Sizing Halo Nuclei with Atomic Isotope Shifts

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OUTLINE

Main Theme:

- Derive nuclear charge radii by combining atomic theory with high precision spectroscopy (especially ^{6}He, ^{8}He, ^{11}Li, ^{11}Be 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.

History

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

^{3}He – ^{4}He Isotope shift (MHz)

Transition	Theory [a]	Experiment [b]	Difference
$2\,^3\mathrm{S}_1 - 2\,^3\mathrm{P}_0$	33 667.734(1)	33 667.968(38)	–0.234(38)
$2\,^3\mathrm{S}_1 - 2\,^3\mathrm{P}_1$	33 667.459(1)	33 667.693(38)	–0.234(38)
$2\,^3\mathrm{S}_1 - 2\,^3\mathrm{P}_2$	33 668.447(1)	33 668.670(38)	–0.223(38)

[a]Assuming $r_\mathrm{c}(^3\mathrm{He}) = 1.875 \pm 0.05$ fm.

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

Adjust $r_\mathrm{c}(^3\mathrm{He}) = 1.925 \pm 0.008$ fm.

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

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

3. Marin, Minardi, Pavone, Inguscio, and Drake, "Hyperfine structure of the $3\,^3$P state of ^{3}He and isotope shift for the $2\,^3\mathrm{S} - 3\,^3\mathrm{P}$ transition," Z. Phys. D **32**, 285–293 (1994).

   Yielded $r_\mathrm{c}(^3\mathrm{He}) = 1.956 \pm 0.042$ fm.

4. Shiner, Dixson, and Vedantham, "Three-Nucleon Charge Radius: A Precise Laser Determination Using ^{3}He," Phys. Rev. Lett. **74**, 3553 (1995).

   Yielded $r_\mathrm{c}(^3\mathrm{He}) = 1.9506 \pm 0.0014$ fm from the $2\,^3\mathrm{S}_1 - 2\,^3\mathrm{P}_0$ transition.

5. Schmitt, Dax, Kirchner, Kluge, Kühl, Tanihata, Wakasugi, Wang, and Zimmermann, Hyperfine Interactions, "Towards the determination of the charge radius of Li-11 by laser spectroscopy" **127**, 111-115 (2000).

   - first communication from Andreas Dax was three years earlier, in 1997.

6. Drake and Goldman, "Bethe logarithms for Ps^-, H^- and heliumlike atoms," Can. J. Phys. **77**, 835 (2000).

   - allowed a complete control of theoretical uncertainties in the isotope shift up to order $\alpha^3\mu/M$ Ryd.

   - similarly for Li-like atoms in Yan and Drake, "Bethe logarithm and QED shift for lithium," Phys. Rev. Lett., **91**, 113004 (2003).

7. 2000: Wilfried Nörtershäuser begins work on the Li-11 experiment at GSI.

8. June 21, 2001: First communication from Z.T. Lu suggesting a measurement of the isotope shift for He-6 at Argonne to determine the nuclear charge radius.

9. L.-B. Wang, P. Mueller, K. Bailey, G.W.F. Drake, 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, M. Paul, K.E. Rehm, J.P. Schiffer, and X.D. Tang, "Laser spectroscopic determination of the 6He nuclear charge radius," Phys. Rev. Lett. **93**, 142501 (2004).

10. R. Sanchez, W. Nördershäuser, G. Ewald, D. Albers, J. Behr, P. Bricault, B. A. Bushaw, A. Dax,, J. Dilling, M. Dombsky, G.W.F. Drake, S. Götte, R. Kirchner, H.-J. Kluge, T. Kühl, J. Lassen, C.D.P. Levi, M.R. Pearson, E.J. Prime, V. Ryjkov, A. Wojtaszek, Z.-C. Yan, and Claus Zimmerman, "Nuclear charge radii of Li-9,Li-11: The influence of halo neutrons," Phys. Rev. Lett. **96**, 033002 (2006).

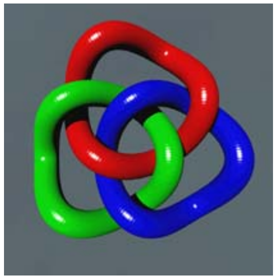
11. K. Pachucki and A.M. Moro, "Nuclear polarizability of helium isotopes in atomic transitions", Phys. Rev. A **75**, 032521(2007).

