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Relativistic, QED, and finite nuclear mass corrections for low-lying states of Li and Be$^+$

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Accurate results for nonrelativistic energy, relativistic, QED, and finite nuclear mass corrections are obtained for $2^1S_{1/2}$, $3^1S_{1/2}$, and $2^1P_{1/2}$ states of the Li atom and Be$^+$ ion. Our computational approach uses the Hylleraas basis set with the analytic integration and recursion relations. From comparison of experimental results for the isotope shifts to theoretical predictions including nuclear polarizabilities, we obtain nuclear charge radii for Li and Be isotopes.

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I. INTRODUCTION

The accurate evaluation of energy levels in atoms and ions requires inclusion of both the electron correlations and quantum electrodynamic (QED) effects. At present, in spite of significant theoretical effort [1] there is no universal computational method which treats accurately correlations and QED effects all together. For heavy few electron systems, electron interactions can be treated perturbatively within systematic QED approach [2]. For light systems involving few electrons, the most fundamental approach is based on the expansion of energy levels in the fine structure constant α, and also in the electron-nucleus mass ratio. At the same time, electron correlations are treated accurately by the use of explicitly correlated basis sets. This method has been advanced significantly in the last years by the calculation of $m\alpha^6$ corrections to helium energy levels [3], $m\alpha^7$ to helium fine structure [4,5], and $m\alpha^5$ corrections in three- and four-electron systems [6–8]. The achieved numerical precision is sufficient to determine nuclear properties from isotope shift measurements of transition energies. For example, the most accurate determination of the deuteron charge radius comes from the measurement of the $1S$-$2S$ transition in hydrogen and deuterium [9]. Recently a series of measurements of isotope shifts in helium [10,11] and lithium isotopes [12,13] together with the intensive calculations of theoretical energy levels [7,14–16] brought the accurate values of charge radii of short-lived nuclei with respect to the stable isotope. However, at present, theoretical methods are not capable of predicting energy levels with such an accuracy, which would make available the absolute determination of nuclear charge radii, except for the hydrogenic systems, where accuracy is limited only by small $m\alpha^2(Z\alpha)^6$ higher order two-loop corrections [17].

The most important in the accurate calculation of (light) atomic energy levels is the precise representation of the nonrelativistic wave function. The frequently used explicitly correlated Gaussian (ECG) functions give very accurate nonrelativistic energies, but the wave function does not satisfy the cusp condition, and for this reason this representation cannot be used for the calculation of $m\alpha^6$ and higher order corrections. Also, the estimation of numerical uncertainties within the ECG method is quite problematic. More difficult to use is the Hylleraas basis set [18–20], but its achieved accuracy exceeds significantly results with ECG for three electron systems. In order to solve accurately Schrödinger equation we use the Hylleraas basis set with the number of functions of about 10 000 for S states and 14 000 for P states. The calculations of matrix elements of nonrelativistic Hamiltonian, as well as relativistic and QED operators are performed analytically using newly developed recursion relations for the Hylleraas integrals [20–23].

In this work we present the most accurate calculations of nonrelativistic, leading relativistic, and QED contributions, including finite nuclear mass corrections and nuclear polarizability, to energy levels of $2^1S_{1/2}$, $3^1S_{1/2}$, and $2^1P_{1/2}$ states of Li and Be$^+$. As a main result, we obtain ionization energies of Li and Be$^+$, transition energies $2^1S_{1/2}$-$3^1S_{1/2}$ and $2^1S_{1/2}$-$2^1P_{1/2}$, and corresponding isotope shifts. In comparison to the former work of Yan *et al.* [7], our results are in agreement for transition frequencies, but in slight disagreement for the isotope shifts in Be$^+$. For the Li isotope shift both Ref. [7] and this work are in agreement with [16]. In all cases our numerical precision is about an order of magnitude higher, with the total uncertainty dominated by higher order terms. The comparison to experimental values [24–27], apart from agreement with experimental transition energies in both Li and Be$^+$, reveals small discrepancy for the Be$^+$ ionization energy with the NIST data [27]. Together with these benchmarking results, from our theoretical predictions and measured isotope shifts [12,13,28] we obtain improved nuclear charge radii for various isotopes including halo nuclei ^{11}Li and ^{11}Be.

