Special Topics on Precision Measurement in Atomic Physics: Lecture 8

Relativistic and QED Effects

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Hydrogenic Atoms

- Uncertainties here limit what can be achieved for more complex systems.
- For hydrogen, the Schrödinger (or Dirac) equation can be solved exactly, and so uncertainties come from QED corrections and the effects of finite nuclear size and structure.
- Relativistic corrections can be expressed as an expansion in powers of $(\alpha Z)^2$, and summed to infinity by solving the Dirac equation.
- QED effects (self energy and vacuum polarization) can be written as a dual expansion in powers of αZ and α, but cannot be summed to infinity.

$$E_{\mathsf{Total}} = E_{\mathsf{NR}} + \Delta E_{\mathsf{rel.}} + \Delta E_{\mathsf{QED}}$$

where $E_{\rm NR}$ is the nonrelativistic energy, and (in atomic units)

$$\begin{aligned} \Delta E_{\mathsf{rel.}} &= \alpha^2 Z^4 \left[E^{(2)}_{\mathsf{rel.}} + (\alpha Z)^2 E^{(4)}_{\mathsf{rel.}} + \cdots \right] \\ \Delta E_{\mathsf{QED}} &= \alpha^3 Z^4 \left[\ln(\alpha Z) E^{(3,1)}_{\mathsf{QED}} + E^{(3,0)}_{\mathsf{QED}} + O(\alpha Z)^2 + O(\alpha/\pi) \right] \end{aligned}$$

- QED Terms are known in their entirety up to $O(\alpha^5 Z^6)$, and so the uncertainty is of $O(\alpha^6 Z^7)$ (at least in the low-Z region), or a few kHz for hydrogen 2s state [K. Pachucki and U. D. Jentschura, Phys. Rev. Lett. **91**,113005 (2003)].
- The proton size discrepancy of 0.84 fm (muonic) – 0.87 fm (electronic) also corresponds to an energy discrepancy of 3 kHz for the 2s state.

High-Z Hydrogenic Ions

- There has been considerable progress in summing the αZ binding energy corrections to infinity [A. Gumberidze et al., Hyperfine Interact. **199**, 59 (2011)]. For U^{91+}, the Lamb shift is
  464.26 ± 0.5 eV theory
  460.2 ± 4.6 eV experiment.

- For excited s-states, the Lamb shifts and uncertainties scale approximately as $1/n^3$ with n and Z^6 with Z. These uncertainties place a fundamental limit on the accuracy of atomic structure computations.

Methods of Theoretical Atomic Physics.

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

Relativistic Corrections

Nonrelativistic Energy: $1/Z$ Expansion

$$E_{\mathsf{NR}} = E^{(0)}_{\mathsf{NR}} Z^2 + E^{(1)}_{\mathsf{NR}} Z + \underline{E^{(2)}_{\mathsf{NR}}} + \cdots$$

Relativistic Corrections: $(\alpha Z)^2$ and $1/Z$ Expansions

$$\begin{aligned} E_{\mathsf{rel}} &= E^{(2,4)}_{\mathsf{rel}} \alpha^2 Z^4 + E^{(4,6)}_{\mathsf{rel}} + \cdots \\ &+ \underline{E^{(2,3)}_{\mathsf{rel}} \alpha^2 Z^3} + \cdots \end{aligned}$$

Cross-over point: $E^{(2)}_{\mathsf{NR}} \simeq E^{(2,3)}_{\mathsf{rel}} \alpha^2 Z^3$ when $\alpha^2 Z^3 \simeq 1$, or $Z \simeq 1/\alpha^{2/3} \simeq 27$

Two Strategies

- $Z < 27$: start from the nonrelativistic Schrödinger equation and treat relativistic effects as a perturbation. Uncertainty dominated by relativistic (and QED) corrections.
- $Z \geq 27$: start from the Dirac equation and treat electron correlation effects as a perturbation. Uncertainty dominated by electron correlation corrections.

Current Status for Helium

- Nonrelativistic Energy: Essentially exact
- Relativistic and QED Corrections:
  - α^2 Breit interaction: essentially exact
  - α^3 QED terms: essentially exact
  - α^4 Douglas and Kroll terms: essentially exact but complicated operators [recently completed by Yerokhin and Pachucki PRA 81, 022507 (2010)].
  - α^5 QED terms: can be estimated from the known hydrogenic terms.
- Final uncertainty: ± 36 MHz for the ground state ionization energy of helium. This scales roughly as $1/n^3$ with n and Z^5 with Z.

High-Z Heliumlike Ions

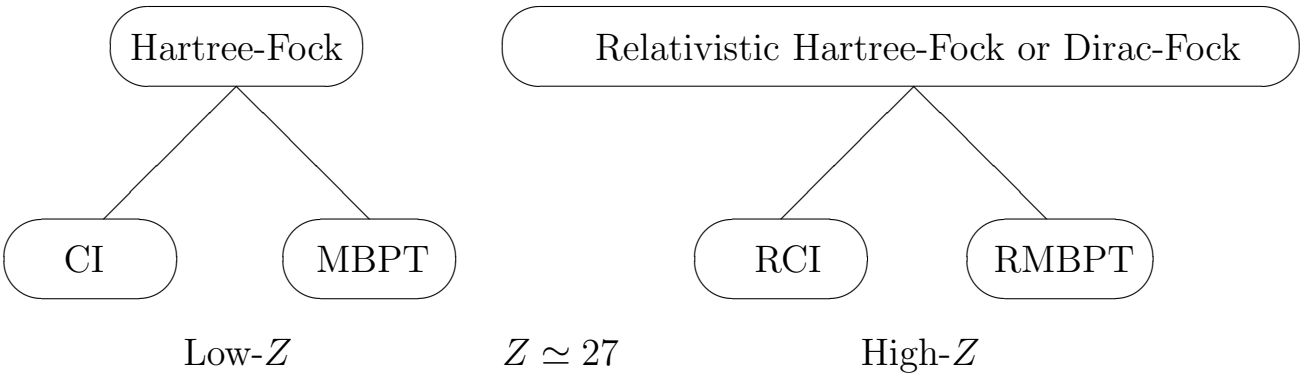
- Start from the Dirac equation and use all-orders methods to sum relativistic and QED effects to infinity.
- Dominant source of uncertainty comes from the combined effects of electron correlation and relativistic effects: leading order $(\alpha Z)^4$.
- Final uncertainty for $n = 2$ is approximately $(Z/10)^4$ cm^{-1} or ± 0.9 eV for U^{90+}.
- This is an order of magnitude larger than the one-electron QED uncertainty.

