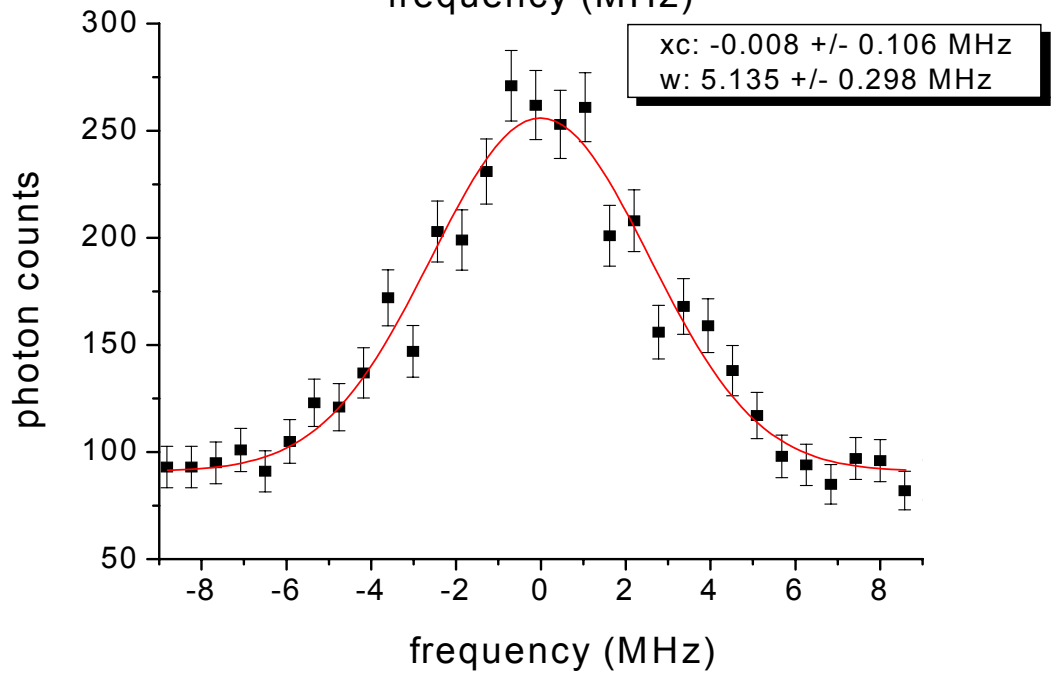
^{4}He

^{6}He

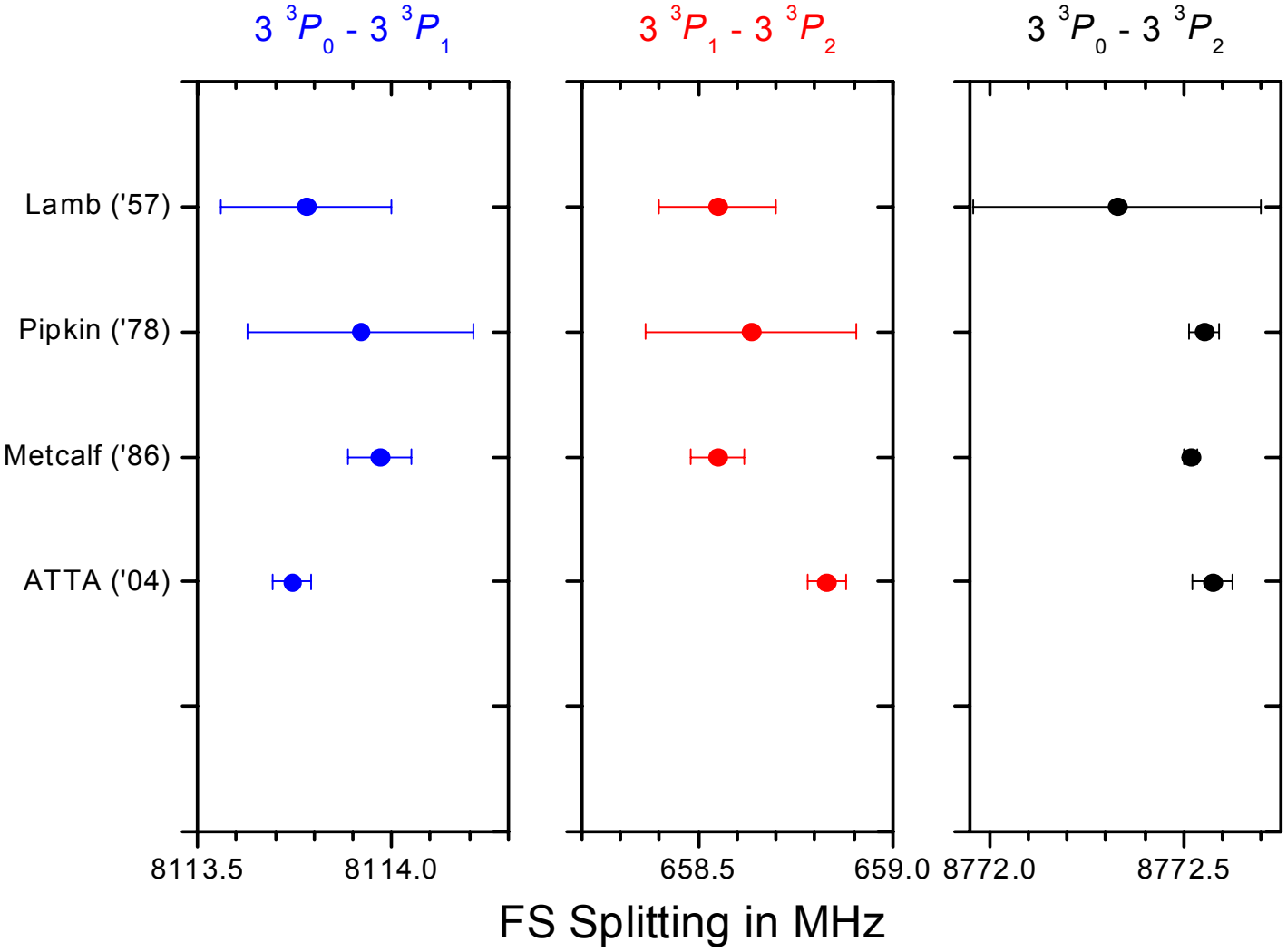
~ 150 ^{6}He atoms in one hour

April 6, 2004



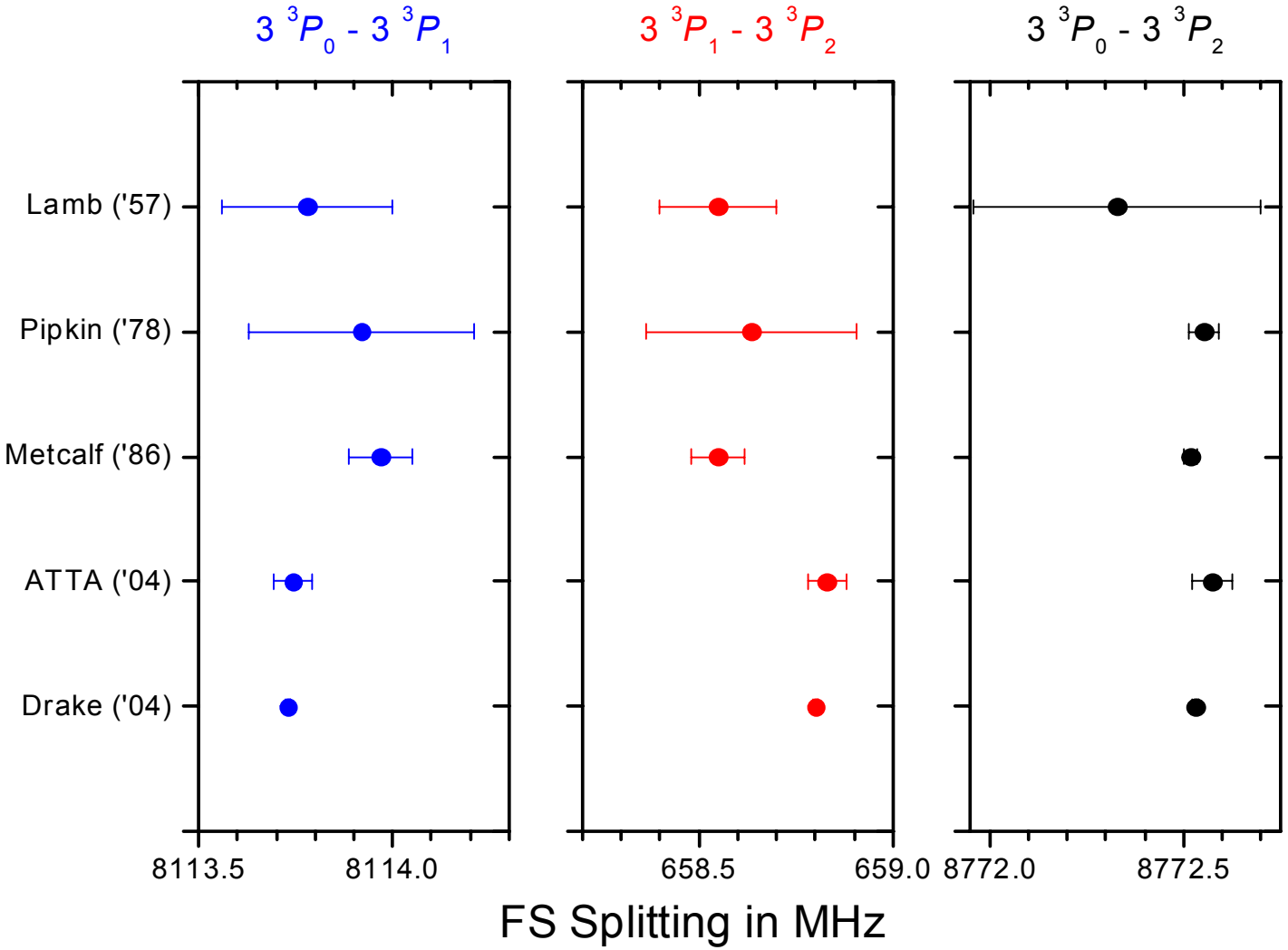


^{4}He Finestructure Splitting in 3p $^3P_{0,1,2}$



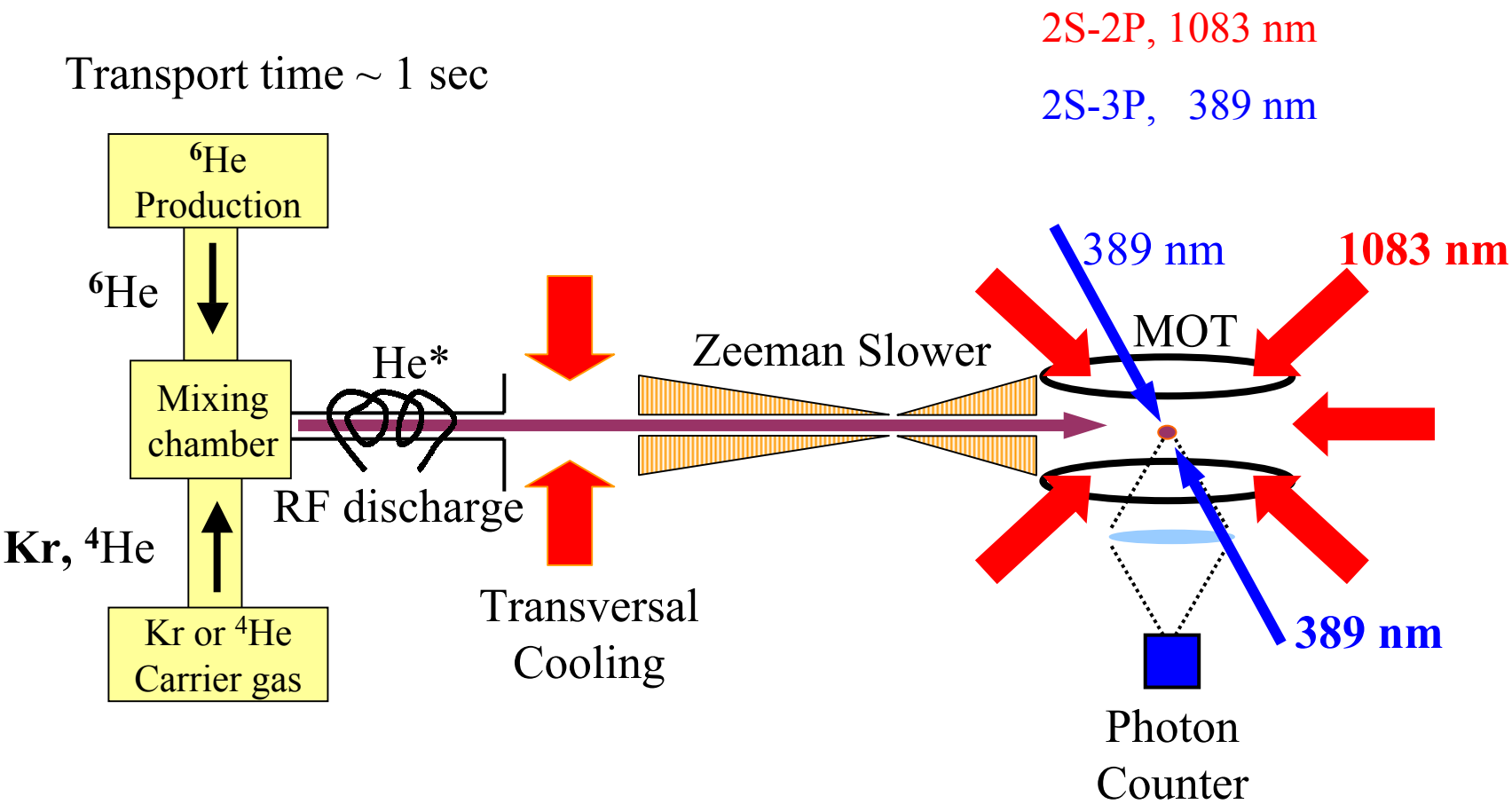
Lamb ('57): I. Wieder and W.E. Lamb, Jr., Phys. Rev. **107**, 125 (1957)
Pipkin ('78): P. Kramer and F. Pipkin, Phys. Rev. **A18**, 212 (1978)
Metcalf ('86): D.-H. Yang, P. McNicholl, and H. Metcalf, Phys. Rev. **A33**, 1725 (1986)
ATTA ('04): this work **Drake ('04): private ommuncation**

^{4}He Finestructure Splitting in 3p $^3P_{0,1,2}$

