High Precision Atomic Theory for Li and Be$^+$: QED Shifts and Isotope Shifts

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High-precision results are presented for calculations of the nonrelativistic energies, relativistic corrections, and quantum electrodynamic corrections for the $2\,^2S$, $2\,^2P$, and $3\,^2S$ states of Li and Be$^+$, using nonrelativistic wave functions expressed in Hylleraas coordinates. Bethe logarithms are obtained for the states of Be$^+$. Finite mass corrections are calculated with sufficient accuracy to extract the nuclear charge radius from measurements of the isotope shift for the $2\,^2S - 2\,^2P$ and $2\,^2S - 3\,^2S$ transitions. The calculated ionization potential for Be$^+$ is $146\,882.923 \pm 0.005$ cm^{-1}.

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The past few years have seen remarkable advances in our ability to achieve spectroscopic accuracy for the energies and transition frequencies of lithium and the lithiumlike ions (or more generally four-body systems). The dominant sources of uncertainty are the higher-order quantum electrodynamic (QED) corrections, rather than the accuracy of calculations for the basic nonrelativistic energy and leading relativistic corrections. This work builds on the much longer history of high-precision calculations for helium and other three-body systems [1–3]. Here we present results suitable for the interpretation of QED shifts and isotope shifts in Li and Be$^+$

The key to obtaining high-precision results that are essentially exact for all practical purposes (in the sense that hydrogenic wave functions and energies are "exact") is the use of explicitly correlated variational wave functions in Hylleraas coordinates. This is a specialized method that has been fully implemented only for the two- and three-electron cases [4–6]. The results are more accurate by many orders of magnitude than the well-known and generally applicable methods of atomic physics, such as configuration interaction. The high accuracy opens the possibility of using the results in combination with high-precision experiments to create unique measurement tools. A prime example is the use of the calculated isotope shift in combination with isotope shift measurements to determine the nuclear charge radius of short-lived halo nuclei such as ^{6}He, ^{8}He, and ^{11}Li [7,8]. New experiments are in progress at GSI [9] and at RIKEN [10] for ^{11}Be$^+$, where the isotope shift in the $2\,^2S_{1/2} - 2\,^2P_J$ transitions will be used. Another example is the testing of the higher-order relativistic and QED corrections to the transition frequencies in atomic systems more complicated than hydrogen. The theory of these effects is still under active development [11–13]. The Bethe logarithm that appears in the lowest-order electron self-energy [14,15] remains one of the most difficult parts of the calculation.

In a previous sequence of papers [1,16–19], we have obtained high-precision results for transitions among the $2\,^2S_{1/2}$, $2\,^2P_J$, and $3\,^2S_{1/2}$ states of lithium. More recently, Puchalski *et al.* [20] have confirmed these results and improved the accuracy of the relativistic recoil corrections. They have also obtained a significant correction to the isotope shift in the case of ^{11}Li due to nuclear polarization. In the present work, we present high-precision results for the low-lying states of Be$^+$. The results will form the theoretical basis for the interpretation of the planned isotope shift measurements [9,10] in terms of the nuclear charge radius for the radioactive isotopes ^{7}Be, ^{10}Be, and ^{11}Be relative to stable ^{9}Be. The ^{11}Be case is especially important and interesting because it is the simplest example of a halo nucleus containing just a single halo neutron. We also improve our previous results for Li by using much larger basis sets containing up to 9577 terms, and by implementing an absolutely convergent method [21] to eliminate numerical instabilities in the calculation of slowly convergent integrals required for the $\langle p^4\rangle$ term in the Breit interaction. This brings our results into agreement with those of Pachucki *et al.* [20] for Li.

For our purposes, the three key parameters controlling the energy levels are α, λ, and $\bar{r}_c$, where α is the fine structure constant, $\lambda = \mu/M \equiv m/(m+M)$ is the ratio of the reduced electron mass to the nuclear mass, and $\bar{r}_c$ is the rms nuclear charge radius for a particular isotope. 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

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

in units of $\alpha^2\mu c^2 = \alpha^2(1-\lambda)mc^2$, where the subscripts denote the nonrelativistic energy (NR), relativistic corrections (rel), quantum electrodynamic corrections (QED), higher-order QED corrections (ho), and finite nuclear size corrections (nuc). The factor of $1-\lambda$ accounts for the normal isotope shift.