Three-electron Atoms

- High precision variational calculations in Hylleraas coordinates are still possible, but the basis sets become much larger (30,000 terms instead of 3000 terms).
- Accuracies are more limited, but spectroscopic accuracy is still possible.
- Only the ground state $1s^2 2s\ ^2S_2$ and a few excited states have been calculated in any detail.

Many-Electron Atoms

- Because of difficulties in calculating integrals in fully correlated Hylleraas coordinates $r_{12}\, r_{23}\, r_{34} \cdots$, no calculations have been done for more than three electrons.
- General methods of atomic structure are needed.



Important progress by
M.S. Safronova et al. Phys. Rev. A **90**, 042513, 052509 (2014), and
B.K. Sahoo et al. Phys. Rev. A **83**, 030503 (2011).

Methods to Estimate Uncertainties

- Study convergence as more configurations (or excitations) are added (SDTQ$\cdots$).
- Compare different methods of calculation.
- Compare with benchmark calculations of higher accuracy, or experimental data.
- Use internal consistency checks, such as length/velocity forms for radiative transitions.
- Estimate order of magnitude for higher-order terms not included in the calculation.

EQUILIVENT NONRELATIVISTIC OPERATORS

Objective: Find equivalent nonrelativistic operators whose expectation values w.r.t. nonrelativistic wave functions give the same results as relativistic operators up to a given order in powers of αZ. Called NRQED in the literature.

Once the operators are known, they can be applied to many-electron wave functions.

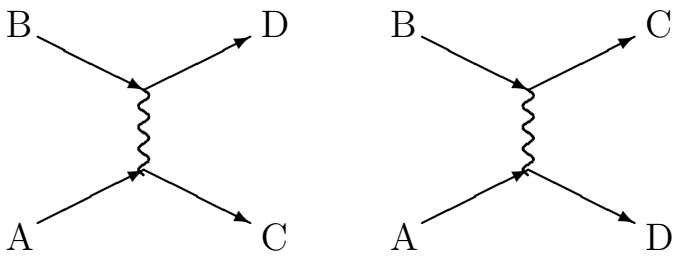
Two sources of terms:

1. Nonrelativistic reduction of the Dirac equation. The Foldy-Wouthuysen transformation provides a general procedure for transforming away the contribution of the small component of the Dirac wave function (see for example Messiah, *Quantum Mechanics Vol. II*. For example a power-series expansion of $E = (c^2p^2 + m^2c^4)^{1/2}$ yields

$$E = mc^2 + \frac{p^2}{2m} + \frac{p^4}{8m^3c^2} + \cdots \tag{1}$$

   In addition, the F.W. transformation yields the spin-orbit interaction and a δ-function term that is characteristic of the Dirac equation.

2. The electron-electron interaction, including dynamical effects due to the motion of the electrons corresponding to the Feynman diagrams



A systematic evaluation of the Feynman diagrams yields the Dirac relativistic form of the Breit interaction (see Akhiezer and Berestetskii, *Quantum Electrodynamics*, Sect. 38.1, and the Sharcnet Notes *Dirac equations 1* and

Relativistic 3.3–3.4)

$$B_{\rm D} = \frac{e^2}{r_{12}} - \frac{e^2}{2r_{12}}\left[\boldsymbol{\alpha}_1\cdot\boldsymbol{\alpha}_2 + \frac{(\boldsymbol{\alpha}_1\cdot\mathbf{r}_{12})(\boldsymbol{\alpha}_2\cdot\mathbf{r}_{12})}{r_{12}^2}\right] \tag{2}$$

Finally, use $\chi = (\boldsymbol{\sigma}\cdot\mathbf{p}/2mc)\phi$ to eliminate the small components in favour of the large components.

BREIT INTERACTION OPERATORS

The leading order relativistic corrections of order α^2 Ry, including the relativistic recoil correction of order $(m_e/M)\alpha^2$ Ry, are calculated by first-order perturbation theory

$$\Delta E_{\rm rel} = \langle\Psi_J|H_{\rm rel}|\Psi_J\rangle, \tag{3}$$

where Ψ_J is an eigenfunction of the nonrelativistic Hamiltonian (**??**) and $H_{\rm rel}$ is the relativistic correction operator defined by

$$\begin{aligned} H_{\rm rel} &= B_1 + B_2 + B_4 + B_{\rm 3Z} + B_{\rm 3e} + B_{\rm ss} + \frac{m_e}{M}\left(\tilde{\Delta}_2 + \tilde{\Delta}_{\rm 3Z}\right) \\ &\quad +\gamma\left(2B_{\rm 3Z} + \frac{4}{3}B_{\rm 3e} + \frac{2}{3}B_{3e\gamma} + 2B_{\rm ss}\right) + \gamma\frac{m_e}{M}\tilde{\Delta}_{\rm 3Z}, \end{aligned} \tag{4}$$

with $\gamma = \alpha/(2\pi) - 0.32847(\alpha/\pi)^2 + \cdots$. The terms containing γ are the corrections due to the electron anomalous magnetic moment. In the above equation,

$$B_1 = -\frac{\alpha^2}{8}\left(\nabla_1^4 + \nabla_2^4 + \nabla_3^4\right), \text{ variation of mass with velocity} \tag{5}$$

$$B_2 = \frac{\alpha^2}{2}\sum_{i>j}^{3}\left[\frac{1}{r_{ij}}\nabla_i\cdot\nabla_j + \frac{1}{r_{ij}^3}\mathbf{r}_{ij}\cdot(\mathbf{r}_{ij}\cdot\nabla_i)\nabla_j\right], \text{ orbit-orbit} \tag{6}$$

$$B_4 = \pi\alpha^2\left[\frac{Z}{2}\sum_{i=1}^{3}\delta(\mathbf{r}_i) - \sum_{i>j}^{3}(1+\frac{8}{3}\mathbf{s}_i\cdot\mathbf{s}_j)\delta(\mathbf{r}_{ij})\right], \text{ Dirac terms} \tag{7}$$

$$B_{\rm 3Z} = \frac{Z\alpha^2}{2}\sum_{i=1}^{3}\frac{1}{r_i^3}\mathbf{r}_i\times\mathbf{p}_i\cdot\mathbf{s}_i, \text{ spin-orbit} \tag{8}$$

$$B_{\rm 3e} = \frac{\alpha^2}{2}\sum_{i\neq j}^{3}\frac{1}{r_{ij}^3}\mathbf{r}_{ji}\times\mathbf{p}_i\cdot(\mathbf{s}_i + 2\mathbf{s}_j), \text{ spin-other-orbit} \tag{9}$$