II. RELATIVISTIC AND QED CORRECTIONS WITH THE NUCLEAR CHARGE RADIUS

The energy level $E(\alpha,\eta)$ as a function of α and $\eta=-\mu/m_N=-m/(m+m_N)$ is expanded in power series in its arguments

$$E(\alpha,\eta) = m\alpha^2[\mathcal{E}^{(2,0)} + \eta\mathcal{E}^{(2,1)} + \eta^2\mathcal{E}^{(2,2)}] + m\alpha^4[\mathcal{E}^{(4,0)} + \eta\mathcal{E}^{(4,1)}] + m\alpha^5[\mathcal{E}^{(5,0)} + \eta\mathcal{E}^{(5,1)}] + m\alpha^6[\mathcal{E}^{(6,0)} + \eta\mathcal{E}^{(6,1)}] + m\alpha^7\mathcal{E}^{(7,0)}, \quad (1)$$

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and each coefficient is calculated separately from the expectation value of the corresponding Hamiltonian or the operator. The leading terms $\mathcal{E}^{(2,0)}$, $\mathcal{E}^{(2,1)}$, and $\mathcal{E}^{(2,2)}$ result from nonrelativistic Hamiltonian for three electrons and the nucleus with Coulomb interactions between them,

$$H_0 = \sum_a \frac{p_a^2}{m} + \frac{p_N^2}{m_N} - \sum_a \frac{Z\alpha}{r_a} + \sum_{a>b} \frac{\alpha}{r_{ab}}. \tag{2}$$

In order to calculate relativistic and nuclear recoil corrections for atomic systems with the finite size nucleus, one should at first properly define the nuclear charge radius. Therefore, let us consider the interaction of the particle having spin $\vec{s}$ and the charge e with the electric field. The leading interaction related to the finite size is

$$\delta H = -\frac{e}{6}(\langle r_{\rm ch}^2\rangle \delta^{ij} + (s^i s^j)^{(2)} Q_E)\partial^j E^i, \tag{3}$$

where $\langle r_{\rm ch}^2\rangle$ is the averaged square of the charge radius, Q_E is related to the electric quadrupole moment Q by $Q_E=3/[s_N(2s_N-1)]Q$, and

$$(s^i s^j)^{(2)} = \frac{1}{2}s^i s^j + \frac{1}{2}s^j s^i - \frac{\delta^{ij}}{3}\vec{s}^2. \tag{4}$$

For the point spin $s=1/2$, particle $\langle r_{\rm ch}^2\rangle$ does not vanish and is equal to $3/(4m^2)$; it is the so-called Darwin term and it depends on the value of the spin s [29]. This term is the source of ambiguity in the definition of nuclear charge radii [30]. If we want the point particle to have the vanishing charge radius, the Darwin term should be excluded from $\langle r_{\rm ch}^2\rangle$. However, the value of the Darwin term for the arbitrary spin point particle with the arbitrary magnetic moment is unknown. Therefore, we propose the universal definition of $\langle r_{\rm ch}^2\rangle$ by Eq. (3), and thus include the Darwin term within the charge radius. A similar, but even more complicated problem appears when QED effects are being included. Now, assuming the definition of charge radius by Eq. (3), the atomic Hamiltonian including relativistic corrections and neglecting magnetic moment anomaly for electrons is of the form [31]