There are two contexts in which this equation can be applied. First, for total transition frequencies, the dominant source of uncertainty comes from the higher-order QED term $\alpha^4\mathcal{E}^{(0)}_{\rm ho}$, where here and throughout the superscript denotes the power of λ. A comparison with experiment therefore provides an effective measurement of this term, assuming that the lower-order terms are known to sufficient accuracy. Second, for isotope shifts, the terms independent of λ do not contribute (except for the last $\bar{r}_c^2$ term), and the term $\alpha^4\lambda\mathcal{E}^{(1)}_{\rm ho}$ contributes only at the level of a few kHz, and so a simple one-electron estimate is sufficient. To sufficient accuracy, the expression for the isotope shift between isotopes A and B in the same atomic state is then

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

where $\lambda_\pm = (\mu/M)_B \pm (\mu/M)_A$. Since all coefficients can now be calculated to sufficient accuracy, it is clear that the difference between theory and experiment for the isotope shift in a particular atomic transition (without the $\bar{r}_c$ terms) yields the rms nuclear charge radius for isotope B relative to a known isotope A.

The expansion coefficients in Eq. (1) all have a simple physical meaning. $\mathcal{E}^{(0)}_{\rm NR}$ is the eigenvalue corresponding to the Schrödinger equation for infinite nuclear mass, and $\lambda\mathcal{E}^{(1)}_{\rm NR}$ and $\lambda^2\mathcal{E}^{(2)}_{\rm NR}$ are the first- and second-order perturbation corrections due to the mass polarization operator $H_{\rm MP} = -\lambda\sum_{i>j}^{3}\nabla_i\cdot\nabla_j$ contained in the total Hamiltonian $H = H^{(0)} + H_{\rm MP}$. The leading relativistic term $\alpha^2\mathcal{E}^{(0)}_{\rm rel}$ follows from the matrix element $\langle\Psi^{(0)}|B|\Psi^{(0)}\rangle$, where B is the usual Breit interaction [17] and $\Psi^{(0)}$ is the wave function for infinite nuclear mass. The relativistic finite mass correction term $\alpha^2\lambda\mathcal{E}^{(1)}_{\rm rel}$ contains contributions from (a) the mass scaling of the terms in B, (b) perturbative corrections to the wave function $\Psi^{(0)}$ due to the mass polarization operator, and (c) recoil corrections resulting from the transformation of the Breit interaction to center-of-mass plus relative coordinates, as first derived by Stone [22] (see Yan and Drake [17]). This term is not so well known, and is often neglected in atomic structure calculations.

The leading QED term $\alpha^3\mathcal{E}^{(0)}_{\rm QED}$ consists of both an electron-nucleus contribution and an electron-electron contribution, denoted previously by $E^{(0)}_{L,1}$ and $E^{(0)}_{L,2}$ [18,19]. The calculation of these terms is straightforward, with the exception of the Bethe logarithm contained in the expression

$$E^{(0)}_{L,1} = \frac{4}{3}Z\alpha^3\langle\delta(\mathbf{r}_i)\rangle^{(0)}\left[\ln(Z\alpha)^{-2} - \beta^{(0)}(nL) + \frac{19}{30}\right], \tag{3}$$

where $\beta^{(0)}(nL) \equiv \ln(k_0/Z^2R_\infty)$ is Bethe's mean excitation energy for the $n\,^2L$ state in question for infinite nuclear mass, and a sum over $i = 1, 2, 3$ is assumed. It is difficult to calculate because it involves virtual excitations summed over all intermediate states, with the dominant contributions lying high in the photoionization continuum. We have recently solved this problem for the cases of helium [15] and lithium [19] by introducing a discrete variational basis set for the intermediate pseudostates that spans a huge range of distance scales. Our results for Be$^+$ are further discussed below.

The finite mass term $\alpha^3\mathcal{E}^{(1)}_{\rm QED}$ contains all the reduced mass and recoil corrections $E^{(1)}_{L,1}$ and $E^{(1)}_{L,2}$ to be expected from $E^{(0)}_{L,1}$ and $E^{(0)}_{L,2}$, as well as radiative recoil terms as discussed previously [18,23]. These are all straightforward to calculate with the exception of the finite mass correction $\beta^{(1)}(nL)$ as further discussed below. The higher-order QED terms $\alpha^4\mathcal{E}^{(0)}_{\rm ho}$ and the finite mass corrections $\alpha^4\mathcal{E}^{(1)}_{\rm ho}$ are estimated from the dominant hydrogenic terms, corrected for the electron density at the nucleus, as described in detail previously [18,20]. Finally, the finite nuclear size correction is given by

$$\bar{r}_c^2\mathcal{E}^{(0)}_{\rm nuc} = \frac{2\pi Ze^2}{3}\bar{r}_c^2\langle\delta(\mathbf{r}_i)\rangle^{(0)} \tag{4}$$

together with a negligibly small finite mass correction.