12. P. Mueller, I. A. Sulai, A. C. C. Villari, J. A. Alcántara-Núñez, R. Alves-Condé, K. Bailey, G. W. F. Drake, M. Dubois, C. Eléon, G. Gaubert, R. J. Holt,1 R. V. F. Janssens, N. Lecesne, Z.-T. Lu, T. P. O'Connor, M.-G. Saint-Laurent, J. P. Schiffer,1 J.-C. Thomas, and L.-B. Wang, "Nuclear charge radius of ^{8}He," Phys. Rev. Lett. **99**, 252501 (2008).

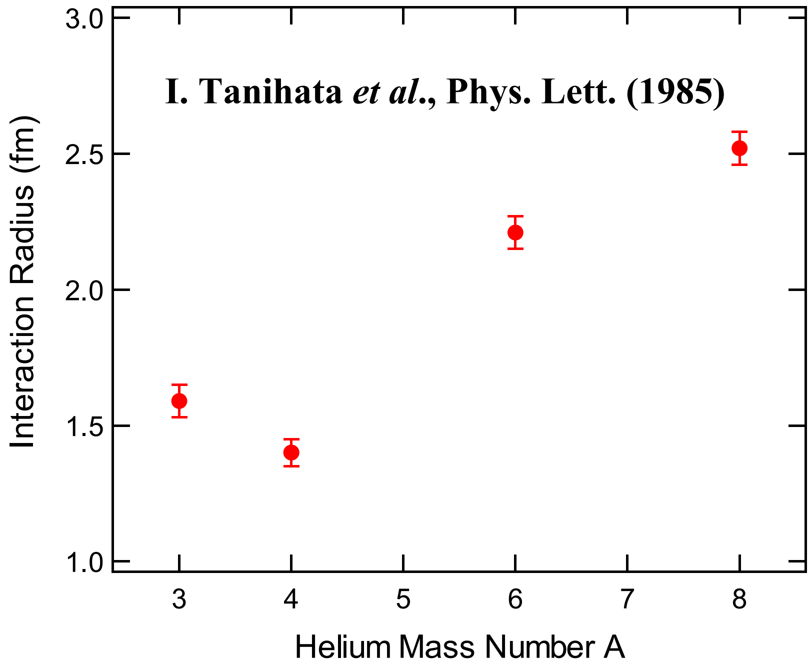
13. W. Nörtershäuser, D. Tiedemann, M. Zakova, Z. Andjelkovic, K. Blaum, M. L. Bissell, R. Cazan, G.W.F. Drake, Ch. Geppert, M. Kowalska, J. Kramer, A. Krieger, R. Neugart, R. Sanchez, F. Schmidt-Kaler, Z.-C. Yan, D. T. Yordanov, and C. Zimmermann, 2008. "Nuclear Charge Radii of ^{7,9,10}Be and the one-neutron halo nucleus ^{11}Be," Phys. Rev. Lett. **102**, 062503 (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

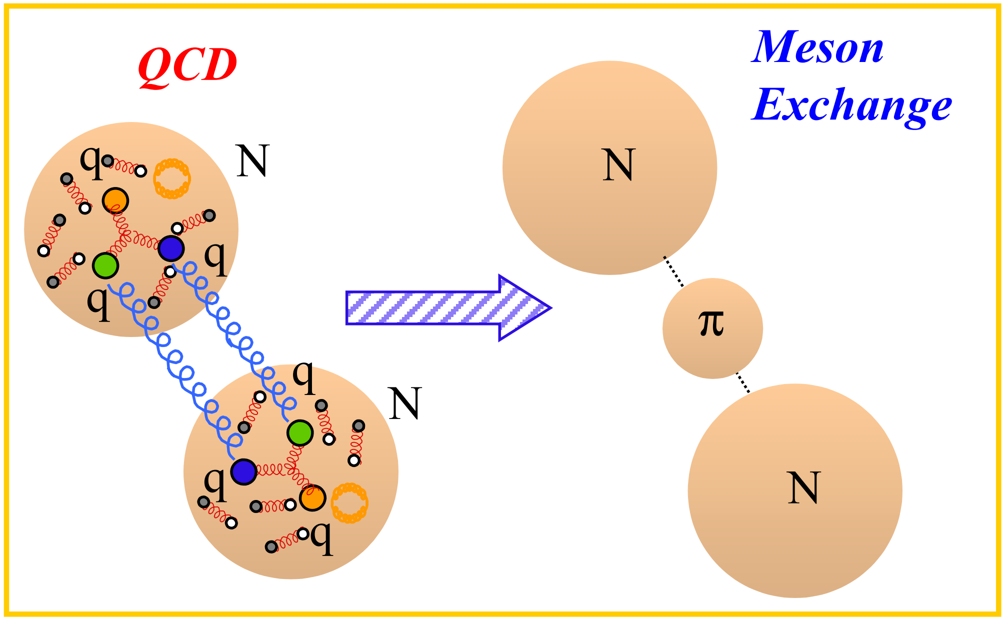
$$\sigma_I(6He) - \sigma_I(4He) = \sigma_{-2n}(6He)$$