$$B_{\rm ss} = \alpha^2\sum_{i>j}^{3}\left[\frac{1}{r_{ij}^3}(\mathbf{s}_i\cdot\mathbf{s}_j) - \frac{3}{r_{ij}^5}(\mathbf{r}_{ij}\cdot\mathbf{s}_i)(\mathbf{r}_{ij}\cdot\mathbf{s}_j)\right], \text{ spin-spin} \tag{10}$$

$$\tilde{\Delta}_2 = \frac{iZ\alpha^2}{2}\sum_{j=1}^{3}\left[\frac{1}{r_j}\mathbf{p}\cdot\nabla_j + \frac{1}{r_j^3}\mathbf{r}_j\cdot(\mathbf{r}_j\cdot\mathbf{p})\nabla_j\right],\ \text{Stone rel. recoil} \tag{11}$$

$$\tilde{\Delta}_{3\mathrm{z}} = Z\alpha^2\sum_{i=1}^{3}\frac{1}{r_i^3}\mathbf{r}_i\times\mathbf{p}\cdot\mathbf{s}_i,\ \text{Stone rel. recoil} \tag{12}$$

$$B_{3e\gamma} = \frac{\alpha^2}{2}\sum_{i\neq j}^{3}\frac{1}{r_{ij}^3}\mathbf{r}_{ji}\times\mathbf{p}_i\cdot(\mathbf{s}_i-\mathbf{s}_j),\ \text{anom. Mag. moment} \tag{13}$$

with $\mathbf{p} = \mathbf{p_1} + \mathbf{p_2} + \mathbf{p_3}$.

Terms involving the singular terms $\langle r_{ij}^{-2}\rangle$, $\langle r_{ij}^{-3}\rangle$ and $\langle r_i^{-3}\rangle$ involve significant computational challenges. See L. M. Wang, Chun Li Z.-C. Yan, and G. W. F. Drake, Phys. Rev. A **95**, 032504 (2017).

1 Leading-order QED corrections

The leading terms or order α^3 a.u. (or $\alpha^5 mC^2$ can be written in the form

$$E_{\mathrm{QED}} = E_{\mathrm{L},1} + E_{\mathrm{M},1} + E_{\mathrm{R},1} + E_{\mathrm{L},2} \tag{14}$$

where

- $E_{\mathrm{L},1}$ is the mass-independent part of the electron-nucleus Lamb shift (the Kabir-Salpeter term [**?**]),
- $E_{\mathrm{M},1}$ contains mass scaling and mass polarization corrections,
- $E_{\mathrm{R},1}$ contains recoil corrections (including radiative recoil),
- $E_{\mathrm{L},2}$ is the electron-electron term originally obtained by Araki [**?**] and Sucher [**?**].

For example,

$$E_{\mathrm{L},1} = \frac{4Z\alpha^3\langle\sum_i\delta(\mathbf{r}_i)\rangle^{(0)}}{3}\left\{\ln(Z\alpha)^{-2} - \beta(n\,L) + \frac{19}{30}\right\} \tag{15}$$

This is the same as the corresponding one-electron case except for the Bethe logarithm term $\beta(n\,L)$ for the two- or three-electron case, the replacement

$$\frac{Z^3}{\pi n^3} \to \sum_i \langle \delta(\mathbf{r}_i) \rangle$$

as the overall multiplying factor.

For a $1snl$ state with large l, the asymptotic expansion [36, 37]

$$\ln k_0(1snl) \sim \ln k_0(1s) + \frac{1}{n^3}\left(\frac{Z-1}{Z}\right)^4 \ln k_0(nl) + 0.316\,205(6) Z^{-6} \langle r^{-4} \rangle_{nl} + \Delta\beta(1snl) \tag{11.41}$$

becomes essentially exact. Here $\ln k_0(nl)$ is the one-electron Bethe logarithm [38] and

$$\langle r^{-4} \rangle_{nl} = \frac{16(Z-1)^4[3n^2 - l(l+1)]}{(2l-1)2l(2l+1)(2l+2)(2l+3)}. \tag{11.42}$$

The correction $\Delta\beta(1snl)$ for higher order terms is

$$\Delta\beta(1snl\ ^1\mathrm{L}) = 95.8(8)\langle r^{-6} \rangle - 845(19)\langle r^{-7} \rangle + 1406(50)\langle r^{-8} \rangle \tag{11.43}$$

$$\Delta\beta(1snl\ ^3\mathrm{L}) = 95.1(9)\langle r^{-6} \rangle - 841(23)\langle r^{-7} \rangle + 1584(60)\langle r^{-8} \rangle . \tag{11.44}$$

For example, for the $1s4f\ ^1\mathrm{F}$ state, $\beta(4\ ^1\mathrm{F}) = 2.984\,127\,1493(3)$.

Hylleraas-B-spline basis set and its application of energies, polarizability and Bethe-logarithm of helium

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Motivation

- Traditional B-spline basis has been widely used to calculate the spectrum of atomic and molecular systems. This basis has great advantages in describing low lying and continuous states. However, for the lower excited states, especially the ground state, in order to obtain sufficient precision in calculations, this basis requires a large partial-wave expansion length, which leads an unacceptable amount of computation.
- To describe the wave-function behavior at two-electron coalescences, through coupling the correlation factor $r_{12} = |\vec{r}_1 - \vec{r}_2|$ with B-spline, we constructed the Hylleraas-B-spline (H-B-spline) basis.

Hylleraas-B-spline

Helium Hamiltonian

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

where Z is the nuclear charge number.

Hylleraas-B-spline basis

$$\phi_{ijcl_1l_2}(\vec{r}_1, \vec{r}_2) = B_i(r_1)B_j(r_2)r_{12}^c\Lambda_{l_1l_2}^{LM}(\hat{r}_1, \hat{r}_2) \pm (1 \rightleftharpoons 2) \tag{2}$$

where $B_i(r)$ is the B-spline function which defined in $(0, r_{max})$, i is the serial number of B-spline, Λ is the vector coupled product of angular momenta.

Table: Comparison of the static dipole polarizabilities for the five lowest singlet and triplet states of helium. Numbers in parentheses are computational uncertainties. Units are a.u.