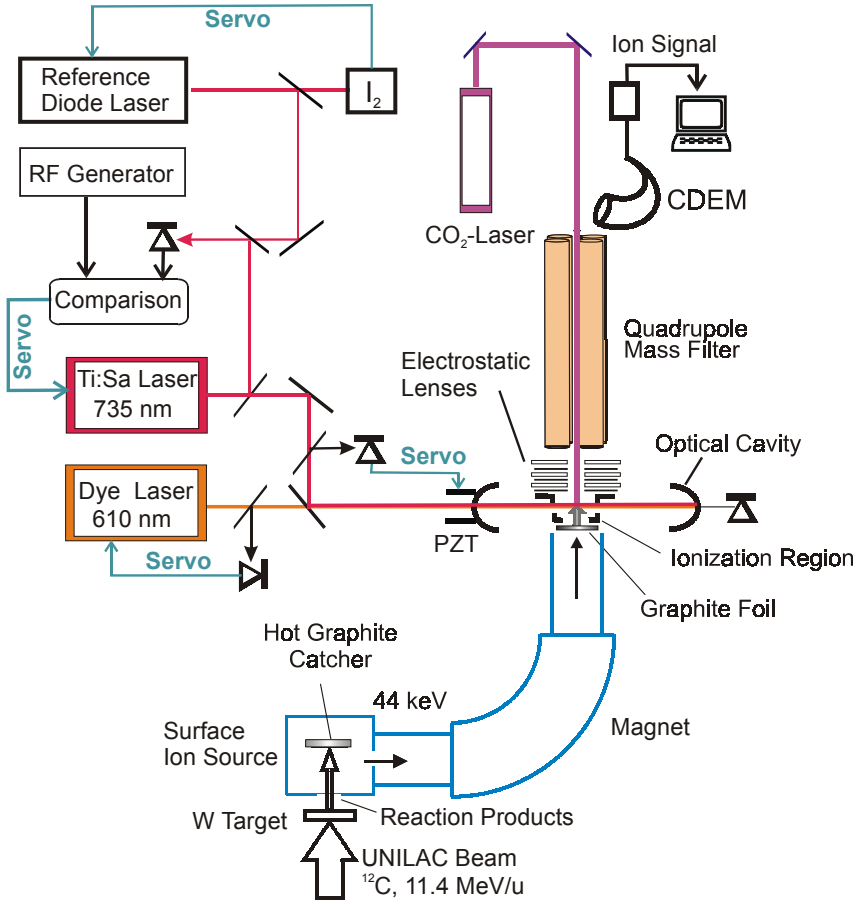


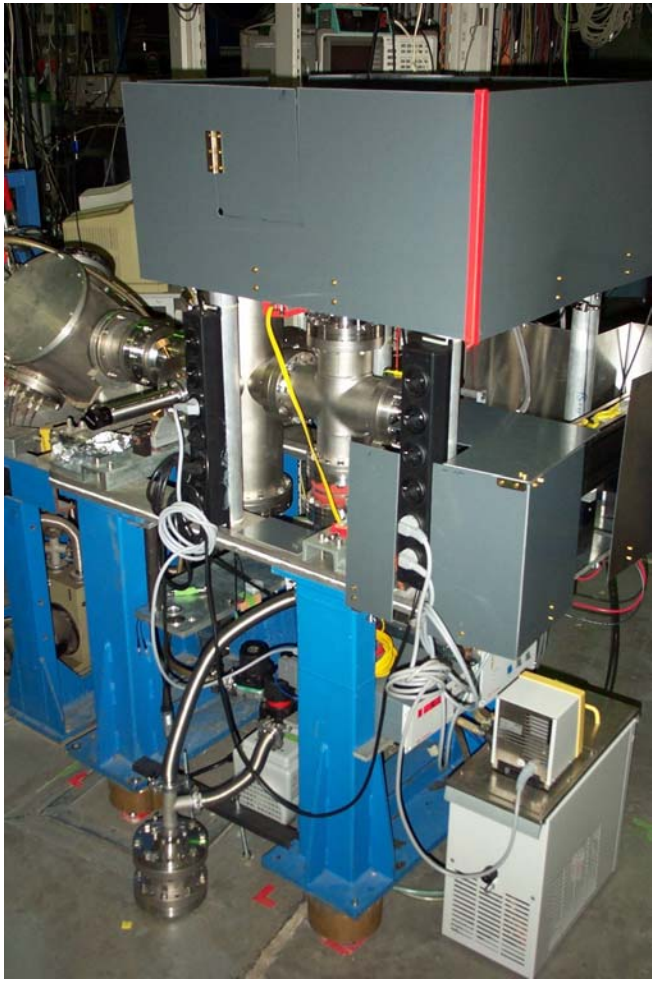
Lamb ('57): I. Wieder and W.E. Lamb, Jr., Phys. Rev. **107**, 125 (1957)
Pipkin ('78): P. Kramer and F. Pipkin, Phys. Rev. **A18**, 212 (1978)
Metcalf ('86): D.-H. Yang, P. McNicholl, and H. Metcalf, Phys. Rev. **A33**, 1725 (1986)
ATTA ('04): this work **Drake ('04): private ommuncation**

Experimental Setup - Schematic



Experimental Arrangement





^{6}He - Nuclear Charge Radius

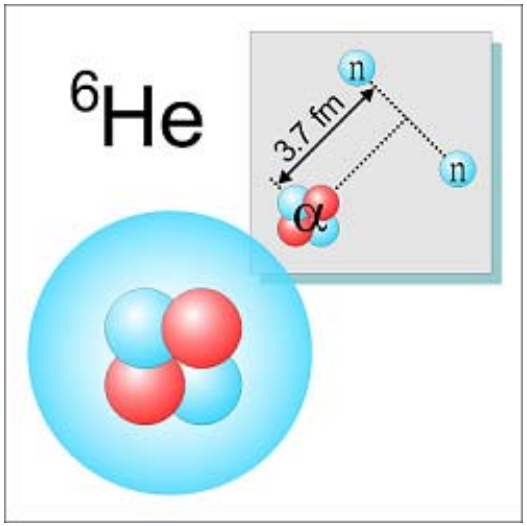
Courtesy of Peter Müller, Argonne Nat. Lab

Isotope shift
(2^3S_1 - 3^3P_2, ^{6}He – ^{4}He)