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

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

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

Nucleon-Nucleon Interaction at Low Energy

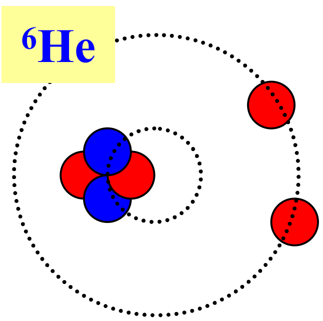


- Fundamental theory QCD not calculable in low-energy regime (nucleus structure)
- Modern nuclear calculation uses "effective potential" between nucleons

Charge Radii Measurements

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

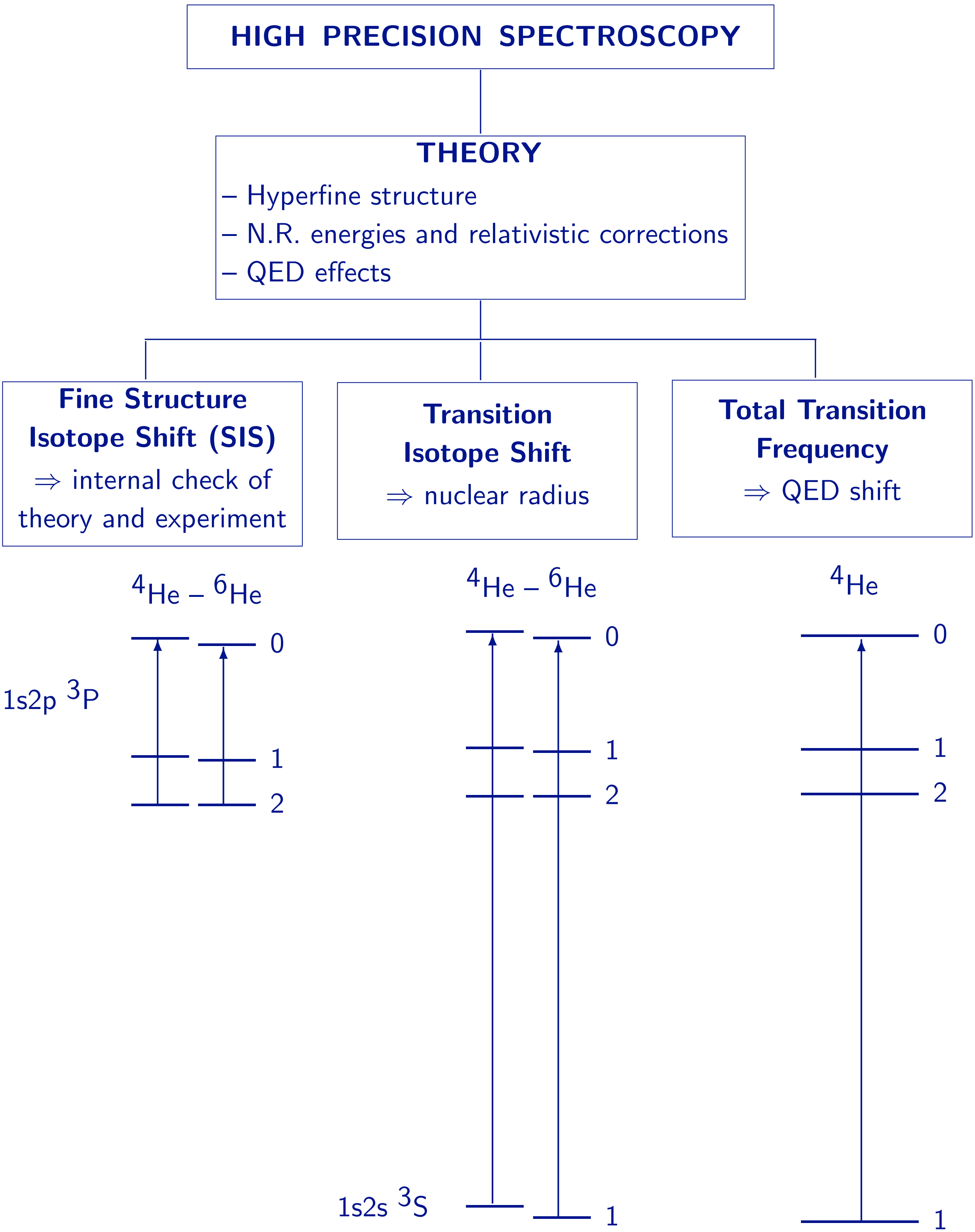
- ❖ Nuclear scattering – model dependent
- ❖ Electron scattering – stable isotope only
- ❖ Muonic atom spectroscopy – stable isotope only
- ❖ Atomic isotope shift