$$H_{BP} = \sum_a H_a + \sum_{a>b} H_{ab} + H_N + \sum_a H_{aN}, \tag{5}$$

$$H_a = \frac{\vec{p}_a^{\,2}}{2m} - \frac{\vec{p}_a^{\,4}}{8m^3}, \tag{6}$$

$$\begin{aligned}H_{ab} = \alpha\Bigg\{ & \frac{1}{r_{ab}} - \frac{1}{2m^2} p_a^i \left(\frac{\delta^{ij}}{r_{ab}} + \frac{r_{ab}^i r_{ab}^j}{r_{ab}^3}\right) p_b^j + \frac{\pi}{m^2}\delta^3(r_{ab}) \\ & + \frac{1}{m^2}\frac{s_a^i s_b^j}{r_{ab}^3}\left(\delta^{ij} - 3\frac{r_{ab}^i r_{ab}^j}{r_{ab}^2}\right) + \frac{1}{2m^2 r_{ab}^3}[2\vec{s}_a\cdot\vec{r}_{ab}\times\vec{p}_b \\ & - 2\vec{s}_b\cdot\vec{r}_{ab}\times\vec{p}_a + \vec{s}_b\cdot\vec{r}_{ab}\times\vec{p}_b - \vec{s}_a\cdot\vec{r}_{ab}\times\vec{p}_a]\Bigg\},\end{aligned} \tag{7}$$

$$H_N = \frac{\vec{p}_N^{\,2}}{2m_N} - \frac{\vec{p}_N^{\,4}}{8m_N^3}, \tag{8}$$

$$\begin{aligned}H_{aN} = -Z\alpha\Bigg\{ & \frac{1}{r_a} - \frac{1}{2mm_N} p_a^i \left(\frac{\delta^{ij}}{r_a} + \frac{r_a^i r_a^j}{r_a^3}\right) p_N^j \\ & - \frac{2\pi}{3}\left(\langle r_{\rm ch}^2\rangle + \frac{3}{4m^2}\right)\delta^3(r_a) - \frac{4\pi g_N}{3mm_N}\vec{s}_a\cdot\vec{s}_N\delta^3(r_a) \\ & + \frac{g_N}{2mm_N}\frac{s_a^i s_N^j}{r_a^3}\left(\delta^{ij} - 3\frac{r_a^i r_a^j}{r_a^2}\right) + \frac{1}{2r_a^3}\bigg[\frac{2}{mm_N}\vec{s}_a\cdot\vec{r}_a\times\vec{p}_N \\ & - \frac{g_N}{mm_N}\vec{s}_N\cdot\vec{r}_a\times\vec{p}_a + \frac{(g_N-1)}{m_N^2}\vec{s}_N\cdot\vec{r}_a\times\vec{p}_N \\ & - \frac{1}{m^2}\vec{s}_a\cdot\vec{r}_a\times\vec{p}_a\bigg] - \frac{Q_E}{6}\frac{(s_N^i s_N^j)^{(2)}}{r_a^3}\left(\delta^{ij} - 3\frac{r_a^i r_a^j}{r_a^2}\right)\Bigg\}.\end{aligned} \tag{9}$$

In practice small relativistic terms involving nuclear mass are treated perturbatively and in this work we neglect all relativistic $O(m/M)^2$ corrections. These terms become much more important in muonic atoms and cannot be neglected there.

Let us now consider leading QED corrections of order $m\alpha^5$, which also include the inelastic contribution $E_{\rm pol}$ due to the nuclear polarizability. Since we do not consider the hyperfine structure, the spin of atomic nucleus can be neglected, and the QED correction takes the form [32,33]

$$\begin{aligned}E^{(5)} = & -\frac{4Z\alpha^2}{3}\left(\frac{1}{m} + \frac{Z}{M}\right)^2 \left\langle \sum_a \delta^3(r_a)\right\rangle \ln k_0 \\ & + \sum_a \langle H_{aN}^{(5)}\rangle + \sum_{a>b}\langle H_{ab}^{(5)}\rangle + E_{\rm pol},\end{aligned} \tag{10}$$