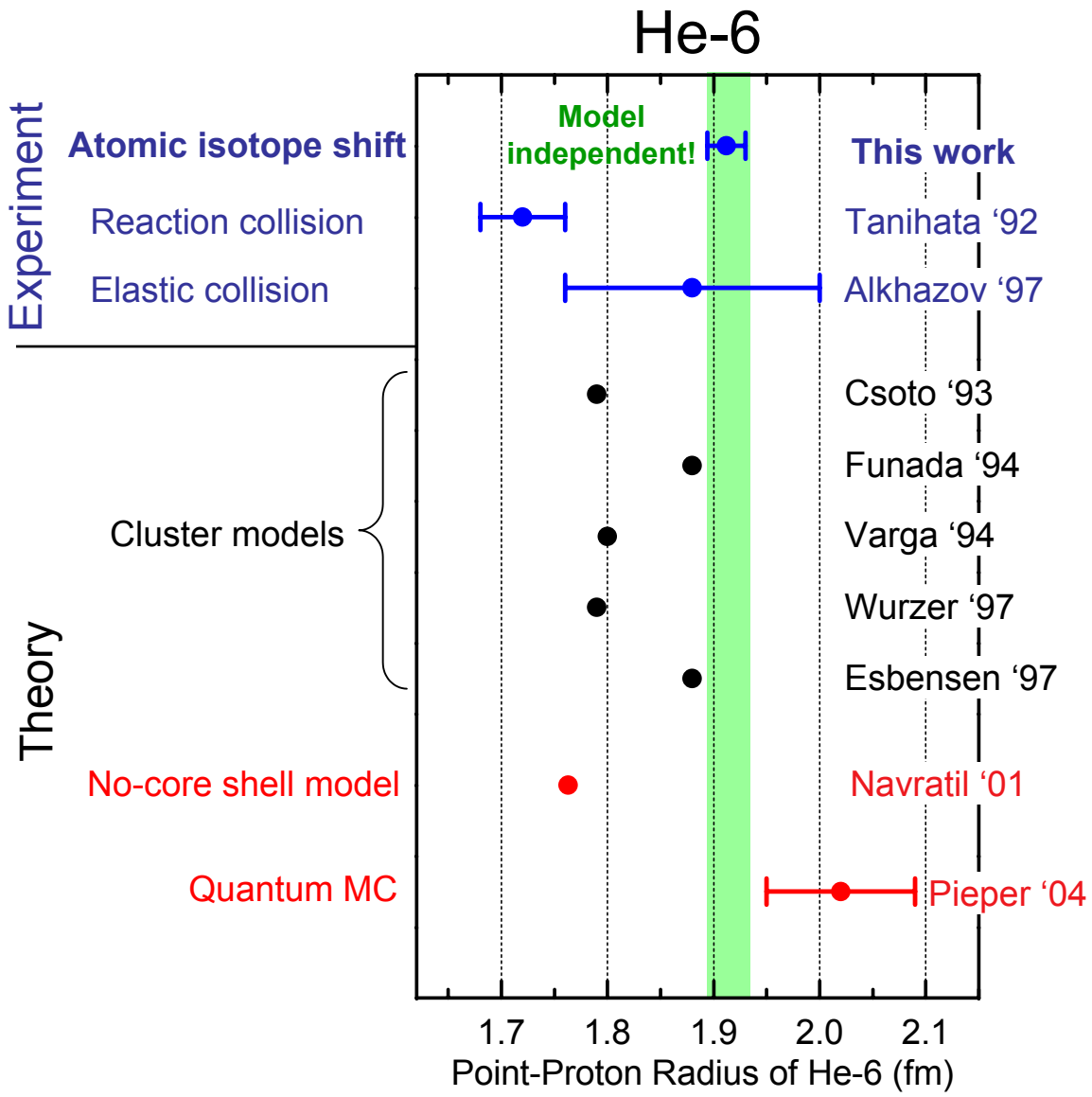
43 194.772(56) MHz

^{6}He rms charge radius

2.054(14) fm (0.7%)



L.-B. Wang *et al.*,
PRL **93**, 142501 (2004)



Determination of the Nuclear Radius for Isotopes of Lithium

$$R^2_{\rm rms}(\,^A{\rm Li}) = R^2_{\rm rms}(\,^6{\rm Li}) + \frac{E^A_{\rm meas} - E^A_0}{C} \qquad (12)$$

where $E^A_{\rm meas}$ is the measured isotope shift for ^{A}Li relative to ^{6}Li, and E^A_0 contains all the calculated contributions to the isotope shift with the exception of the shift due to finite nuclear size.

Values of E^A_0 to determine $R^2_{\rm rms}$ from the measured isotope shift in various transitions. Units are MHz.

Isotopes	$E^A_0(2\,^2P_{1/2} - 2\,^2S)$	$E^A_0(2\,^2P_{3/2} - 2\,^2S)$	$E^A_0(3\,^2S - 2\,^2S)$
^{7}Li–^{6}Li	10 532.19(7)	10 532.58(7)	11 453.00(6)
^{8}Li–^{6}Li	18 472.86(12)	18 473.55(12)	20 088.10(10)
^{9}Li–^{6}Li	24 631.11(16)	24 632.03(16)	26 785.01(13)
^{10}Li–^{6}Li	29 575.46(20)	29 576.56(20)	32 161.92(17)
^{11}Li–^{6}Li	33 615.19(24)	33 616.45(24)	36 555.11(21)

$C = -2.4565$ MHz/fm^2 for the $2\,^2{\rm P}_J - 2\,^2{\rm S}_{1/2}$ I.S.
$C = -1.5661$ MHz/fm^2 for $3\,^2{\rm S}_{1/2} - 2\,^2{\rm S}_{1/2}$ I.S.

Contributions to the ^{7}Li $1s^2 3s\ ^2\mathrm{S} - 1s^2 2s\ ^2\mathrm{S}$ transition energy and $1s^2 2s\ ^2\mathrm{S}$ ionization potential (I.P.), in units of cm^{-1}.

Term	$3\ ^2\mathrm{S}_{1/2} - 2\ ^2\mathrm{S}_{1/2}$	$2\ ^2\mathrm{S}_{1/2}$ I.P.
Nonrelativistic	27 206.492 856(4)	43 488.220 2449(16)
Nonrel., μ/M	–2.295 854 30(16)	–3.621 707 668(4)
Nonrel., $(\mu/M)^2$	0.000 165 962	0.000 315 803
Relativistic, α^2	2.089 0(4)	2.811 33(2)
Rel. recoil, $\alpha^2 \mu/M$	–0.000 04(1)	–0.000 011(9)
QED(e$^-$–nucl.), α^3	–0.198 6(3)	–0.258 32(3)
QED(e$^-$–e$^-$), α^3	0.010 747	0.013 884
QED higher order, $\alpha^4 \cdots$	–0.005 4(4)	–0.007 0(4)
Nuclear size, R^2	–0.000 298(8)	–0.000 389(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.	–0.001 6(9)	–0.001 0(5)

[a] L. J. Radziemski, R. Engleman, Jr., and J. W. Brault, Phys. Rev. A **52**, 4462 (1995).

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

[c] C. E. Moore, NSRDS-NBS Vol. 14 (U.S. Department of Commerce, Washington, DC, 1970.

[d] Bruce Bushaw, preliminary value.

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

Contribution	$2\,^2P_{1/2}$–$2\,^2S$	$2\,^2P_{3/2}$–$2\,^2S$
	Theory	
μ/M	10 533.501 92(60)[a]	10 533.501 92(60)[a]
$(\mu/M)^2$	0.057 3(20)	0.057 3(20)
$\alpha^2\,\mu/M$	–1.397(66)	–1.004(66)
$\alpha^3\,\mu/M$, anom. magnetic	–0.000 175 3(84)	0.000 087 5(84)
$\alpha^3\,\mu/M$, one-electron	0.0045(10)	0.0045(10)
$\alpha^3\,\mu/M$, two-electron	0.010 5(20)	0.010 5(20)
$r^2_{\rm rms}$	1.94(61)	1.94(61)
$r^2_{\rm rms}\,\mu/M$	–0.000 73(11)	–0.000 73(11)
Total	10 534.12(7)±0.61	10 534.51(7)±0.61
	Experiment	
Sansonetti *et al.*[b]	10 532.9(6)	10 533.3(5)
Windholz *et al.*[c]	10 534.3(3)	10 539.9(1.2)
Scherf *et al.*[d]	10 533.13(15)	10 534.93(15)
Walls *et al.*[e]	10 534.26(13)	

[a]The additional uncertainty from the atomic mass determinations is ±0.008 MHz.

[b]C. J. Sansonetti, B. Richou, R. Engleman, Jr., and L. J. Radziemski, Phys. Rev. A **52**, 2682 (1995).

[c]L. Windholz and C. Umfer, Z. Phys. D **29**, 121 (1994).

[d]W. Scherf, O. Khait, H. Jäger, and L. Windholz, Z. Phys. D **36**, 31, (1996).

[e]J. Walls, R. Ashby, J. J. Clarke, B. Lu, and W. A. van Wijngaarden, Eur. Phys. J **D 22** 159 (2003).

Rayleigh-Schrödinger Variational Principle

Diagonalize H in the

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

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.

Rescale distances and energies according to

$$\begin{aligned} \boldsymbol{\rho} &= \mathbf{r}/a_\mu \\ \mathcal{E} &= E/(e^2/a_\mu) \end{aligned}$$

where $a_\mu = \dfrac{\hbar^2}{\mu e^2}$ is the reduced mass Bohr radius,

and $\dfrac{e^2}{a_\mu} = 2R_\mu = 2\dfrac{\mu}{m}R_\infty = 2\left(1 - \dfrac{\mu}{M}\right)R_\infty.$

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

$$\left\{-\frac{1}{2}\nabla^2_{\rho_1} - \frac{1}{2}\nabla^2_{\rho_2} - \frac{\mu}{M}\nabla_{\rho_1}\cdot\nabla_{\rho_2} - \frac{Z}{\rho_1} - \frac{Z}{\rho_2} + \frac{1}{|\boldsymbol{\rho}_1 - \boldsymbol{\rho}_2|}\right\}\Psi = \mathcal{E}\Psi$$

Convergence of the nonrelativistic energies for the $1s^2 2s\,^2S$ and $1s^2 2p\,^2P$ states of lithium, in atomic units.