RMS point proton radii (fm) from theory and experiment

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

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

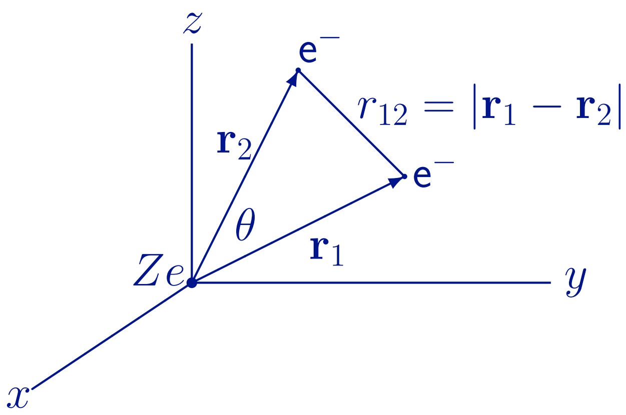


Flow diagram for types of measurements.

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

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

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

Rayleigh-Schrödinger Variational Principle

Diagonalize H in the

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

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.

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

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

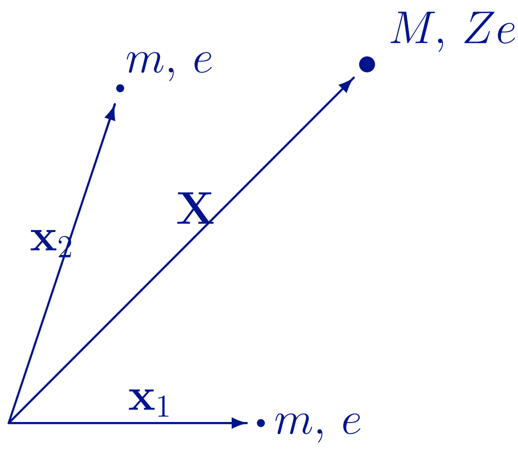
for $t = 1$, 2, with $\langle \Psi_{\mathsf{tr}} \mid \Psi_{\mathsf{tr}}\rangle = 1$.
$\Psi(\mathbf{r}_1,\mathbf{r}_2;\alpha_t) =$ terms in Ψ_{tr} which depend explicitly on α_t.

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).

Mass Scaling



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

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

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

and ignore centre-of-mass motion. Then

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

Expand

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

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

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

The “normal” isotope shift is

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

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 $\alpha^4 \mathcal{E}_{\rm ho}^{(0)} \simeq 10^{-8}$, where here and throughout the superscript denotes the power of λ.

II. For isotope shifts

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

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

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

Variational Basis Set for Lithium

Solve for Ψ_0 and Ψ_1 by expanding in Hylleraas coordinates

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

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

Include all terms from (1) such that

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

and study the eigenvalues as Ω is progressively increased.