State	H-B-spline (length gauge)	H-B-spline (velocity gauge)	Hylleraas [4]
$1\,^1S$	1.3831921742(3)	1.3831921744(1)	1.38319217440(5)[5]
$2\,^1S$	800.3162331(1)	800.3162332(1)	800.31633(7)
$3\,^1S$	16887.18563(1)	16887.18564(1)	16887.17(1)
$4\,^1S$	135851.5811(1)	135851.5812(1)	135851.430(1)
$5\,^1S$	669586.064(1)	669586.0653(1)	669585.8982(2)
$2\,^3S$	315.63147233(5)	315.6314723632(4)	315.63147(1)
$3\,^3S$	7937.585923(3)	7937.5859256(5)	7937.58(1)
$4\,^3S$	68650.20892(2)	68650.20897(4)	68650.061(2)
$5\,^3S$	351796.228(1)	351796.2291(1)	351796.060(2)
$6\,^3S$	1314954.976(1)	1314954.979(3)	1314954.806(3)

The second and third column listed the results of polarizabilities in two gauges respectively. The different gauges results have at least 9 digits effective number. Comparing with the results in the fourth column, the results of two basis agree well with each other.

Nonrelativistic Bethe-logarithm

In the calculation of energy levels of light few body systems using NRQED approach, the Bethe-logarithm (BL) type correction terms need to be consider

f the extrapolated values are the computational uncertainties. Units are a.u.

H-B-spline [1]	B-spline [2]	Hylleraas [3]
−2.9037243771(2)	−2.9035774	−2.9037243770341195
−2.14597404608(4)	−2.1459649	−2.145974046054419(6)
−2.06127198976(3)	−2.0612681	−2.061271989740911(5)
−2.03358671705(3)	−2.0335850	−2.03358671703072(1)
−2.02117685159(3)	−2.021175	−2.021176851574363(5)
−2.17522937826(4)	−2.1752288	−2.17522937823679130
−2.068689067469(3)	−2.0686888	−2.06868906747245719
−2.0365120831(1)	−2.0365120	−2.03651208309823630(2)
−2.0226188723(1)	−2.0226188	−2.0226188723023122 7(1)
−2.0153774530(1)		−2.0153774529928621 9(3)

econd column of this table are the extrapolated value of H-B-spline under $l_{max} = 4$.). Comparing to the results of B-spline listed in the third column, especially for states, the accuracy of results is obviously improved. According to the benchmark ained by Hylleraas basis, our results arrived at least 11 digits effective number. ound state, our result has 7 effective number digits improved comparing to the asis. And in the aspect of rate of energy eigenvalues convergence, H-B-spline is ntage.

Dipole polarizabilities

ipole polarizability for an atom is defined by (in length gauge)

$$\alpha_l^l = 2e^2\Sigma' \frac{|\langle\psi_0|Z|\psi_n\rangle|^2}{(E_n - E_0)} \tag{3}$$

s the direction of electric field. Using $[H, p_i] = r_i$, one can get the dipole polariz- elocity gauge.

$$\alpha_l^v = 2e^2\Sigma' \frac{|\langle\psi_0|p_z|\psi_n\rangle|^2}{(E_n - E_0)^3} \tag{4}$$

calculations of helium polarizabilities, pseudo-states-sum-over approach is effec- eraas-B-spline basis can simultaneously describe higher and lower excited states following table contains the results of helium static polarizabilities in two gauges. See the following table.

Table: Comparison of nonrelativistic BL for $n\,^{1,3}S$, n up to 6, states of helium. Numbers in parentheses are computational uncertainties. Units are a.u.

State	H-B-spline	Hylleraas [6]	$1/n$ *expansion* [7]
$1\,^1S$	4.370159(1)	4.370160218(3)	
$2\,^1S$	4.3664123(1)	4.36641272(7)	4.3664127
$3\,^1S$	4.3691644(2)	4.369164871(8)	4.3691648
$4\,^1S$	4.3698902(3)	4.36989066(1)	4.3698906
$5\,^1S$	4.3701514(3)	4.3701516(1)	4.3701520
$6\,^1S$	4.3702666(3)		4.3702673
$2\,^3S$	4.364036*4(1)*	4.36403682(1)	4.3640354
$3\,^3S$	4.368666*6(1)*	4.36866692(2)	4.3686665
$4\,^3S$	4.369723*0(2)*	4.36972344(5)	4.3697229
$5\,^3S$	4.3700782(2)	4.37007831(8)	4.3700791
$6\,^3S$	4.370228*6(4)*		4.3702300

Acknowledgments

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Bethe logarithm for the helium atom

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The Bethe logarithm for a large set of states of the helium atom is calculated with a precision of 12–14 significant digits. The numerical data are obtained for the case of infinite mass of a nucleus. Then we study the mass dependence and provide coefficients of the m_e/M expansion, which allows us to calculate accurate values for the Bethe logarithm for any finite mass. An asymptotic expansion for the Rydberg states is analyzed, and a high-quality numerical approximation is found, which ensures 7–8-digit accuracy for the S, P, and D states of the helium atom.

TABLE I. The Bethe logarithm calculations for the ground and excited states of the helium atom with infinite nuclear mass $M_{\mathrm{He}} \to +\infty$ and comparison with most precise previous calculations.

n	$n\,^1S$	$n\,^3S$	$n\,^1P$	$n\,^3P$
1	4.370 160 223 0703(3)			
	4.370 160 218(3)[a]			
	4.370 160 222 9(1)[b]			
	4.370 160 223 06(2)[c]			
2	4.366 412 726 417(1)	4.364 036 820 476(1)	4.370 097 743 554(2)	4.369 985 364 549(3)
	4.366 412 72(7)[a]	4.364 036 82(1)[a]	4.370 097 82(3)[a]	4.369 985 20(2)[a]
	4.366 412 726 2(1)[b]	4.364 036 820 41(2)[b]	4.370 097 743 5(1)[b]	4.369 985 364 4(2)[b]
3	4.369 164 860 824(2)	4.368 666 996 159(2)	4.370 295 862 299(4)	4.370 235 654 775(4)
	4.369 164 871(8)[a]	4.368 666 92(2)[a]	4.370 295 75(9)[a]	4.370 233 9(2)[a]
4	4.369 890 632 356(3)	4.369 723 392 715(4)	4.370 363 160 331(5)	4.370 334 604 477(5)
	4.369 890 66(1)[a]	4.369 723 44(5)[a]	4.370 363 2(2)[a]	4.370 334 16(5)[a]
5	4.370 151 796 310(4)	4.370 078 509 668(4)	4.370 390 514 367(5)	4.370 375 352 464(5)
	4.370 151 7(1)[a]	4.370 078 31(8)[a]	4.370 390 54(4)[a]	4.370 374 6(2)[a]
6	4.370 266 974 319(5)	4.370 229 062 747(5)	4.370 403 502 993(6)	4.370 394 624 37(2)
7	4.370 325 261 772(5)	4.370 303 319 792(5)		
n	$n\,^1D$	$n\,^3D$	$n\,^1F$	$n\,^3F$
3	4.370 413 478 422(3)	4.370 420 247 640(2)		
	4.370 413 470(7)[d]	4.370 420 247(2)[c]		
4	4.370 417 339 045(4)	4.370 421 238 038(4)	4.370 421 511 306(3)	4.370 421 527 144(3)
5	4.370 419 597 74(2)	4.370 421 809 90(2)		

[a]Drake and Goldman [8].
[b]Yerokhin and Pachucki [19].
[c]Korobov [16].
[d]Wienczek *et al.* [20].