Ω	No. of terms	$E(\Omega)$	$E(\Omega) - E(\Omega-1)$	$R(\Omega)$[a]
		$1s^2 2s\,^2S$		
2	19	–7.477 555 720 321 8		
3	51	–7.477 995 835 140 8	–0.000 440 114 819 0	
4	121	–7.478 053 567 299 9	–0.000 057 732 159 1	7.623
5	257	–7.478 059 464 463 7	–0.000 005 897 163 8	9.790
6	503	–7.478 060 228 080 1	–0.000 000 763 616 4	7.723
7	919	–7.478 060 311 092 9	–0.000 000 083 012 9	9.199
8	1590	–7.478 060 321 724 7	–0.000 000 010 631 8	7.808
9	2626	–7.478 060 323 416 8	–0.000 000 001 692 1	6.283
10	3502	–7.478 060 323 618 9	–0.000 000 000 202 1	8.371
∞		–7.478 060 323 650 3(71)		
		$1s^2 2p\,^2P$		
2	20	–7.410 088 210 427		
3	56	–7.410 146 240 952	–0.000 058 030 525	
4	139	–7.410 155 057 909	–0.000 008 816 956	6.582
5	307	–7.410 156 274 821	–0.000 001 216 912	7.245
6	623	–7.410 156 490 483	–0.000 000 215 662	5.643
7	1175	–7.410 156 524 272	–0.000 000 033 789	6.383
8	1846	–7.410 156 530 070	–0.000 000 005 798	5.828
9	2882	–7.410 156 531 534	–0.000 000 001 464	3.960
10	3463	–7.410 156 531 721	–0.000 000 000 187	7.813
∞		–7.410 156 531 763(42)		

[a] $R(\Omega) = \dfrac{R(\Omega-1) - R(\Omega-2)}{R(\Omega) - R(\Omega-1)}$

The Recoil Term

The recoil term $a(n\,^2L)$ corresponds, in the hydrogenic case, to the term $\tilde{a}(nL)$ given by

$$\tilde{a}(nL) = -2\left(\ln\frac{2}{n} + \sum_{q=1}^{n} q^{-1} + 1 - \frac{1}{2n}\right)\delta_{L,0} + \frac{1-\delta_{L,0}}{L(L+1)(2L+1)}\,. \tag{4}$$

In the multi-electron case, it corresponds to the term

$$a(n\,^2L) = \frac{2Q_1}{\langle\delta(\mathbf{r}_i)\rangle^{(0)}} + 2\ln Z - 3\,. \tag{5}$$

where Q_1 is the matrix element

$$Q_1 = (1/4\pi)\lim_{\epsilon\to 0}\langle r_i^{-3}(\epsilon) + 4\pi(\gamma_{\rm eu} + \ln\epsilon)\delta(\mathbf{r}_i)\rangle\,,$$

$\gamma_{\rm eu}$ is Euler's constant, ϵ is the radius of a sphere about $r_i = 0$ excluded from the integration, and a summation over i from 1 to 3 is assumed for lithium.

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High precision variational calculations for H_2^+

Mark M Cassar and G W F Drake

University of Windsor, Windsor, ON N9B 3P4, Canada

E-mail: cassar1@uwindsor.ca

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Abstract

A double basis set in Hylleraas coordinates is used to obtain improved variational upper bounds for the nonrelativistic energy of the $1\,^1S$ ($v = 0, R = 0$), $2\,^1S$ ($v = 1, R = 0$) and $2\,^3P$ ($v = 0, R = 1$) states of H_2^+. This method shows a remarkable convergence rate for relatively compact basis set expansions. A comparison with the most recent work is made. The accuracy of the wavefunctions is tested using the electron–proton Kato cusp condition.

2. Calculations

After isolating the centre-of-mass motion, the Hamiltonian for H_2^+ may be written (in reduced mass atomic units) as

$$H = -\frac{1}{2}\nabla_{r_1}^2 - \frac{1}{2}\nabla_{r_2}^2 - \frac{\mu}{m_e}\nabla_{r_1}\cdot\nabla_{r_2} - \frac{1}{r_1} - \frac{1}{r_2} + \frac{1}{r_{12}}, \tag{3}$$

where μ is the reduced electron mass; the electron has been chosen to be at the origin of the coordinate system. The main task now is to solve the Schrödinger equation

$$H\Psi(\mathbf{r}_1, \mathbf{r}_2) = E\Psi(\mathbf{r}_1, \mathbf{r}_2), \tag{4}$$

for the stationary states of the Hamiltonian H.

For our modified double basis set, the trial function for S-states is given by

$$\Psi^S(\mathbf{r}_1, \mathbf{r}_2) = \sum_{p=1}^{2}\sum_{i,j=0}^{\Omega_1}\sum_{k=\Omega_{low}}^{\Omega_{high}} a_{ijk}^{(p)} r_1^i r_2^j r_{12}^k \exp(-\alpha^{(p)} r_1 - \beta^{(p)} r_2 - \gamma^{(p)} r_{12}) \pm (\text{exchange}), \tag{5}$$

where $\Omega_1 \geqslant i + j$, that is, Ω_1 is the maximum sum of powers of r_1 and r_2,

$$\Omega_{\text{low}} = \mathcal{M} - \Omega_1 + (i + j),$$
$$\Omega_{\text{high}} = \mathcal{M} + \Omega_1 - (i + j),$$

and the integer $\mathcal{M} > \Omega_1$ is an adjustable parameter; and for states with $L > 0$,

$$\Psi^{L>0}(\mathbf{r}_1, \mathbf{r}_2) = \sum_{\text{ang}} \Psi^{\text{S}}(\mathbf{r}_1, \mathbf{r}_2)\mathcal{Y}^{LM}_{l_1 l_2}(\hat{\mathbf{r}}_1, \hat{\mathbf{r}}_2), \tag{6}$$

where $\mathcal{Y}^{LM}_{l_1 l_2}(\hat{\mathbf{r}}_1, \hat{\mathbf{r}}_2)$ is a vector-coupled product of spherical harmonics [16] and $\sum_{\text{ang}}$ means that all distinct angular couplings are included according to the scheme in [17].

Normally, all distinct combinations of powers $\{i, j, k\}$ would be included in expansions (5) and (6); however, in order to avoid problems of near linear dependence for S-states, all terms with $i > j$ are omitted only in (5). In addition, we employed a form of truncation first introduced by Kono and Hattori [18] in which terms with $i+j+|\mathcal{M}-k|-|l_1-l_2|+|j-i| > \Omega_1$ are avoided.

Table 1. Convergence study for the ground state of H_2^+. Ω ($=\mathcal{M}+\Omega_1$) is the highest power of r_{12} and N is the total number of terms in the basis set. Atomic units are used.

Ω	N	$E(\Omega)$	Ratio[a]
42	33	−0.597 138 979 257 696 807 296 095	
43	57	−0.597 139 061 191 160 229 487 982	
44	90	−0.597 139 062 954 250 154 856 869	46.47
45	134	−0.597 139 063 120 531 138 258 260	10.60
46	190	−0.597 139 063 123 316 985 447 178	59.69
47	260	−0.597 139 063 123 402 568 522 508	32.55
48	345	−0.597 139 063 123 404 987 310 249	35.38
49	447	−0.597 139 063 123 405 072 038 078	28.55
50	567	−0.597 139 063 123 405 074 674 920	32.13
51	707	−0.597 139 063 123 405 074 825 966	17.46
52	868	−0.597 139 063 123 405 074 834 205	18.33
53	1052	−0.597 139 063 123 405 074 834 331	65.43
Extrapolation		−0.597 139 063 123 405 074 834 338(3)	19.80
[b]	2200	−0.597 139 063 123 405 0740	
[c]		−0.597 139 063 123 405 076(2)	
[d]	3500	−0.597 139 063 123 405 074 83	
[e]	1330	−0.597 139 063 123 405 0741	
[f]		−0.597 139 063 123 405 074 5(4)	

[a] Ratio is the ratio of successive differences $[E(\Omega-1)-E(\Omega-2)]/[E(\Omega)-E(\Omega-1)]$.
[b] Korobov variational bound [10].
[c] Korobov extrapolation [10].
[d] Bailey and Frolov variational bound [9].
[e] Yan *et al* variational bound [11].
[f] Yan *et al* extrapolation [11].

Table 3. Convergence study for the 2^1S state of H_2^+. Ω $(=\mathcal{M}+\Omega_1)$ is the highest power of r_{12} and N is the total number of terms in the basis set. Atomic units are used.

Ω	N	$E(\Omega)$	Ratio[a]
39	20	−0.587 151 043 016 274 880 167	
40	40	−0.587 155 435 230 538 473 190	
41	70	−0.587 155 671 003 177 129 307	18.63
42	112	−0.587 155 678 540 275 385 079	31.28
43	168	−0.587 155 679 208 721 236 702	11.28
44	240	−0.587 155 679 212 575 658 166	173.42
45	330	−0.587 155 679 212 741 279 834	23.27
46	440	−0.587 155 679 212 746 648 696	30.85
47	572	−0.587 155 679 212 746 807 755	33.75
48	728	−0.587 155 679 212 746 811 406	43.56
49	910	−0.587 155 679 212 746 812 118	5.13
50	1015	−0.587 155 679 212 746 812 191	9.65
51	1240	−0.587 155 679 212 746 812 205	5.57
52	1496	−0.587 155 679 212 746 812 211	2.03
Extrapolation		−0.587 155 679 212 746 812 212(2)	6.18
[b]		−0.587 155 679 212(1)	
[c]		−0.587 155 679 2127	
[d]		−0.587 155 679 213 6(5)	

[a] Ratio is the ratio of successive differences $[E(\Omega-1)-E(\Omega-2)]/[E(\Omega)-E(\Omega-1)]$.
[b] Hilico *et al* [15].
[c] Moss variational bound [26].
[d] Taylor *et al* [27].

Table 4. Convergence study for the 2^3P state of H_2^+. Ω ($=\mathcal{M}+\Omega_1$) is the highest power of r_{12} and N is the total number of terms in the basis set. Atomic units are used.

Ω	N	$E(\Omega)$	Ratio[a]
40	39	−0.596 872 821 718 250 761 31	
41	82	−0.596 873 728 191 903 938 74	
42	149	−0.596 873 738 113 177 432 23	91.37
43	244	−0.596 873 738 822 338 108 35	13.99
44	373	−0.596 873 738 832 029 635 19	73.17
45	540	−0.596 873 738 832 750 200 25	13.45
46	751	−0.596 873 738 832 762 355 10	59.28
47	1010	−0.596 873 738 832 764 668 79	5.25
48	1323	−0.596 873 738 832 764 729 56	38.07
49	1694	−0.596 873 738 832 764 734 80	11.60
Extrapolation		−0.596 873 738 832 764 734 96(5)	32.92
[b]		−0.596 873 738 832 8(5)	
[c]		−0.596 873 738 832 8	
[d]		−0.596 873 738 832 764 733(1)	

[a] Ratio is the ratio of successive differences $[E(\Omega-1)-E(\Omega-2)]/[E(\Omega)-E(\Omega-1)]$.
[b] Taylor *et al* [27].
[c] Moss variational bound [26].
[d] Yan *et al* extrapolation [11].