$$\begin{aligned}H_{aN}^{(5)} = & \frac{Z\alpha^2}{2\pi m^2 r_a^3}\left[\vec{s}_a\cdot\vec{r}_a\times\vec{p}_a - \frac{m}{M}\vec{s}_a\cdot\vec{r}_a\times\vec{p}_N\right] \\ & + \left[\frac{19}{30} + \ln(\alpha^{-2})\right]\frac{4\alpha^2 Z}{3m^2}\delta^3(r_a) \\ & + \left[\frac{62}{3} + \ln(\alpha^{-2})\right]\frac{(Z\alpha)^2}{3mM}\delta^3(r_a) \\ & - \frac{7}{6\pi}\frac{m^2}{M}(Z\alpha)^5 P\left[\frac{1}{(m\alpha r_a)^3}\right] + \frac{4}{3}\frac{Z^3\alpha^2}{M^2}\ln\left(\frac{M}{m\alpha^2}\right)\delta^3(r_a),\end{aligned} \tag{11}$$

$$\begin{aligned}H_{ab}^{(5)} = & \frac{\alpha^2}{\pi m^2}\bigg[\frac{s_a^i s_b^j}{r_{ab}^3}\left(\delta^{ij} - 3\frac{r_{ab}^i r_{ab}^j}{r_{ab}^2}\right) \\ & - \frac{1}{2r_{ab}^3}(\vec{s}_a + \vec{s}_b)\cdot\vec{r}_{ab}\times(\vec{p}_a - \vec{p}_b)\bigg] \\ & + \frac{\alpha^2}{m^2}\left[\frac{164}{15} + \frac{14}{3}\ln\alpha\right]\delta^3(r_{ab}) - \frac{7}{6\pi}m\alpha^5 P\left[\frac{1}{(m\alpha r_{ab})^3}\right],\end{aligned} \tag{12}$$

where

$$\ln k_0 \equiv \frac{\left\langle \sum_a \vec{p}_a (H_0 - E_0)\ln\left[\frac{2(H_0-E_0)}{\alpha^2 m}\right]\sum_b \vec{p}_b\right\rangle}{2\pi\alpha Z\langle\Sigma_c\delta^3(r_c)\rangle}, \tag{13}$$

$$\langle\phi|P\left[\frac{1}{r^3}\right]|\psi\rangle = \lim_{a\to 0}\int d^3r\,\phi^*(\vec{r})\left[\frac{1}{r^3}\Theta(r-a) + 4\pi\delta^3(r)(\gamma+\ln a)\right]\psi(\vec{r}). \tag{14}$$

The electron-electron terms have been simplified in the above, since $\delta^3(r_{ab})$ does not vanish only for singlet states, therefore $\vec{s}_a\cdot\vec{s}_b\delta^3(r_{ab})=-3/4\,\delta^3(r_{ab})$. We included in H_{aN} the leading logarithmic contribution that comes from the nuclear self-energy, but neglected all nonlogarithmic $(m/M)^2$ terms which are proportional to $\delta^3(r_a)$. They are not known for a general nucleus since they depend on the nuclear spin and charge distribution within the nucleus. For the calculation of the isotope shift in Li and Be^+ we again neglect all $O(m/M)^2$ terms. These terms are important for muonic atoms, but their calculation requires proper definition of the nuclear charge radius including QED effects, and its relation to the charge radius obtained from a different type of measurements such as the elastic electron scattering off nuclei.

The last term in Eq. (10), E_{pol}, is the nuclear polarizability correction. It is significant for halo nuclei such as $^{11}\mathrm{Li}$ [16], or whenever the isotope shift transition in the optical range reaches sub-MHz precision, for example, in the $1S$-$2S$ transition in deuterium [9]. The nuclear polarizability correction is expected to be significant also for $^{11}\mathrm{Be}$, as this nucleus has the largest known $B(E1)$ line strength among all nuclei. For this reason, we calculate it using experimental [34] and theoretical [35] data for the electric dipole excitation of the $^{11}\mathrm{Be}$ nucleus.