The explicit mass-dependence of E is

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

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)

$$\tilde\Delta_2 = -\frac{Z\alpha^2}{2}\left\{\frac{1}{r_1}(\mathbf{p}_1+\mathbf{p}_2)\cdot\mathbf{p}_1 + \frac{1}{r_1^3}br_1\cdot[\mathbf{r}_1\cdot(\mathbf{p}_1+\mathbf{p}_2)]\mathbf{p}_1 + \frac{1}{r_2}(\mathbf{p}_1+\mathbf{p}_2)\cdot\mathbf{p}_2 + \frac{1}{r_2^3}br_2\cdot[\mathbf{r}_2\cdot(\mathbf{p}_1+\mathbf{p}_2)]\mathbf{p}_2\right\}$$

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

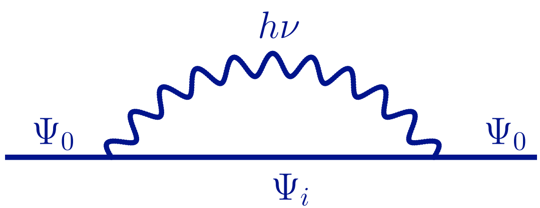
Two-Electron QED Shift

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

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

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

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



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:

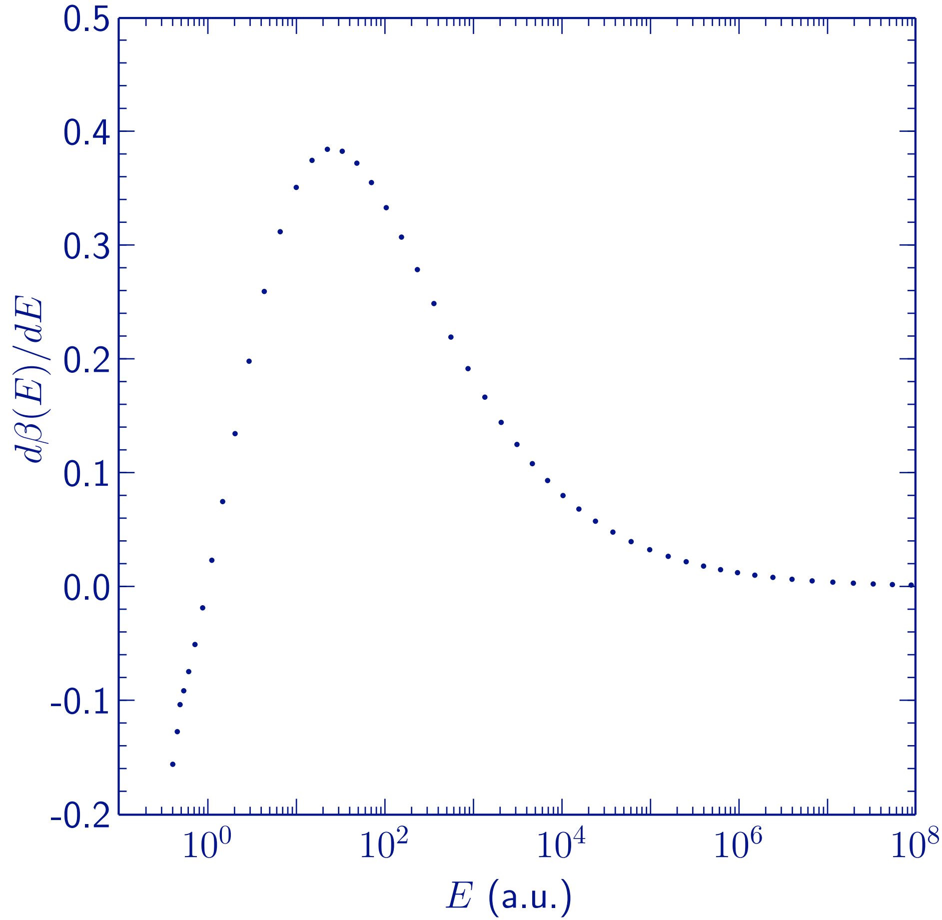
$$\Omega = 1; \; N = 1:$$
$$e^{-\alpha r}$$

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

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

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

$$e^{-\alpha r}, \quad re^{-\alpha r}, \quad r^2 e^{-\alpha r}, \quad r^3 e^{-\alpha r}$$