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

Contribution	$2\,^2P_{1/2}$–$2\,^2S$	$2\,^2P_{3/2}$–$2\,^2S$
	Theory	
μ/M	10 533.501 92(60)[a]	10 533.501 92(60)[a]
$(\mu/M)^2$	0.057 3(20)	0.057 3(20)
$\alpha^2\,\mu/M$	–1.397(66)	–1.004(66)
$\alpha^3\,\mu/M$, anom. magnetic	–0.000 175 3(84)	0.000 087 5(84)
$\alpha^3\,\mu/M$, one-electron	0.0045(10)	0.0045(10)
$\alpha^3\,\mu/M$, two-electron	0.010 5(20)	0.010 5(20)
$r^2_{\rm rms}$	1.94(61)	1.94(61)
$r^2_{\rm rms}\,\mu/M$	–0.000 73(11)	–0.000 73(11)
Total	10 534.12(7)±0.61	10 534.51(7)±0.61
	Experiment	
Sansonetti *et al.*[b]	10 532.9(6)	10 533.3(5)
Windholz *et al.*[c]	10 534.3(3)	10 539.9(1.2)
Scherf *et al.*[d]	10 533.13(15)	10 534.93(15)
Walls *et al.*[e]	10 534.26(13)	
Noble *et al.*[f]	10 534.039(70)	

[a] The additional uncertainty from the atomic mass determinations is ±0.008 MHz.

[b] C. J. Sansonetti, B. Richou, R. Engleman, Jr., and L. J. Radziemski, Phys. Rev. A **52**, 2682 (1995).

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[e] J. Walls, R. Ashby, J. J. Clarke, B. Lu, and W. A. van Wijngaarden, Eur. Phys. J. **D 22** 159 (2003).

[f] G.A. Noble, B.E. Schultz, H. Ming, W.A. van Wijngaarden, Phys. Rev. A submitted.

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	Theory	
μ/M	10 533.501 92(60)[a]	10 533.501 92(60)[a]
$(\mu/M)^2$	0.057 3(20)	0.057 3(20)
$\alpha^2\,\mu/M$	–1.397(66)	–1.004(66)
$\alpha^3\,\mu/M$, anom. magnetic	–0.000 175 3(84)	0.000 087 5(84)
$\alpha^3\,\mu/M$, one-electron	0.0045(10)	0.0045(10)
$\alpha^3\,\mu/M$, two-electron	0.010 5(20)	0.010 5(20)
$r^2_{\rm rms}$	1.94(61)	1.94(61)
$r^2_{\rm rms}\,\mu/M$	–0.000 73(11)	–0.000 73(11)
Total	10 534.12(7)±0.61	10 534.51(7)±0.61
	Experiment	
Sansonetti *et al.*[b]	10 532.9(6)	10 533.3(5)
Windholz *et al.*[c]	10 534.3(3)	10 539.9(1.2)
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Walls *et al.*[e]	10 534.26(13)	
Noble *et al.*[f]	10 534.039(70)	

[a]The additional uncertainty from the atomic mass determinations is ±0.008 MHz.

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[f]G.A. Noble, B.E. Schultz, H. Ming, W.A. van Wijngaarden, Phys. Rev. A submitted.

Comparison between theory and experiment for the fine structure splittings and ^{7}Li–^{6}Li splitting isotope shift (SIS). Units are MHz.

Reference	^{7}Li $2\,^2P_{3/2} - 2\,^2P_{1/2}$	^{6}Li $2\,^2P_{3/2} - 2\,^2P_{1/2}$	SIS
Present work	10 051.24(2)±3[a]	10 050.85(2)±3[a]	0.393(6)
Brog *et al.* [b]	10 053.24(22)	10 052.76(22)	0.48(31)
Scherf *et al.* [c]	10 053.4(2)	10 051.62(20)	1.78(28)
Walls *et al.* [d]	10 052.37(11)	10 053.044(91)	–0.67(14)
Orth *et al.* [e]	10 053.184(58)		
Noble *et al.* [f]	10 053.119(58)	10 052.964(50)	0.155(76)
Recommended value	10 053.2(1)	10 052.8(1)	

[a] Includes uncertainty of ±3 MHz due to mass-independent higher-order terms not yet calculated.

[b] K.C. Brog, Phys. Rev. **153**, 91 (1967).

[c] W. Scherf, O. Khait, H. Jager, and L. Windholz, Z. Phys. D **36**, 31 (1996).

[d] J. Walls, R. Ashby, J. J. Clarke, B. Lu, and W. A. van Wijngaarden, Eur. Phys. J **D 22** 159 (2003).

[e] H. Orth, H. Ackermann, and E.W. Otten, Z. Phys. A **273**, 221 (1975).

[f] G.A. Noble, B.E. Schultz, H. Ming, W.A. van Wijngaarden, Phys. Rev. A submitted.

```
7Li-11Li     2- 1
      nr mu/M          25104.803934335          0.000062605          0.114928928
      nr (mu/M)^2         -2.967598804          0.000006864          0.000010569
      rel mu/M             0.415505222          0.121140432
      anom mu/M            0.000000000          0.000000000
^3 Bethe log corr         -0.013934996          0.004087835
^3 mu/M 2-e EL2            0.024632937          0.004480293
^3 mu/M                   -0.131023010          0.000857103
^3 mu/M 1-e TOTAL         -0.144958006          0.004176724
   H.O. sum > a^3         -0.120325070          0.006125197     25102.131515683
      totals
         mu/M             25105.099114488          0.121226300          0.114930280
         (mu/M)^2            -2.967598804          0.000006864          0.000010569
         R^2                  0.000000000          0.000000000          0.000000000
         R^2mu/M              0.000000000
         TOTAL            25102.131515741          0.121226300          0.114930280
         TOTALerr             0.167047254
```

High Precision Theory and Isotope Shifts for Li and Be^+

Gordon W.F. Drake
University of Windsor, Canada

Zong-Chao Yan
University of New Brunswick, Canada

Collaborators

Mark Cassar (AIP)
Zheng Zhong (Ph.D. student)
Qixue Wu (Ph.D. student)
Atef Titi (Ph.D. student)

Financial Support: NSERC and SHARCnet

DAMOP, Knoxville
May 2006

Studies of Light Halo Nuclei from Atomic Isotope Shifts

Gordon W.F. Drake

University of Windsor, Canada

Collaborators

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Mark Cassar (PDF)
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Gordon W.F. Drake

University of Windsor, Canada

Collaborators

Zong-Chao Yan (UNB)
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15 June 2006

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Gordon W.F. Drake

University of Windsor, Canada

Collaborators

Zong-Chao Yan (UNB)
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Gordon W.F. Drake
University of Windsor, Canada

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Collaborators

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Table 5. Optimized scale factors for the three lowest states of H_2^+. Units are $\mu/(m_e a_0)$, where a_0 is the Bohr radius and μ is the reduced electron mass.

N	$\alpha^{(1)}$	$\beta^{(1)}$	$\gamma^{(1)}$	$\alpha^{(2)}$	$\beta^{(2)}$	$\gamma^{(2)}$
			$1\,^1\mathrm{S}$			
33	1.298 28	0.407 35	18.325 44	1.153 75	0.418 33	19.539 86
57	1.221 68	0.500 00	19.395 75	1.173 89	0.430 97	18.863 71
90	1.257 81	0.895 63	18.472 11	1.167 91	0.483 40	19.375 37
134	1.311 40	0.594 18	20.289 73	1.188 48	0.382 26	19.579 10
190	1.171 08	0.858 52	20.037 17	1.108 34	0.507 81	19.788 76
260	1.250 67	1.020 69	19.286 25	1.166 26	0.482 97	18.987 00
345	1.552 86	1.034 36	19.294 43	1.191 77	0.370 36	18.999 33
447	1.543 88	1.121 52	19.184 94	1.178 28	0.368 96	19.313 42
567	1.561 65	1.289 79	18.935 79	1.166 69	0.392 82	19.413 27
707	1.625 18	1.409 12	19.105 22	1.225 89	0.441 89	18.634 83
868	1.703 25	1.459 29	19.806 95	1.206 54	0.429 32	19.418 52
1052	1.718 81	1.471 98	19.984 99	1.192 87	0.425 05	17.587 71
			$2\,^1\mathrm{S}$			
20	1.446 66	0.194 21	16.939 94	1.071 29	0.300 90	17.510 99
40	1.219 73	0.373 60	16.521 73	1.104 80	0.388 55	18.238 34
70	1.529 42	0.360 84	16.595 21	1.158 02	0.359 80	18.129 58
112	1.465 09	0.286 93	16.856 57	1.297 97	0.344 54	17.879 27
168	1.166 99	0.718 99	17.654 54	1.130 68	0.594 79	17.733 70
240	1.307 74	0.811 04	17.186 04	1.181 15	0.601 38	17.444 89
330	1.531 86	0.931 95	16.537 48	1.162 90	0.586 06	17.150 76
440	1.730 41	0.985 84	16.496 95	1.167 66	0.560 06	17.844 85
572	1.646 24	1.027 95	18.023 19	1.109 80	0.568 73	18.673 34
728	1.572 94	1.071 66	20.452 64	1.121 64	0.573 85	18.974 49
910	1.556 15	1.060 24	20.235 23	1.133 61	0.580 02	19.176 27
1015	1.854 06	1.161 50	20.277 28	1.133 00	0.581 05	19.166 02
1240	1.844 67	1.156 62	20.254 94	1.135 19	0.584 11	19.188 42
1496	1.825 93	1.144 84	20.045 78	1.146 73	0.590 21	19.387 57
			$2\,^3\mathrm{P}$			
39	1.320 92	0.360 35	18.009 83	0.790 34	0.692 75	18.090 76
82	1.254 88	0.442 32	18.609 19	0.703 31	0.558 35	18.896 85
149	1.369 38	0.512 70	17.930 54	0.812 81	0.651 79	17.989 99
244	1.183 53	0.698 00	18.510 25	1.001 65	0.709 29	18.479 31
373	1.289 61	0.694 76	18.655 88	1.056 34	0.792 30	18.554 69
540	1.325 07	0.764 34	18.638 00	0.908 45	0.735 66	18.963 75
751	1.536 62	0.826 97	18.446 84	0.882 32	0.716 98	18.716 86
1010	1.528 87	0.831 18	18.532 29	0.878 36	0.719 06	18.633 06
1323	1.536 50	0.833 92	18.619 51	0.874 21	0.715 70	18.545 72
1694	1.536 07	0.851 56	18.824 04	0.864 07	0.713 99	18.344 18

The 20-, 21- and 24-figure accuracies of the nonrelativistic energy eigenvalues presented above, although more than sufficient for comparison with experiment, lay a firm foundation for the calculation of higher order relativistic and QED corrections to the nonrelativistic energy levels of H_2^+. The 10-figure accuracy of the electron–proton cusp quoted here represents, to our knowledge, an improvement of about five orders of magnitude over the best available value in the literature [12, 20]. This further shows the reliability of the wavefunctions to compute observables, other than the energy, to high precision, and especially the highly singular operators that appear in the relativistic and QED corrections.