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Testing fundamental interactions on the helium atom

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We critically examine the current status of theoretical calculations of the energies, the fine structure, and the isotope shift of the lowest-lying states of helium, searching for unresolved discrepancies with experiments. Calculations are performed within the quantum electrodynamics expansion in powers of the fine structure constant α and the electron-to-nucleus mass ratio m/M. For energies, theoretical results are complete through orders $\alpha^6 m$ and $\alpha^6 m^2/M$, with the resulting accuracy ranging from 0.5 to 2 MHz for the $n = 2$ states. The fine-structure splitting of the $2\,^3P$ state is predicted with a much better accuracy, 1.7 kHz, as a consequence of a calculation of the next-order $\alpha^7 m$ effect. An excellent agreement of the theoretical predictions with the recent measurements of the fine structure provides one of the best tests of the bound-state QED in few-electron systems. The isotope shift between ^{3}He and ^{4}He is treated with a subkilohertz accuracy, which allows for a high-precision determination of the differences of the nuclear charge radii δr^2. Several such determinations, however, yield results that are in a 4σ disagreement with each other, which remains unexplained. Apart from this, we find no significant discrepancies between theory and experiment for the helium atom. A further calculation of the yet unknown $\alpha^7 m$ correction to energy levels will provide a sensitive test of universality in electromagnetic interactions of leptons by comparison of nuclear charge radii obtained by the helium and muonic helium spectroscopy.

TABLE II. Comparison of the theoretical predictions for various transitions in ^{4}He with the experimental results, in MHz. IE denotes the ionization energy.

	Experiment/Theory/Difference	Ref.
1^1S_0 (IE)	5 945 204 212. (6)	[26]
	5 945 204 173. (36.)	
	39. (36.)	
2^1S_0 (IE)	960 332 041.01(15)	[27]
	960 332 038.0 (1.9)	
	3.0(1.9)	
1^1S_0–2^1S_0	4 984 872 315. (48.)	[28]
	4 984 872 135. (36.)	
	180. (60.)	
2^3S_1–3^3D_1	786 823 850.002 (56)	[29]
	786 823 848.4 (1.3)[a]	
	1.6 (1.3)	
2^1S_0–2^1P_1	145 622 892.886 (183)	[30]
	145 622 891.5(2.3)	
	1.4(2.3)	
2^1P_1–3^1D_2	448 791 399.113 (268)	[31]
	448 791 397.4(0.4)[b]	
	1.7(0.5)	
2^3P_0–3^3D_1	510 059 755.352 (28)	[32]
	510 059 754.0 (0.7)[a]	
	1.4 (0.7)[a]	
2^3P–2^3S_1	276 736 495.649 (2)[c]	[33]
	276 736 495.4 (2.0)	
	0.2 (2.0)	
2^3S_1–2^1P_1	338 133 594.4 (5)	[34]
	338 133 594.9 (1.4)	
	−0.5 (2.2)	
2^1S_0–2^3S_1	192 510 702.145 6 (18)	[35]
	192 510 703.4 (0.8)	
	−1.3 (0.8)	

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TABLE IV. Comparison of the theoretical predictions for the 2^3P fine-structure intervals of ^{4}He with the experimental results, in kHz.

	2^3P_0–2^3P_2	2^3P_1–2^3P_2	2^3P_0–2^3P_1
Theory			
Pachucki and Yerokhin [22]	31 908 131.4 (1.7)	2 291 178.9 (1.7)	29 616 952.5 (1.7)
Experiment			
Zheng *et al.* [46]	31 908 130.98 (13)	2 291 177.56 (19)	
Feng *et al.* [47]		2 291 177.69 (36)	
Smiciklas *et al.* [48]	31 908 131.25 (30)		
Smiciklas *et al.* [48] reevaluated in Ref. [45]	31 908 131.25 (32)		
Borbely *et al.* [49]		2 291 177.53 (35)	
Borbely *et al.* [49] reevaluated in Ref. [45]		2 291 177.55 (35)	
Zelevinsky *et al.* [50]	31 908 126.8 (0.9)	2 291 175.6 (0.5)	29 616 951.7 (0.7)
Zelevinsky *et al.* [50] reevaluated in Ref. [45]	31 908 126.8 (3.0)	2 291 176.8 (1.1)	29 616 951.7 (3.0)
Guisfredi *et al.* [51]			29 616 952.7 (1.0)
Guisfredi *et al.* [51] reevaluated in Ref. [45]			29 616 953. (10.0)
George *et al.* [52]			29 616 950.9 (0.9)
George *et al.* [52] reevaluated in Ref. [45]			29 616 950.8 (0.9)
Castillega *et al.* [53]		2 291 175.9 (1.0)	
Castillega *et al.* [53] reevaluated in Ref. [45]		2 291 177.1 (1.0)	

Ultrahigh-Precision Measurement of the $n=2$ Triplet P Fine Structure of Atomic Helium Using Frequency-Offset Separated Oscillatory Fields

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For decades, improved theory and experiment of the $n = 2\ ^3P$ fine structure of helium have allowed for increasingly precise tests of quantum electrodynamics, determinations of the fine-structure constant α, and limitations on possible beyond-the-standard-model physics. Here we use the new frequency-offset separated-oscillatory-fields technique to measure the $2^3P_2 \rightarrow 2^3P_1$ interval. Our result of 2 291 176 590(25) Hz represents a major step forward in precision for helium fine-structure measurements.