Considering $m\alpha^6$ corrections, they are well known for the hydrogen. Results for few-electron atoms are expressed in terms of the effective Hamiltonian [36]. Corresponding calculations have been performed only for low-lying states of helium [3]. Calculations for three-electron systems are at present too difficult and therefore we use an approximate formula on the basis of hydrogenic values,

$$E^{(6)} = \left\{\frac{Z^2\alpha^3}{m^2}\left[\frac{427}{96} - 2\ln(2)\right] + \frac{Z^2\alpha^3}{mm_N}\left[\frac{35}{36} - \frac{448}{27\pi^2} - 2\ln(2) + \frac{6\zeta(3)}{\pi^2}\right] + \frac{Z^3\alpha^3}{mm_N}\left[4\ln(2) - \frac{7}{2}\right]\right\}\pi\left\langle\sum_a \delta^3(r_a)\right\rangle. \tag{15}$$

It includes dominating electron-nucleus one-loop radiative, radiative recoil, and pure recoil corrections [37]. We neglect electron-electron radiative corrections and the purely relativistic corrections, as we expect them to be relatively small, of order 10%. The relativistic $m\alpha^6$ corrections are also very difficult to calculate. Its neglect is the leading source of uncertainty in the theoretical predictions for transition frequencies. Similarly, the nuclear recoil correction $m^2/M\alpha^6$, which is still significant for the isotope shift, is also estimated on the basis of the known hydrogenic value in the above formula. This introduced some uncertainty in the determination of the isotope shift, from which nuclear charge radii are obtained.

Due to numerical importance, one calculates approximately $m\alpha^7$ contribution which is known exactly only for hydrogenic systems [37],

$$E_{\mathrm{H}}^{(7)}(n) = m\frac{\alpha}{\pi}\frac{(Z\alpha)^6}{n^3}[A_{60}(n) + \ln(Z\alpha)^{-2}A_{61}(n) + \ln^2(Z\alpha)^{-2}A_{62}] + m\left(\frac{\alpha}{\pi}\right)^2\frac{(Z\alpha)^5}{n^3}B_{50} + m\left(\frac{\alpha}{\pi}\right)^3\frac{(Z\alpha)^4}{n^3}C_{40}. \tag{16}$$

It includes one-, two-, and three-loop corrections, and values of A, B, and C coefficients may be found in [37]. Following Ref. [32] these hydrogenic values of order $m\alpha^7$ are extrapolated to lithium, according to

$$\mathcal{E}^{(7)}(Z) = [2\mathcal{E}^{(7)}(1S,Z) + \mathcal{E}^{(7)}(nX,Z-2)] \times\frac{\langle\delta^3(r_1)+\delta^3(r_2)+\delta^3(r_3)\rangle_{\mathrm{Li}}}{2\langle\delta^3(r)\rangle_{1S,Z} + \langle\delta^3(r)\rangle_{nX,Z-2}}, \tag{17}$$

for $X=S$, and for states with higher angular momenta $\mathcal{E}^{(7)}(nX,Z)$ is neglected. We expect this approximate formula to be accurate to 25%. This completes QED corrections to transition frequencies and the isotope shifts in light atomic systems.

III. COMPUTATIONAL METHOD AND NUMERICAL RESULTS

In the construction of the wave function we closely follow the works of Yan and Drake in [19]. The global wave function Ψ for both S and P states is expressed as a linear combination of ψ, the antisymmetrized product $\mathcal{A}$ of the spatial function φ and the spin function χ,

$$\psi = \mathcal{A}[\phi(\vec{r}_1,\vec{r}_2,\vec{r}_3)\chi], \tag{18}$$

$$\psi_a^i = \mathcal{A}[\phi_a^i(\vec{r}_1,\vec{r}_2,\vec{r}_3)\chi], \tag{19}$$

$$\phi(\vec{r}_1,\vec{r}_2,\vec{r}_3) = e^{-w_1r_1-w_2r_2-w_3r_3}\,r_{23}^{n_1}\,r_{31}^{n_2}\,r_{12}^{n_3}\,r_1^{n_4}\,r_2^{n_5}\,r_3^{n_6}, \tag{20}$$

$$\phi_a^i(\vec{r}_1,\vec{r}_2,\vec{r}_3) = r_a^i\,\phi(\vec{r}_1,\vec{r}_2,\vec{r}_3), \tag{21}$$