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HIGH PRECISION SPECTROSCOPY

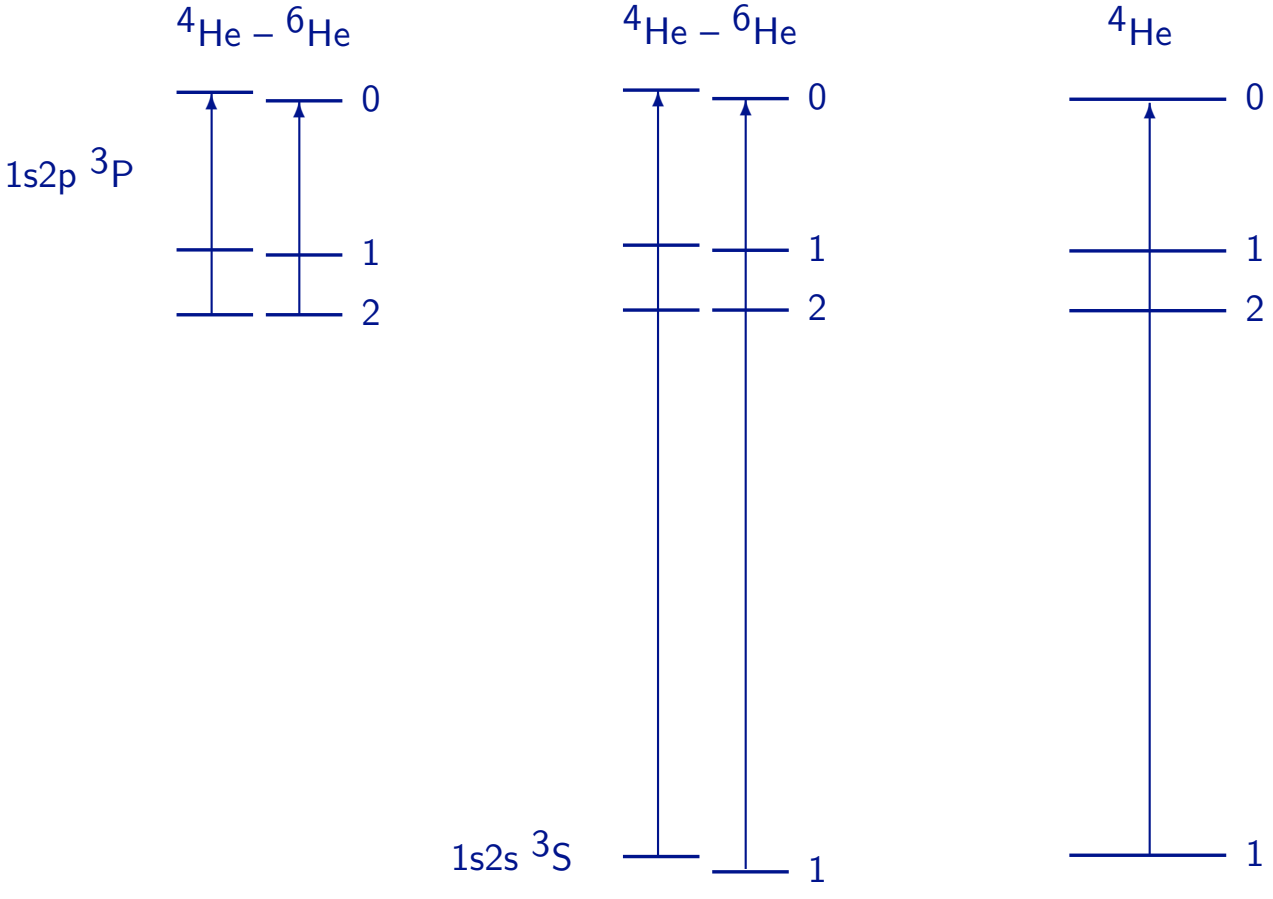
THEORY

– Hyperfine structure
– N.R. energies and relativistic corrections
– QED effects

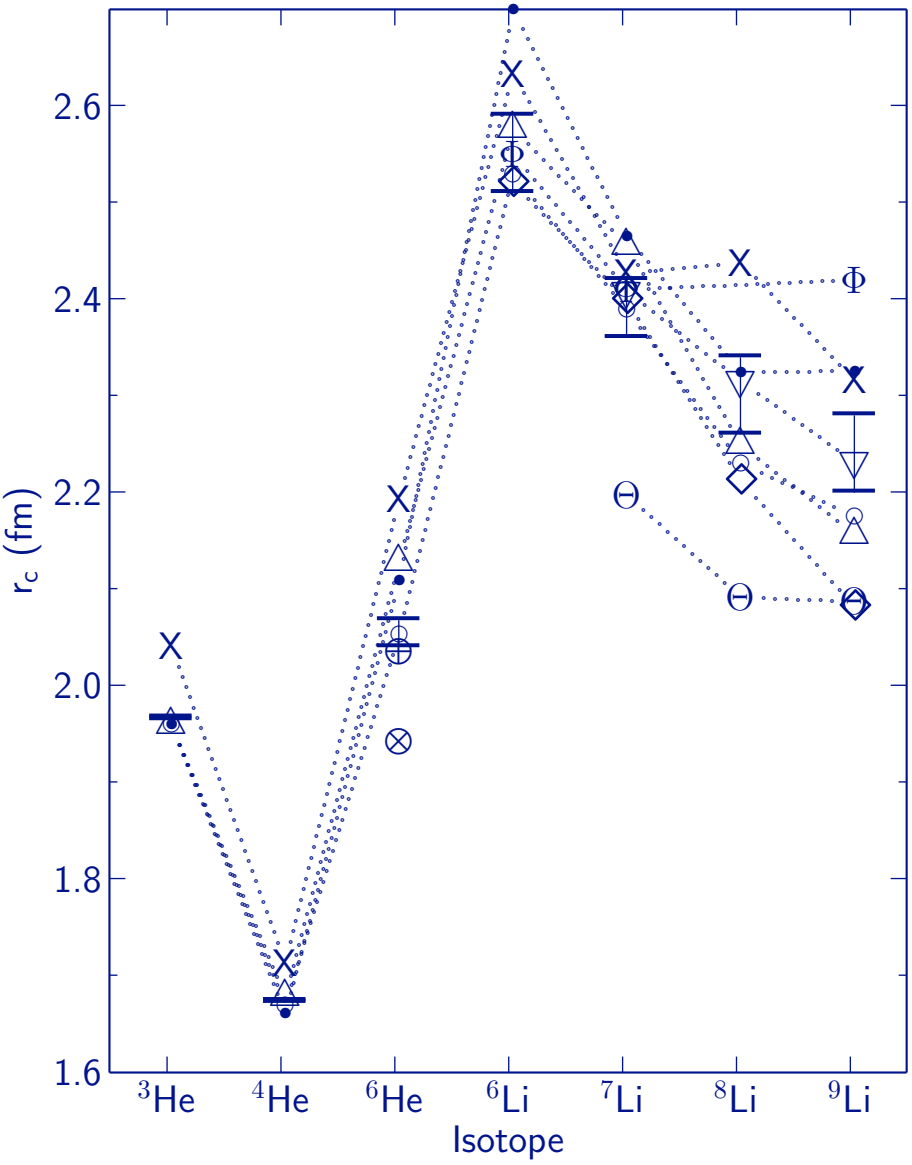
Fine Structure Isotope Shift
$\Rightarrow$ internal check of theory and experiment