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	2.041334736712356432007		
3	6	2.255625010210503788880	0.214290273498147356672	
4	10	2.286605838061750809919	0.030980827851247020039	6.917
5	15	2.290467318738008208061	0.003861480676257399942	8.023
6	21	2.290924656589168318580	0.000457337851160109997	8.443
7	28	2.290975289804262786500	0.000050633215094467920	9.032
8	36	2.290980746794663559290	0.000005456990400772790	9.279
9	45	2.290981311450116771570	0.000000564655453212280	9.664
10	55	2.290981368905904892320	0.000000057455788120750	9.828
11	66	2.290981374589832446030	0.000000005683927553700	10.108
12	78	2.290981375146506428110	0.000000000556673982080	10.211
13	91	2.290981375199918957690	0.000000000053412529570	10.422
14	105	2.290981375205022051190	0.000000000005103093500	10.467
15	120	2.290981375205502360460	0.000000000000480309280	10.625
16	136	2.290981375205547638810	0.000000000000045278340	10.608
17	153	2.290981375205551863030	0.000000000000004224220	10.719
18	171	2.290981375205552260320	0.000000000000000397290	10.633
19	190	2.290981375205552297460	0.000000000000000037140	10.697
20	210	2.290981375205552300960	0.000000000000000003510	10.594
Extrap.		2.290981375205552301330		

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 94
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 06
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(
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 01
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(
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(
5 ^{1}S	2.983 857 4(1)	2.983 513 01(2)	2.983 267 901(6)	2.983 094 85(5)	2.982 968 66(
5 ^{3}S	2.983 784 02(8)	2.983 422 50(2)	2.983 180 677(6)	2.983 015 17(3)	2.982 896 13(
5 ^{1}P	2.984 096 174(9)	2.984 038 03(5)	2.983 992 23(1)	2.983 958 67(5)	2.983 933 65(
5 ^{3}P	2.984 080 3(2)	2.984 014 4(4)	2.983 968 9(4)	2.983 937 2(4)	2.983 914 07(

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

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

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

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

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

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

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

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

e

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	$2\,{}^{3}\mathrm{S}_1$	$3\,{}^{3}\mathrm{P}_2$	$2\,{}^{3}\mathrm{S}_1 - 3\,{}^{3}\mathrm{P}_2$
E_{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
$E_{\mathrm{nuc}}^{\mathrm{a}}$	–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 $r_{\mathrm{nuc}}({}^{6}\mathrm{He}) = 2.04$ fm.

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

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

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

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

Nuclear Charge Radius of ^{8}He

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(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

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

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

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

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

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

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

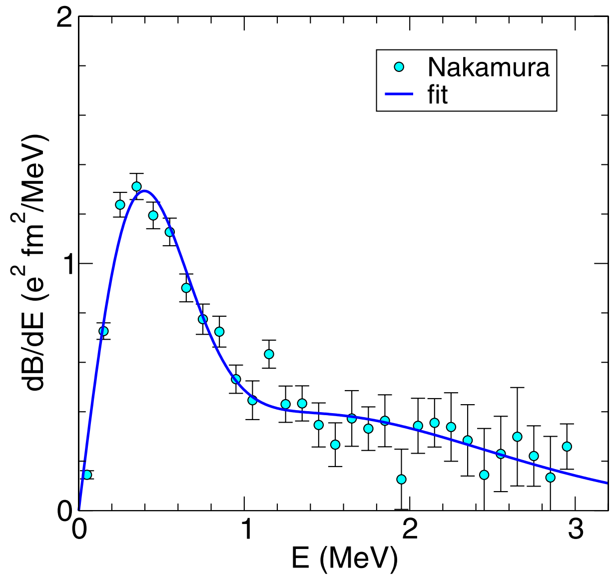
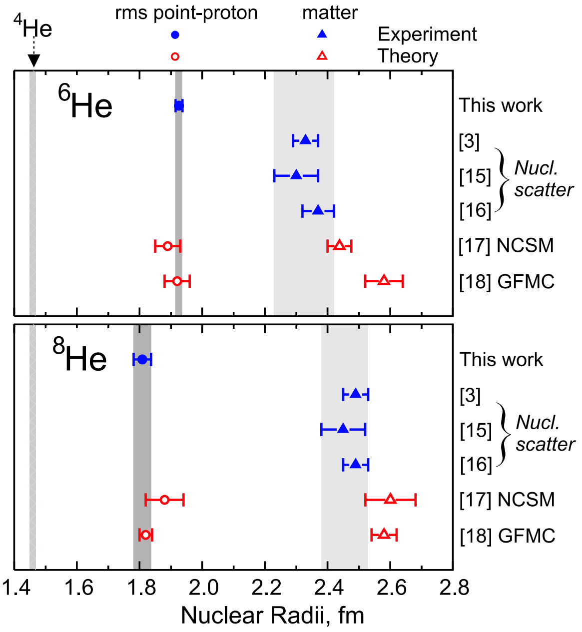


FIG. 1 (color online). Electric dipole line strength by Nakamura *et al.* [20] adapted to the new value of E_T from Ref. [7].