$$\chi = \alpha(1)\beta(2)\alpha(3) - \beta(1)\alpha(2)\alpha(3), \tag{22}$$

with n_i being non-negative integers, $w_i\in R_+$, and the subscript $a=1,2,3$. The matrix element of the nonrelativistic Hamiltonian H_0 in Eq. (2) or of any spin independent operator can be expressed after eliminating spin variables as

$$\begin{aligned}\langle\psi|H_0|\psi'\rangle = \langle 2\phi(r_1,r_2,r_3) + 2\phi(r_2,r_1,r_3) - \phi(r_3,r_1,r_2)\\ - \phi(r_2,r_3,r_1) - \phi(r_1,r_3,r_2)\\ - \phi(r_3,r_2,r_1)|H_0|\phi'(r_1,r_2,r_3)\rangle,\end{aligned} \tag{23}$$

$$\begin{aligned}\langle\psi_a^i|H_0|\psi_b'^i\rangle = \langle 2\phi_a^i(r_1,r_2,r_3) + 2\phi_a^i(r_2,r_1,r_3) - \phi_a^i(r_3,r_1,r_2)\\ - \phi_a^i(r_2,r_3,r_1) - \phi_a^i(r_1,r_3,r_2)\\ - \phi_a^i(r_3,r_2,r_1)|H_0|\phi_b'^i(r_1,r_2,r_3)\rangle.\end{aligned} \tag{24}$$

While for S states Hamiltonian matrix elements can be written in one form, for P states with the help of an additional r_1,r_2,r_3 permutation they can take two different forms: $\langle\phi_3^i|H_0|\phi_3'^i\rangle$ or $\langle\phi_2^i|H_0|\phi_3'^i\rangle$. Next, all these spatial matrix el-

TABLE I. Nonrelativistic energy and relativistic and finite nuclear mass corrections in Li and Be$^+$, $\Omega=\infty$ is a result of extrapolation.

Ω	$\mathcal{E}^{(2,0)}$	$\mathcal{E}^{(2,1)}$	$\mathcal{E}^{(2,2)}$	$\mathcal{E}^{(4,0)}$	$\mathcal{E}^{(4,1)}$
Li $2\ {}^1S_{1/2}$					
10	−7.478 060 323 786 3	−7.779 903 106 67	−1.801 631 491	−12.049 918 25	10.010 910 3
11	−7.478 060 323 861 5	−7.779 903 105 96	−1.801 631 553	−12.049 914 16	10.010 935 1
12	−7.478 060 323 889 7	−7.779 903 104 98	−1.801 631 587	−12.049 913 45	10.010 940 4
∞	−7.478 060 323 906(8)	−7.7792 903 104 4(7)	−1.801 631 62(4)	−12.049 913 0(4)	10.010 945(4)
Li $3\ {}^1S_{1/2}$					
10	−7.354 098 421 004 0	−7.646 138 262 557	−1.677 971 728 8	−11.871 192 0	10.014 596
11	−7.354 098 421 302 1	−7.646 138 262 527	−1.677 971 758 0	−11.871 177 9	10.014 649
12	−7.354 098 421 379 9	−7.646 138 262 612	−1.677 971 775 7	−11.871 171 5	10.014 687
∞	−7.354 098 421 426(19)	−7.646 138 262 65(3)	−1.677 971 789(11)	−11.871 168(8)	10.014 72(4)
Li $2\ {}^1P_{1/2}$					
10	−7.410 156 532 150 2	−7.656 895 306 5	−1.806 107	−11.801 371 0	9.685 503
11	−7.410 156 532 586 0	−7.656 895 217 6	−1.806 275	−11.801 365 9	9.685 230
12	−7.410 156 532 628 6	−7.656 895 191 1	−1.806 407	−11.801 363 5	9.685 356
∞	−7.410 156 532 665(14)	−7.656 895 176(9)	−1.806 51(8)	−11.801 362(2)	9.685 43(8)
Be$^+$ $2\ {}^1S_{1/2}$					
10	−14.324 763 176 616 3	−14.777 682 315 84	−3.634 056 961 9	−43.688 039 3	26.932 300
11	−14.324 763 176 725 0	−14.777 682 314 48	−3.634 057 065 9	−43.688 034 4	26.932 382
12	−14.324 763 176 763 5	−14.777 682 313 66	−3.634 057 095 3	−43.688 026 3	26.932 370
∞	−14.324 763 176 784(11)	−14.777 682 313 0(5)	−3.634 057 110(11)	−43.688 023(4)	26.932 37(2)
Be$^+$ $2\ {}^1S_{1/2}$					
10	−13.922 789 268 385 7	−14.351 840 883 53	−3.294 071 80	−42.344 339 8	27.308 080 8
11	−13.922 789 268 530 7	−14.351 840 888 66	−3.294 073 32	−42.344 323 8	27.308 224 8
12	−13.922 789 268 554 2	−14.351 840 890 68	−3.294 073 94	−42.344 318 4	27.308 210 6
∞	−13.922 789 268 570(10)	−14.351 840 891 8(8)	−3.294 074 4(4)	−42.344 317(3)	27.308 21(2)
Be$^+$ $2\ {}^1P_{1/2}$					
10	−14.179 333 292 319 7	−14.345 507 657	−3.728 487	−42.123 997 4	24.352 898
11	−14.179 333 293 202 9	−14.345 507 560	−3.728 679	−42.123 985 4	24.352 585
12	−14.179 333 293 342 7	−14.345 507 534	−3.728 739	−42.123 978 2	24.352 564
∞	−14.179 333 293 42(3)	−14.345 507 52(3)	−3.728 78(4)	−42.123 976(6)	24.352 55(4)