Transition Isotope Shift
$\Rightarrow$ nuclear radius

Total Transition Frequency
$\Rightarrow$ QED shift

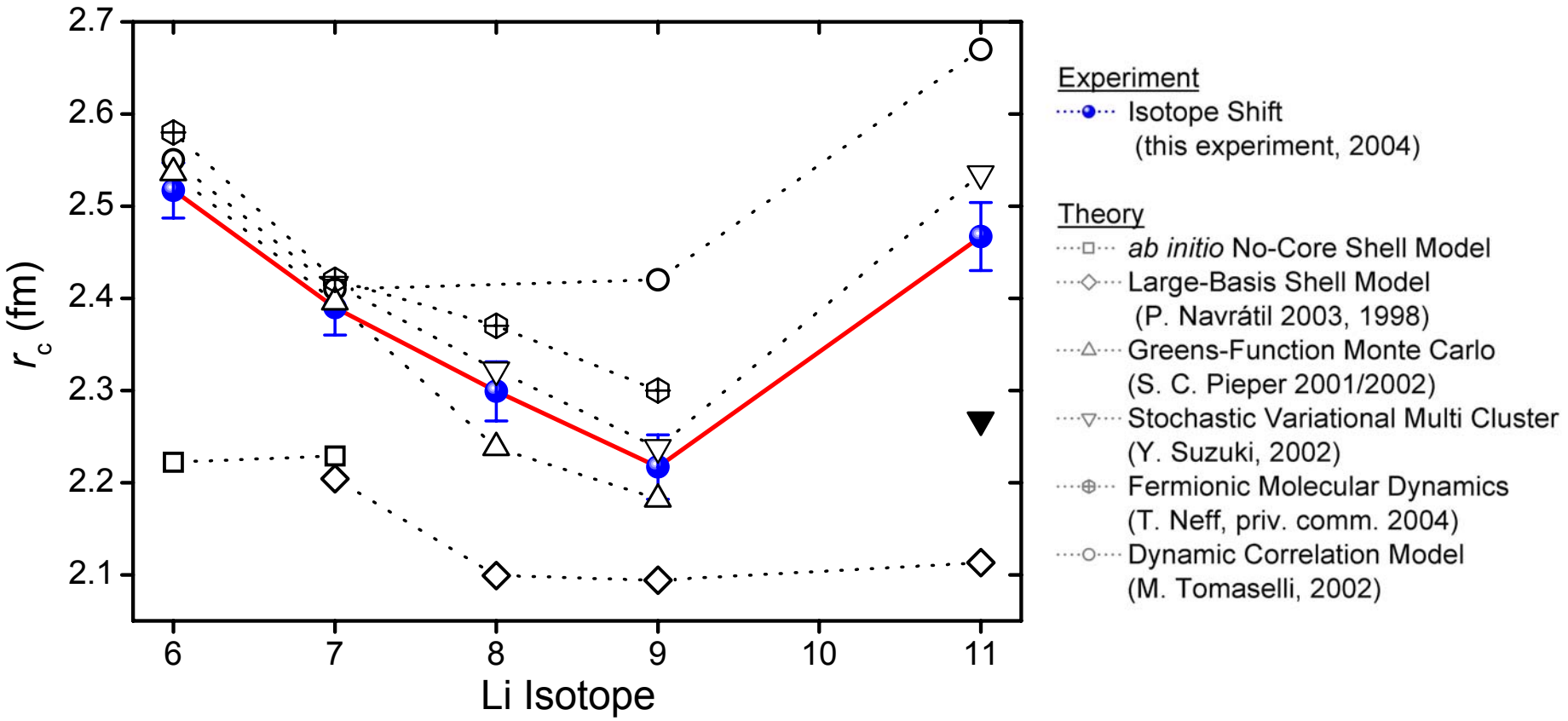


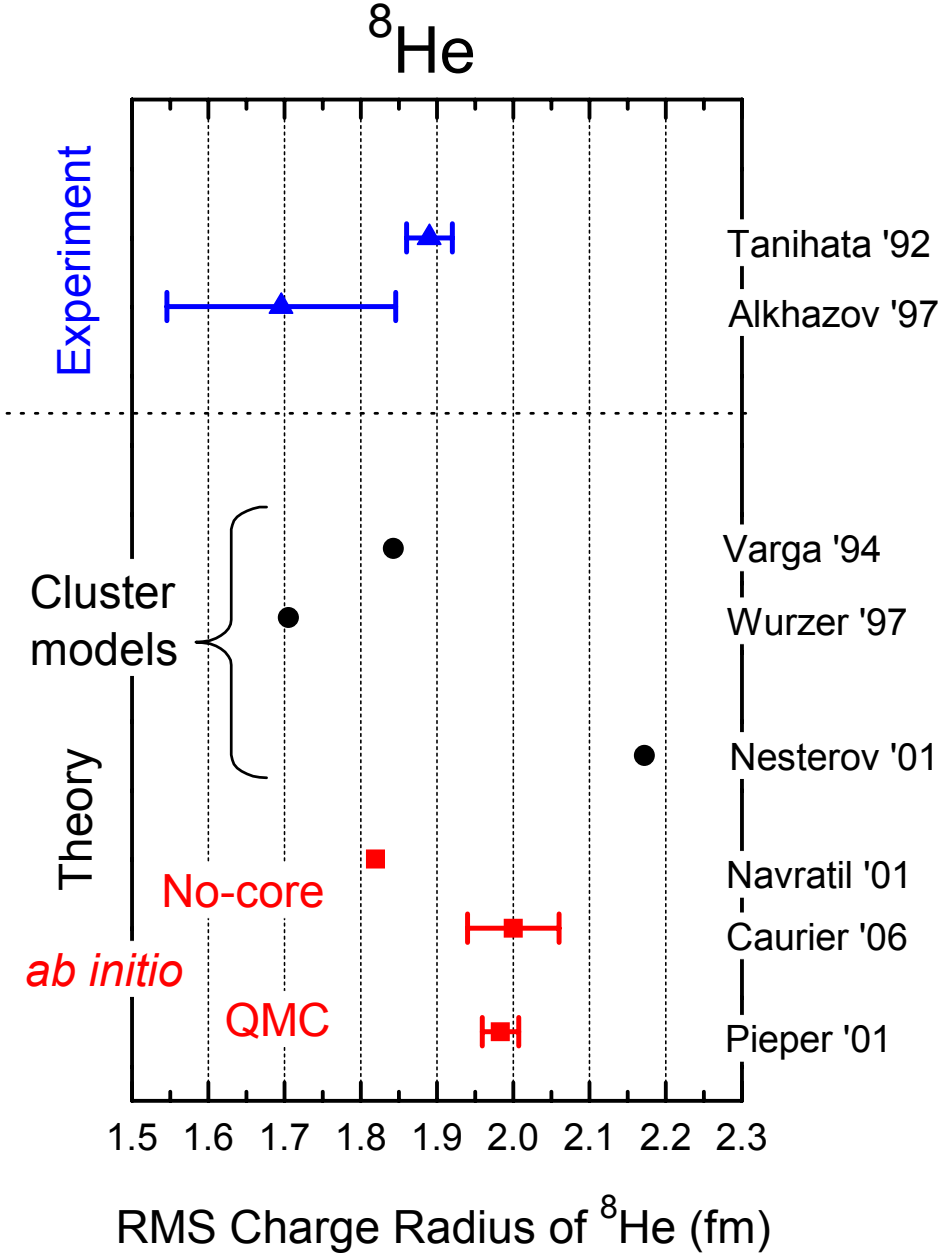
Flow diagram for types of measurements.

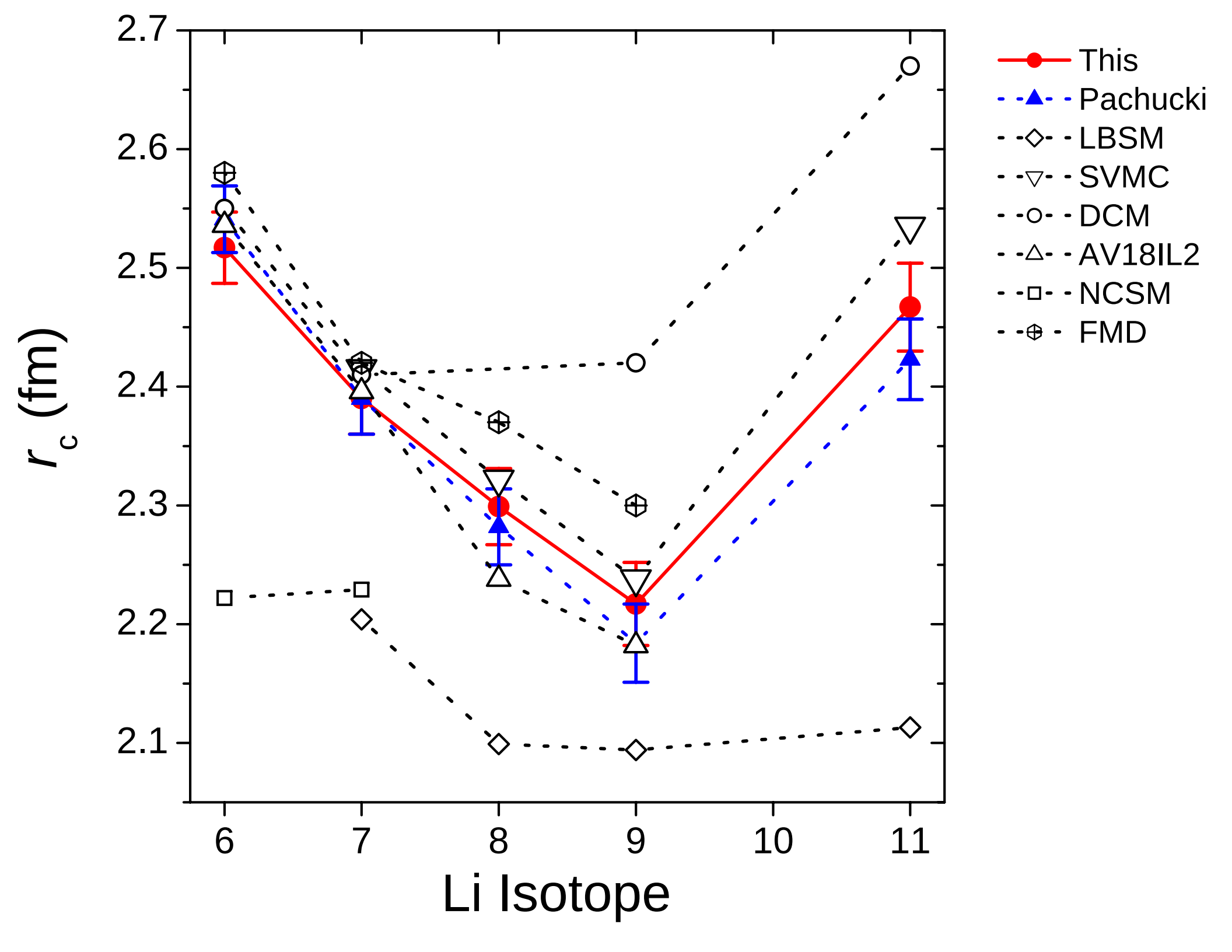


Comparison of nuclear structure theories with experiment for the rms nuclear charge radius r_c. The dotted lines connect sequences of calculations for different nuclei, and the error bars denote the experimental values, relative to the ^{4}He and ^{7}Li reference nuclei. The points are grouped as ($\otimes$)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

Nuclear Charge Radii




^{8}He
Experiment
Tanihata '92
Alkhazov '97
Theory
Cluster models
Varga '94
Wurzer '97
Nesterov '01
No-core
ab initio
QMC
Navratil '01
Caurier '06
Pieper '01
1.5 1.6 1.7 1.8 1.9 2.0 2.1 2.2 2.3
RMS Charge Radius of ^{8}He (fm)


2.7
2.6
2.5
2.4
2.3
2.2
2.1
r_c (fm)
6
7
8
9
10
11
Li Isotope
This
Pachucki
LBSM
SVMC
DCM
AV18IL2
NCSM
FMD