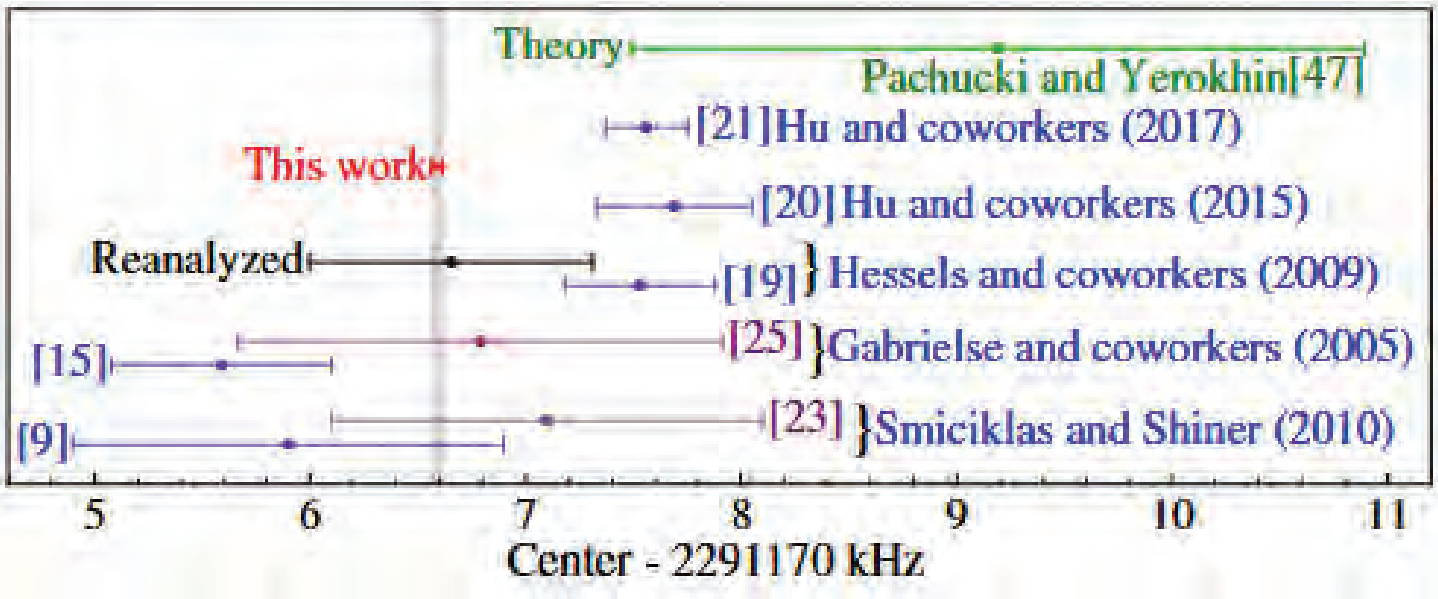

TABLE V. Determinations of the nuclear charge difference of ^{3}He and ^{4}He, $\delta r^2 \equiv r^2(^3\mathrm{He}) - r^2(^4\mathrm{He})$ from different measurements. Units are kHz if not stated otherwise. δE is the part of the isotope shift induced by the finite nuclear size, represented as $\delta E = C\,\delta r^2$, with C being the coefficient calculated from theory.

Determination from Rooij *et al.* [35]		
$E(^3\mathrm{He}, 2\,^1S^{F=1/2} - 2\,^3S^{F=3/2}) - E(^4\mathrm{He}, 2\,^1S - 2\,^3S)$	−5 787 719.2(2.4)	Expt. [35]
$\delta E_{\mathrm{hfs}}(2\,^3S^{3/2})$	−2 246 567.059(5)	Expt. [57,58]
$-\delta E_{\mathrm{iso}}(2\,^1S - 2\,^3S)$ (point nucleus)	8 034 065.91 (19)	Theory [20,21]
δE	−220.4(2.4)	
C	−214.66 (2) kHz/fm^2	[14]
δr^2	1.027 (11) fm^2	[21]
Determination from Cancio Pastor *et al.* [33,55]		
$E(^3\mathrm{He}, 2\,^3P - 2S)$ (centroid)	276 702 827 204.8 (2.4)	Expt. [55]
$-E(^4\mathrm{He}, 2\,^3P - 2S)$ (centroid)	−276 736 495 649.5 (2.1)	Expt. [33,48]*
$-\delta E_{\mathrm{iso}}(2\,^3P - 2\,^3S)$ (point nucleus)	33 667 149.3 (0.9)	Theory [20,21]
δE	−1 295.4 (3.3)	
C	−1212.2 (1) kHz/fm^2	[14]
δr^2	1.069 (3) fm^2	[20]
Determination from Shiner *et al.* [56]		
$E(^3\mathrm{He}, 2\,^3P_0{}^{1/2} - 2\,^3S_1{}^{3/2}) - E(^4\mathrm{He}, 2\,^3P_2 - 2\,^3S_1)$	810 599.0 (3.0)	Expt. [56]
$\delta E_{\mathrm{hfs}}(2\,^3S_1{}^{3/2})$	−2 246 567.059 (5)	Expt. [57,58]
$\delta E_{\mathrm{fs}}(2\,^3P_2)$	−4 309 074.2 (1.7)	Theory [22]
$-\delta E_{\mathrm{fs,hfs}}(2\,^3P_0{}^{1/2})$	−27 923 393.7 (1.7)	Theory [20,21]
$-\delta E_{\mathrm{iso}}(2\,^3P - 2\,^3S)$ (point nucleus)	33 667 149.3 (0.9)	Theory [20,21]
δE	−1286.7 (3.5)	
C	−1212.2 (1) kHz/fm^2	[14]
δr^2	1.061 (3) fm^2	[20]

*The centroid energy E is obtained as $E = (6\,E_0 + 3\,E_1 - 5\,E_{02})/9$, where $E_{0,1} \equiv E(2\,^3S_1 - 2\,^3P_{0,1})$ from Ref. [33] and $E_{02} \equiv E(2\,^3P_0 - 2\,^3P_2)$ from Ref. [48].

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Higher-order recoil corrections for singlet states of the helium atom

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We investigate the finite nuclear mass corrections in the helium atom in order to resolve a significant disagreement between the $2\,^3S$-$2\,^3P$ and $2\,^3S$-$2\,^1S$ transition isotope shifts. These two transitions lead to discrepant results for the nuclear charge radii difference between ^{4}He and ^{3}He. The accurate treatment of the finite nuclear mass effects is quite complicated and requires the use of the quantum field theoretical approach. We derive the $\alpha^6\, m^2/M$ correction with the help of nonrelativistic QED and dimensional regularization of the three-body Coulombic system and present accurate numerical results for low-lying states. The previously reported $4\,\sigma$ discrepancy in the nuclear charge radius difference between ^{3}He and ^{4}He from two different atomic isotope shift transitions is confirmed, which calls for verification of experimental transition frequencies.

TABLE VII. Determination of the nuclear charge difference δr^2 from the measurement by van Rooij *et al.* in Ref. [11], in kHz.