The method of generating the wave functions is the same as the multiple basis set method originally developed by Yan and Drake [16], and subsequently used in a sequence of other papers, including the recent work by Puchalski and Pachucki [5]. The key idea is to start with a fully correlated variational basis set in Hylleraas coordinates of the form

$$r_1^{j_1}r_2^{j_2}r_3^{j_3}r_{12}^{j_{12}}r_{23}^{j_{23}}r_{31}^{j_{31}}e^{-\alpha r_1-\beta r_2-\gamma r_3}\mathcal{Y}^{LM}_{(\ell_1\ell_2)\ell_{12},\ell_3}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)\chi_1, \tag{5}$$

where $\mathcal{Y}^{LM}_{(\ell_1\ell_2)\ell_{12},\ell_3}$ is a vector-coupled product of spherical harmonics for the three electrons to form a state of total angular momentum L, and χ_1 is a spin function with spin angular momentum $1/2$. The basis set is then replicated several times with different nonlinear scale parameters α,

TABLE I. Bethe logarithms, expressed in the form $\beta = \beta^{(0)} + (\mu/M)\beta^{(1)} + \ln(Z^2\mu/m)$.

Atom/ion	$\beta^{(0)}$	$\beta^{(1)}$
Li$(1s^22s\,^2S)$	2.981 06(1)	0.113 05(5)
Li$(1s^23s\,^2S)$	2.982 36(6)	0.1105(3)
Li$(1s^22p\,^2P)$	2.982 57(6)	0.1112(5)
Li$^+(1s^2\,^1S)$	2.982 6246[a]	0.109 55(4)[a]
Be$^+(1s^22s\,^2S)$	2.979 26(2)	0.125 58(4)
Be$^+(1s^23s\,^2S)$	2.981 62(1)	0.1171(1)
Be$^+(1s^22p\,^2P)$	2.982 27(6)	0.1217(6)
Be$^{2+}(1s^2\,^1S)$	2.982 5031[a]	0.116 93(4)[a]

[a] Drake and Goldman [15].

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

Atom/ion transition	$\mathcal{E}_{\rm tot}^{(0)}$	$\mathcal{E}_{\rm tot}^{(1)}$	$\mathcal{E}_{\rm tot}^{(2)}$
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($^2S_{1/2}$) 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)	0.339 983 00(2)
Be$^+$($2\,^2S_{1/2}$) I.P.	0.669 290 555(24)	−0.701 626 33(7)	0.721 963 94(1)

β, and γ, and the scale parameters fully optimized for each sector. The wave function $\Psi^{(0)}$ is then a linear combination of such terms with variationally determined coefficients so as to minimize the energy. The method is numerically stable, requiring at most quadruple precision arithmetic. Our best variational bounds for the ground states with 9577 terms in the basis set are

$$\mathcal{E}_{\rm NR}^{(0)}({\rm Li}; 2\,^2S) = -7.478\,060\,323\,892\,4$$

$$\mathcal{E}_{\rm NR}^{(0)}({\rm Be}^+; 2\,^2S) = -14.324\,763\,176\,766\,8.$$

The result for Li is slightly lower than that obtained by Puchalski and Pachucki [5], while the result for Be$^+$ is much more accurate than any previous calculation.

The calculation of the Bethe logarithm is the most difficult part of the calculation. The $2\,^2S$ state requires a summation over only the virtual $n\,^2P$ states, but the $2\,^2P$ state requires complete sets of ^2S, $^2P^e$, and ^2D intermediate states. These lengthy calculations will be described elsewhere. We quote here only the final results in Table I. Note that with the $\ln(Z^2)$ term subtracted, the numbers are all nearly equal, and close to the value 2.984 128 56 for the ground state of hydrogen.

We turn now to a discussion of the final results and their significance. Table II lists the total expansion coefficients for each power of λ, defined by $\mathcal{E}_{\rm tot}^{(k)} = \mathcal{E}_{\rm NR}^{(k)} + \alpha^2\mathcal{E}_{\rm rel}^{(k)} + \alpha^3\mathcal{E}_{\rm QED}^{(k)} + \alpha^4\mathcal{E}_{\rm ho}^{(k)}$. Since $\lambda \simeq 10^{-4}$, the sum $E = \sum_{k=0}^{2}\lambda^k\mathcal{E}_{\rm tot}^{(k)}$ gives the total energy accurate to a few parts in 10^{12} for any particular isotope. The values of the nuclear masses are as listed in Ref. [24], with the exception of the more recent measurements for ^{11}Li and ^{11}Be by Bachelet *et al.* [25]. Their values are 11.043 716(5) u and 11.021 654(4) u, respectively.

Table III compares theory and experiment for the calculated transition frequencies for the stable isotopes ^{7}Li and ^{9}Be$^+$. It is particularly noteworthy that the ionization potential for Li is now in good agreement with the recent high-precision measurement of Bushaw *et al.* [28], but there is a substantial disagreement with the NIST tabulation for the ionization potential of ^{9}Be$^+$. In view of the good agreement for the other transitions, it seems likely that the theoretical ionization energy of 146 882.923(5) cm^{-1} is more accurate than the experimental value by an order of magnitude.