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


4He
rms point-proton
matter
Experiment
Theory
6He
This work
[3]
[15]
[16]
Nucl.
scatter
[17] NCSM
[18] GFMC
8He
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 ^{9}Be$^+$. Units are cm^{-1}.

[See Z.-C. Yan, W. Nörtershäuser, and G.W.F. Drake, PRL 100, 243002 (2008)].

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 (Pachucki)	14 903.648 4(10)		27 206.093 7(6)	43 487.159 0(8)
^{7}Li (this work)	14 903.648 5(10)	14 903.983 8(10)	27 206.093 9(10)	43 487.159 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 4(10)	0.000 2(10)	–0.000 3(10)	–0.000 1(10)
^{9}Be$^+$ (Pachucki)	31 928.734(8)		88 231.919(5)	146 882.918(7)
^{9}Be$^+$ (this work)	31 928.738(5)	31 935.310(5)	88 231.920(6)	146 882.923(5)
^{9}Be$^+$ (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.*

[f]M. Puchalski and K. Pachucki, Phys. Rev. A **78**, 052501 (2008).

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]	23 082.645(11)	23 083.513(11)	25 101.472(10)
Pachucki[b]			25 101.471(7)[c]
^{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	31 560.31(6)	31 563.89(6)	31 104.60(6)
Pachucki[b]	31 560.30(3)		

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

[b]M. Puchalski and K. Pachucki, Phys. Rev. A **78**, 052501 (2008).

[c]Value with nuclear mass adjusted to 11.043 716(5) u instead of 11.043 723 61(69) u.

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

and for Be^+:

$C(2\,^2P-2\,^2S) = 16.912$ MHz/fm^2

$C(3\,^2S-2\,^2S) = 10.376$ MHz/fm^2

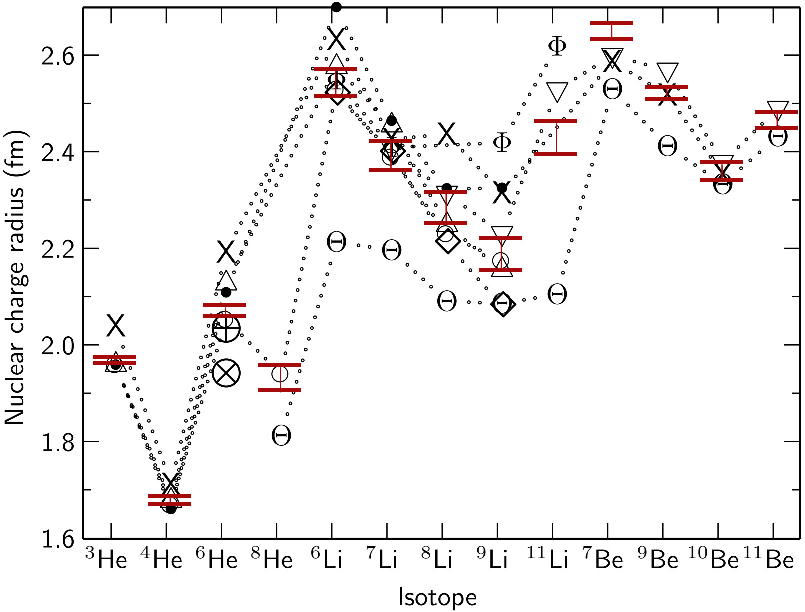


Fig. 4. Comparison of various nuclear structure theories with experiment for the rms nuclear charge radius r_c. The points are grouped as (⊗) variational microcluster calculations[41–43] and a no-core shell model;[44,45] (⊕) effective three-body cluster models;[46,47] (Θ) large-basis shell model;[48]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

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 ± 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.