$E(^3\mathrm{He}, 2\,^1S^{F=1/2}\text{-}2\,^3S^{F=3/2}) - E(^4\mathrm{He}, 2\,^1S\text{-}2\,^3S)$	−5 787 719.2(2.4)	Ref. [11]
$\delta E_{\mathrm{hfs}}(2\,^3S^{3/2})$	−2 246 567.059(5)	Refs. [19,20]
$-\delta E_{\mathrm{iso}}(2\,^1S\text{-}2\,^3S)$ (point nucleus)	8 034 065.91(19)	Theory, Table VI
δE	−220.4(2.4)	
C	−214.66(2) kHz/fm^2	Ref. [7]
$\delta r^2 = r^2(^3\mathrm{He}) - r^2(^4\mathrm{He})$	1.027(11) fm^2	

TABLE I. Expectation values of operators Q_i with $i = 1, \ldots, 30$ for the $1\,^1S_0$, $2\,^1S_0$, and $2\,^1P_1$ states.

	$1\,^1S_0$	$2\,^1S_0$	$2\,^1P_1$
$Q_1 = 4\pi\delta^3(r_1)$	22.750 526	16.455 169	16.014 493
$Q_2 = 4\pi\delta^3(r)$	1.336 375	0.108 679	0.009 238
$Q_3 = 4\pi\delta^3(r_1)/r_2$	33.440 565	5.593 743	3.934 081
$Q_4 = 4\pi\delta^3(r_1)\,p_2^2$	49.160 046	7.578 158	3.866 237
$Q_5 = 4\pi\delta^3(r)/r_1$	5.019 713	0.440 864	0.012 785
$Q_6 = 4\pi\,\delta^3(r)\,P^2$	18.859 765	1.800 294	0.070 787
$Q_7 = 1/r$	0.945 818	0.249 683	0.245 024
$Q_8 = 1/r^2$	1.464 771	0.143 725	0.085 798
$Q_9 = 1/r^3$	0.989 274	0.067 947	0.042 405
$Q_{10} = 1/r^4$	−3.336 384	−0.312 402	0.008 956
$Q_{11} = 1/r_1^2$	6.017 409	4.146 939	4.043 035
$Q_{12} = 1/(r_1 r_2)$	2.708 655	0.561 861	0.491 245
$Q_{13} = 1/(r_1 r)$	1.920 944	0.340 634	0.285 360
$Q_{14} = 1/(r_1 r_2 r)$	4.167 175	0.398 366	0.159 885
$Q_{15} = 1/(r_1^2 r_2)$	9.172 094	1.472 014	1.063 079
$Q_{16} = 1/(r_1^2 r)$	8.003 454	1.348 761	1.002 157
$Q_{17} = 1/(r_1 r^2)$	3.788 791	0.337 891	0.105 081
$Q_{18} = (\vec{r}_1 \cdot \vec{r})/(r_1^3 r^3)$	3.270 472	0.278 353	0.010 472
$Q_{19} = (\vec{r}_1 \cdot \vec{r})/(r_1^3 r^2)$	1.827 027	0.159 078	0.043 524
$Q_{20} = r_1^i r_2^j (r^i r^j - 3\delta^{ij} r^2)/(r_1^3 r_2^3 r)$	0.784 425	0.063 677	−0.004 747
$Q_{21} = p_2^2/r_1^2$	14.111 960	2.064 285	1.127 058
$Q_{22} = \vec{p}_1/r_1^2\,\vec{p}_1$	21.833 598	16.459 209	16.067 214
$Q_{23} = \vec{p}_1/r^2\,\vec{p}_1$	4.571 652	0.499 768	0.190 797
$Q_{24} = p_1^i\,(r^i r^j + \delta^{ij} r^2)/(r_1 r^3)\,p_2^j$	0.811 933	0.065 354	0.053 432
$Q_{25} = P^i\,(3r^i r^j - \delta^{ij} r^2)/r^5\,P^j$	−3.765 488	−0.252 967	0.013 743
$Q_{26} = p_2^k\,r_1^i/r_1^3(\delta^{jk} r^i/r - \delta^{ik} r^j/r - \delta^{ij} r^k/r - r^i r^j r^k/r^3)\,p_2^j$	−0.266 894	−0.038 928	−0.039 976
$Q_{27} = p_1^2\,p_2^2$	7.133 710	1.428 213	0.973 055
$Q_{28} = p_1^2/r_1\,p_2^2$	37.010 643	5.955 767	3.102 248
$Q_{29} = \vec{p}_1 \times \vec{p}_2/r\,\vec{p}_1 \times \vec{p}_2$	4.004 703	0.638 960	0.216 869
$Q_{30} = p_1^k\,p_2^l\,(-\delta^{jl} r^i r^k/r^3 - \delta^{ik} r^j r^l/r^3 + 3r^i r^j r^k r^l/r^5)\,p_1^i\,p_2^j$	−1.591 864	−0.252 663	−0.126 416

Quantum-electrodynamic corrections to the $1s3d$ states of the helium atom

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We perform quantum-electrodynamic calculations of the ionization energy of the $1s3d$ states of the ^{4}He atom, including a complete evaluation of the $m\alpha^6$ correction. We find a large contribution from the nonradiative part of this correction, which has not been accounted for in previous investigations. The additional contribution shifts theoretical predictions for ionization energies by about 10σ. Despite this shift, we confirm the previously reported systematic deviations between measured experimental results and theoretical predictions for transitions involving $3D$ states. The reason for these deviations remains unknown.

Drake & Morton (2006)

TABLE VII. Comparison of different theoretical predictions with experimental results for various transition energies in ^{4}He, in MHz. Theoretical ionization energies of the $n = 2$ states in the column "Present theory" are taken from Ref. [5].