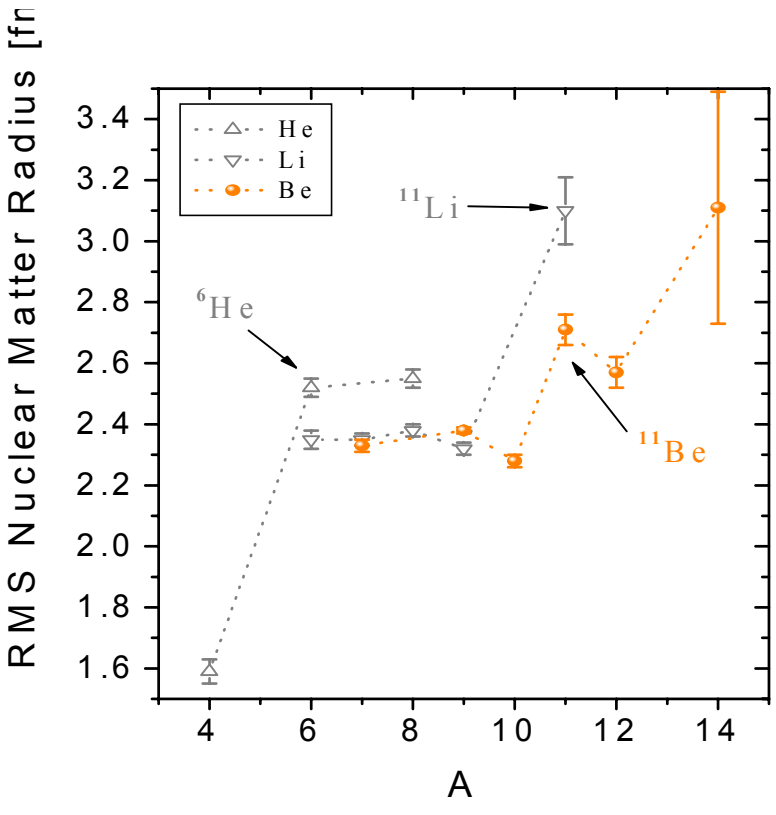
4:00 PM, Wednesday, May 17, 2006
Knoxville Convention Center - Ballroom AB, 4:00pm - 6:00pm

Abstract: G1.00036 : Towards a Laser Spectroscopic Determination of the ^{8}He Nuclear Charge Radius

Authors:

. Mueller K. Bailey R.J. Holt R.V.F. Janssens Z.-T. Lu T.P. O'Connor I. Sulai (Argonne National Lab)	M.-G. Saint Laurent J.-Ch. Thomas A.C.C. Villari (GANIL)	O. Naviliat-Cuncic X. Flechard (Laboratoire de Physique Corpusculaire Caen)
S.-M. Hu (University of Science and Technology of China)	G.W.F. Drake (University of Windsor)	M. Paul (Hebrew University)

We will report on the progress towards a laser spectroscopic determination of the ^{8}He nuclear charge radius. ^{8}He (t$_{1/2}$ = 119 ms) has the highest neutron to proton ratio of all known isotopes. Precision measurements of its nuclear structure shed light on nuclear forces in neutron rich matter, e.g. neutron stars. The experiment is based on our previous work on high-resolution laser spectroscopy of individual helium atoms captured in a magneto-optical trap. This technique enabled us to accurately measure the atomic isotope shift between ^{6}He and ^{4}He and thereby to determine the ^{6}He rms charge radius to be 2.054(14) fm. We are currently well on the way to improve the overall trapping efficiency of our system to compensate for the shorter lifetime and lower production rates of ^{8}He as compared to ^{6}He. The ^{8}He measurement will be performed on-line at the GANIL cyclotron facility in Caen, France and is planned for late 2006.



7Be		9Be	10Be	11Be	12Be		14Be
53.12 d		∞	1.5×10^6 a	13.81 s	21.5 ms		4.84 ms
3/2-		3/2-	0+	1/2+	0+		0+

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 $\pm$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.

Relativistic and QED Effects in Helium and Lithium: Isotope Shifts

Gordon W.F. Drake

University of Windsor, Canada

Collaborators

Zong-Chao Yan (UNB)
Zheng Zhong (Ph.D. student)
Qixue Wu (Ph.D. student)
Atef Titi (Ph.D. student)
Roman Atanasof (M.Sc. student)
Eva Schulhof (M.Sc. student)

Financial Support: NSERC and SHARCnet

A Tribute to Walter Johnson
Notre Dame, April 4–5, 2008.

Objectives

1. Calculate nonrelativistic eigenvalues for helium, lithium and Be^+ of spectroscopic accuracy.
2. Include finite nuclear mass (mass polarization) effects up to second order by perturbation theory.
3. Include relativistic and QED corrections by perturbation theory.
4. Compare the results with high precision measurements.
5. Use the results to measure the nuclear radius of exotic "halo" isotopes of helium, lithium and beryllium such as ^{6}He, ^{11}Li, and $^{11}Be^+$.

What's New?

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

High precision measurements for helium and He-like ions.

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

Main Theme:

Create new measurement tools by combining high precision theory and experiment.

Examples:

- Interpretation of parity nonconservation (24 papers by Johnson et al.)
- Cosmological variation of fundamental constants (Flambaum).
- Interpretation of isotope shifts (with M. Safronova).

Focus on Isotope Shifts for Halo Nuclei

1. Calculate nonrelativistic eigenvalues for helium, lithium and Be^+ of spectroscopic accuracy.
2. Include finite nuclear mass (mass polarization) effects up to second order by perturbation theory.
3. Include relativistic and QED corrections by perturbation theory.
4. Compare the results with high precision measurements.
5. Use the results to measure the nuclear radius of exotic "halo" isotopes of helium, lithium and beryllium such as ^{6}He, ^{8}He, ^{11}Li, and $^{11}Be^+$ (Drake, 1993).

Nonrelativistic and Relativistic Contributions to the Energy

$$
\begin{array}{rc|cccccc}
 & & E_{\rm NR} & \langle B_{\rm P}\rangle & \text{QED} & & & \\
 & & \downarrow & \downarrow & \downarrow & & & (\alpha Z)^2 \longrightarrow \\
\hline
E_{\rm Dirac} & \longrightarrow & E_0^0 Z^2 & + E_0^2\alpha^2 Z^4 & + E_0^4\alpha^4 Z^6 & + E_0^6\alpha^6 Z^8 & + & \cdots \\
\langle e^2/r_{12} + B_{\rm D}\rangle & \longrightarrow & + E_1^0 Z^1 & + E_1^2\alpha^2 Z^3 & + E_1^4\alpha^4 Z^5 & + E_1^6\alpha^6 Z^7 & + & \cdots \\
 & & + E_2^0 Z^0 & + E_2^2\alpha^2 Z^2 & + \underline{E_2^4\alpha^4 Z^4} & + E_2^6\alpha^6 Z^6 & + & \cdots \\
 & & + E_3^0 Z^{-1} & + E_3^2\alpha^2 Z^1 & + & \cdots & & \\
Z^{-1} & & + E_4^0 Z^{-2} & + E_4^2\alpha^2 Z^0 & + & \cdots & & \\
\downarrow & & + & \cdots & + & \cdots & &
\end{array}
$$

where

$$
\begin{aligned}
E_{\rm NR} &= \text{nonrelativistic energy,} \\
\langle B_{\rm P}\rangle &= \text{Pauli form of the Breit interaction,} \\
E_{\rm Dirac} &= \text{sum of one-electron Dirac energies,} \\
\langle B_{\rm D}\rangle &= \text{relativistic Dirac form of the Breit interaction.}
\end{aligned}
$$

Two regions: $(\alpha Z)^2 = Z^{-1}$ when $Z \approx 27$.

- For $Z < 27$ start with $H_{\rm NR}$ and sum column-wise with relativistic corrections as a perturbation.
- For $Z > 27$ start with $H_{\rm Dirac}$ and sum row-wise with the electron-electron interaction as a peturbation.
- Unified Method: Sum the first two rows and the first two columns and subtract the terms that are counted twice.

What's New?

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

Energy Levels and Isotope shifts

The three key parameters controlling the energy levels are

$$\begin{aligned} \alpha &= \text{fine structure constant} \\ \lambda &= \mu/M = m_{\rm e}/(m_{\rm e}+M) \\ \bar{r}_{\rm c} &= \text{nuclear charge radius} \end{aligned}$$

In terms of these parameters, the theoretical contributions to the energy levels of an atom or ion such as Be^+ can be expanded in the form

$$\begin{aligned} E &= \mathcal{E}^{(0)}_{\rm NR} + \lambda\mathcal{E}^{(1)}_{\rm NR} + \lambda^2\mathcal{E}^{(2)}_{\rm NR} + \alpha^2\left(\mathcal{E}^{(0)}_{\rm rel} + \lambda\mathcal{E}^{(1)}_{\rm rel}\right) \\ &\quad + \alpha^3\left(\mathcal{E}^{(0)}_{\rm QED} + \lambda\mathcal{E}^{(1)}_{\rm QED}\right) + \alpha^4\left(\mathcal{E}^{(0)}_{\rm ho} + \lambda\mathcal{E}^{(1)}_{\rm ho}\right) \\ &\quad + \bar{r}_{\rm c}^2\left(\mathcal{E}^{(0)}_{\rm nuc} + \lambda\mathcal{E}^{(1)}_{\rm nuc}\right) + \cdots \end{aligned}$$

in units of $\alpha^2\mu c^2 = \alpha^2(1-\lambda)mc^2$

The subscripts are:

NR = nonrelativistic energy

rel = relativistic corrections

QED = quantum electrodynamic corrections

ho = higher order QED corrections (ho)

nuc = shift due to finite nuclear size.

TABLE VIII. Isotope shifts $\delta\nu^{22,23}$ (MHz) for $n=3$ states of Na.

	NMS+SMS	FS	Total IS	Expt.
$3s$	1448.8	−7.5	1441.3	
$3p_{1/2}$	707.9	0.3	708.2	
$3p_{3/2}$	707.3	0.3	707.6	
$3d_{3/2}$	391.8	0.0	391.8	
$3d_{5/2}$	391.8	0.0	391.8	
$3p_{3/2}$-$3s$	−740.9	7.9	−733.0	−758.5(7)[a]
				−756.9(1.9)[b]
$3p_{5/2}$-$3s$	−741.5	7.9	−733.6	−757.72(24)[c]

[a]Pescht *et al.* [4].
[b]Huber *et al.* [28].
[c]Gangrsky *et al.* [25].

QED and Isotope Shifts in Lithium and Be^+

Gordon W.F. Drake

University of Windsor,

Zong-Chao Yan

University of New Brunswick

Collaborators

Zheng Zhong (Ph.D. student)
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Financial Support: NSERC and SHARCnet

CAP Annual Congress
Quebec City, June 11, 2008.