For purposes of applying the calculated results to the relative determination of nuclear charge radii, it is convenient to express the results in the form

$$\Delta\nu_{B-A} = \Delta\nu_{B-A}^{(0)} + C[(\bar{r}_{c,B})^2 - (\bar{r}_{c,A})^2], \qquad (6)$$

where the left-hand side is the total (measured) isotope shift between isotopes A and B for some atomic transition frequency, $\Delta\nu_{B-A}^{(0)}$ is the calculated isotope shift excluding the effect of finite nuclear size, and C represents the change in the coefficient $\mathcal{E}_{\rm nuc}^{(0)}$ defined in Eq. (4). For completeness, we give updated results for $\Delta\nu_{B-A}^{(0)}$ in Table IV for the transitions in Li, as well as new results for Be$^+$. With the inclusion of the nuclear polarization correction calculated by Pachucki [20] for the $3\,^2S - 2\,^2S$ transition in ^{11}Li relative to ^{7}Li, the results agree to within the estimated uncertainty of his value 25 101.473(9) MHz. The corresponding $\Delta\nu_{B-A}^{(0)}$ and C parameters for Be$^+$ have not been published before. The values of the C coefficient for the

TABLE III. Comparison between theory and experiment for the total transition frequencies of ^{7}Li and ^{9}Be$^+$. Units are cm^{-1}. Numbers in square brackets are reference numbers.

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)	14 903.6479(10)	14 903.9832(10)	27 206.0930(10)	43 487.1583(10)
^{7}Li (experiment)	14 903.648 130(14) [26]	14 903.983 648(14) [26]	27 206.094 20(10) [27]	43 487.159 40(18) [28]
Difference	−0.0002(10)	−0.0004(10)	−0.0012(10)	−0.0011(10)
^{9}Be$^+$ (this work)	31 928.738(5)	31 935.310(5)	88 231.920(6)	146 882.923(5)
^{9}Be$^+$ (experiment)	31 928.744 [29]	31 935.320 [29], 31 935.310(47) [10]	88 231.915 [29]	146 882.86 [29]
Difference	−0.006(5)	−0.010(5), 0.000(47)	0.005(6)	0.063(5)

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

Isotopes	$2\,^2P_{1/2} - 2\,^2S$	$2\,^2P_{3/2} - 2\,^2S$	$3\,^2S - 2\,^2S$
^{7}Li − ^{6}Li	−10 532.111(6)	−10 532.506(6)	−11 452.821(2)
^{7}Li − ^{8}Li	7940.627(5)	7940.925(5)	8634.989(2)
^{7}Li − ^{9}Li	14 098.840(14)	14 099.369(14)	15 331.799(13)
^{7}Li − ^{11}Li[a]	23 082.642(24)	23 083.493(24)	25 101.470(22)
^{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 [20] of 62 kHz for the $2\,^2P_J - 2\,^2S$ transitions, and 39 kHz for the $3\,^2S - 2\,^2S$ transition.

transitions in Be$^+$ are $C(2\,^2P - 2\,^2S) = 16.912$ MHz/fm^2 and $C(3\,^2S - 2\,^2S) = 10.376$ MHz/fm^2.

Turning now to the fine structure splittings, the splitting isotope shift (SIS) provides an important consistency check on the experimental data because the theoretical value is nearly independent of both QED and nuclear volume effects, but there remain serious disagreements between theory and experiment. The best studied example is the isotope shift in the $2\,^2P_{3/2} - 2\,^2P_{1/2}$ splitting, where the predicted value is larger in ^{7}Li than in ^{6}Li by 0.396 MHz (from Table IV), but there is a large amount of scatter in the experimental values. The two most recent measurements yield −0.863(79) MHz [30] and +0.155(77) MHz [31], in clear disagreement with each other, and with theory. The predicted SIS for ^{11}Be$^+$ relative to ^{9}Be$^+$ is 3.878 MHz. The planned isotope shift measurements for Be$^+$ at ISOLDE will provide an important new opportunity to measure the SIS and compare with theory.

In summary, this Letter sets a new standard of accuracy for the comparison between theory and experiment for transition frequencies of Be$^+$, and it establishes the theoretical framework needed to interpret isotope shifts in terms of the nuclear charge radius of the single-neutron halo isotope Be$^+$. It seems likely that the calculated ionization energy of ^{9}Be$^+$ is more accurate than the experimental value by an order of magnitude. However, there remains a significant problem in case of the SIS for lithium, where the experimental values do not agree with each other or with theory. Further measurements in Be$^+$ may help to resolve the discrepancy.

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