	Experiment	Ref.	Present theory	Difference from experiment	Other theory [9]	Difference from experiment
			$3L'$–$2L$ transitions			
$3\,^1D_2$–$2\,^1S_0$	594 414 291.803 (13)	[20]	594 414 289.3 (1.9)	2.5 (1.9)	594 414 292. (5.)	0. (5.)
$3\,^3D_1$–$2\,^3S_1$	786 823 850.002 (56)	[25]	786 823 848.7 (1.3)	1.3 (1.3)	786 823 845. (7.)	4. (7.)
$3\,^3D_1$–$2\,^3P_0$	510 059 755.352 (28)	[22]	510 059 754.2 (0.7)	1.2 (0.7)	510 059 749. (2.)	6. (2.)
$3\,^1D_2$–$2\,^1P_1$	448 791 399.113 (268)	[26]	448 791 397.8 (0.4)	1.3 (0.5)	448 791 400.5 (2)	−1.4 (2)
			$2L'$–$2L$ transitions			
$2\,^3P_0$–$2\,^3S_1$	276 764 094.657 2 (14)	[3]	276 764 094.5 (2.0)	0.2 (2.0)	276 764 096. (7.)	2. (7.)
$2\,^1S_0$–$2\,^3S_1$	192 510 702.148 72 (20)	[21]	192 510 703.4 (0.8)	−1.3 (0.8)	192 510 697. (9.)	5. (9.)
$2\,^1P_1$–$2\,^1S_0$	145 622 892.886 (183)	[27]	145 622 891.5 (2.3)	1.4 (2.3)	145 622 892. (5.)	0. (5.)
$2\,^1P_1$–$2\,^3S_1$	338 133 594.4 (5)	[28]	338 133 594.9 (1.4)	−0.5 (2.2)	338 133 589. (7.)	5. (7.)
			$3L'$–$3L$ transitions			
$3\,^1D_2$–$3\,^3D_1$	101 143.943 (31)	[3,20–22]	101 144.029 (23)	0.086 (37)	101 143.95 (3)	0.01 (4)

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Isotope shifts and transition frequencies for the S and P states of lithium: Bethe logarithms and second-order relativistic recoil

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Isotope shifts and total transition frequencies are calculated for the 2^2S-3^2S transition of the lithium isotopes ^{6}Li, ^{7}Li, ^{8}Li, ^{9}Li, and the halo nucleus ^{11}Li. The accuracy is improved for previously calculated relativistic and quantum electrodynamic corrections, and in particular a disagreement for the Bethe logarithm is resolved for the ground ^2S state. Our previous result is confirmed for the 2^2P state. We use the pseudostate expansion method to perform the sum over virtual intermediate states. Results for the second-order relativistic recoil term of order $\alpha^2(\mu/M)^2$ Ry are shown to make a significant contribution relative to the theoretical uncertainty, but because of accidental cancellations the final result for the isotope shift is nearly unchanged. However, the spin-orbit term makes an unexpectedly large contribution to the splitting isotope shift (SIS) for the $2^2P_{1/2}$-$2^2P_{3/2}$ fine structure, increasing the theoretical value for the ^{6}Li-^{7}Li isotopes to 0.556 31(7) ± 0.001 MHz. A comparison is made with high-precision measurements and other calculations for the SIS and for the total 2^2S-3^2S transition frequency.

TABLE IV. Bethe logarithms for $1s^2 2s\,^2S$, $1s^2 3s\,^2S$, and $1s^2 2p\,^2P$ states of lithium, expressed in the form $\beta = \beta^{(0)} + (\mu/M)\beta^{(1)} + \ln(Z^2\mu/m_e)$.

N_1	N_2	$\beta^{(0)}$	$R(\Omega)$	$\beta^{(1)}$	$R(\Omega)$
		$1s^2 2s\,^2S$			
3910	1452	2.980 833 469	9.587	0.113 790 737	15.526
3910	2445	2.980 923 592	8.791	0.113 793 610	17.772
3910	4109	2.980 937 643	6.414	0.113 801 327	0.372
3910	6809	2.980 941 416	3.724	0.113 809 084	0.995
∞		2.980 943(1)		0.113 81(1)	
Yan *et al.* [24]		2.980 925(3)		0.113 6(2)	
Yan *et al.* [6]		2.981 06(1)		0.113 05(5)	
Puchalski *et al.* [7]		2.980 944(4)		0.113 81(3)	
Stanke *et al.* [27]		2.980 93			
		$1s^2 3s\,^2S$			
3910	2445	2.982 187 350	8.908	0.110 628 587	–0.1989
3910	4109	2.982 209 101	10.29	0.110 549 049	2.372
3910	6809	2.982 210 691	13.68	0.110 520 286	2.764
∞		2.982 210(1)		0.110 50(2)	
Yan *et al.* [24]		2.982 40(4)		0.111(1)	
Yan *et al.* [6]		2.982 36(6)		0.110 5(3)	
Stanke *et al.* [27]		2.982 12			
		$1s^2 2p\,^2P$			
4172	6070	2.982 243 400	5.902	0.111 183 023	3.726
4172	10735	2.982 549 536	6.435	0.111 118 489	6.697
4172	18708	2.982 565 711	7.142	0.111 109 241	6.978
∞		2.982 568(3)		0.111 107(2)	
Yan *et al.* [6]		2.982 57(6)		0.111 08(5)	
Puchalski *et al.* [7]		2.982 58(7)		0.111 3(5)	

TABLE XI. ^{6}Li-^{7}Li isotope shift in the $2\,^2P_{3/2}$-$2\,^2P_{1/2}$ finestructure splitting (SIS). Anom. is the anomalous magnetic moment contribution. All values are in MHz.

Term	Present work	Puchalski *et al.* [7]
$\alpha^2\lambda$	0.385 38(1)	0.397 5(6)
$\alpha^2\lambda^2$	0.023 94(7)	
Anom.	0.000 638	
Mixing [7]	0.146 99	0.146 99
Total	0.556 31(7)± 0.001[a]	0.544 7(1)± 0.001[a]
	Recent Experiment	
Sansonetti *et al.* [42]	0.594(30)	
Brown *et al.* [36]	0.531(24)[b]	

[a]Additional uncertainty due to higher-order QED terms of order $\alpha^4\lambda$ Ry is not included in the calculation.
[b]Includes the effects of quantum interference between unresolvable overlapping lines and laser polarization.

Theoretical contributions to the $1s^2 2s\ ^2S - 1s^2 3s\ ^2S$ transition energy (cm^{-1}) of ^{7}Li [Yan & Drake 2008, Puchalski et al. 2010], and comparison with experiment [Sanchez et al. 2006]. $\mu/M \simeq 7.820 \times 10^{-5}$ is the ratio of the reduced electron mass to the nuclear mass for an atomic mass, and $\alpha \simeq 1/137$ is the fine structure constant.

Contribution	Transition Energy (cm^{-1})
Infinite mass	27 206.492 847 9(5)
μ/M	–2.295 854 362(2)
$\mu/M)^2$	0.000 165 9774
α^2	2.089 120(23)
$\alpha^2\mu/M$	–0.000 003 457(9)
α^3	–0.187 03(26)
$\alpha^3\mu/M$	0.000 009 74(13)
α^4 (Est.)	–0.005 7(6)
α^5 (Est.)	0.000 52(13)
Nucl. size	–0.000 390(10)
Total	27 206.093 7(6)
Exp't. [**?**]	27 206.094 082(6)

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