ements are expressed as linear combination of Hylleraas integrals, namely the integrals with respect to r_i of the form

$$f(n_1,n_2,n_3,n_4,n_5,n_6) = \int\frac{d^3r_1}{4\pi}\int\frac{d^3r_2}{4\pi}\int\frac{d^3r_3}{4\pi} \times e^{-w_1r_1-w_2r_2-w_3r_3}r_{23}^{n_1-1}r_{31}^{n_2-1}r_{12}^{n_3-1}r_1^{n_4-1}r_2^{n_5-1}r_3^{n_6-1}, \tag{25}$$

with non-negative integers n_i. They are performed analytically for $n_1,n_2,n_3=0,1$ and by recursion relations for larger n_i using formulas derived in [20]. These recursions give the most accurate numerical values of Hylleraas integrals among all the methods developed so far. Nevertheless, multiple precision arithmetic has to be used in generating the Hamiltonian matrix, in order to avoid near linear dependence of Hylleraas basis functions.

The total wave function is generated from all ϕ in Eq. (23) with n_i satisfying a condition

$$\sum_{i=1}^{6} n_i \leqslant \Omega, \tag{26}$$

for Ω between 3 and 12. For each Ω we minimize energy with respect to the free parameters w_i in Eq. (23). In order to increase the accuracy of the nonrelativistic wave function, following Yan and Drake [19], we divide the whole basis set into five sectors (six sectors for P states), each one with its own set of w_i's. To avoid numerical instabilities, within each sector we drop the terms with $n_4>n_5$ (or $n_4<n_5$) and for $n_4=n_5$ drop terms with $n_1>n_2$ (or $n_1<n_2$). This division allows for a significant improvements of nonrelativistic energies by optimization of all, five for S and six for P states, sets of w_i's. Numerical results for $2^1S_{1/2}$, $3^1S_{1/2}$, and $2^1P_{1/2}$

TABLE II. Relativistic and QED operators in Li and Be$^+$. Implicit sum over a and sum over $a \neq b$ pairs are assumed. Bethe logarithms are that from Yan *et al.* [7] All values are in atomic units.

Operator	Li $2S_{1/2}$	Li $S_{1/2}$	Li $2P_{1/2}$
$p_a p_b$	0.301 842 780 3(6)	0.292 039 841 2(2)	0.246 738 644(9)
$p_a p_b/(E-H)' p_c p_d$	−1.499 788 83(4)	−1.385 931 96(2)	−1.559 77(7)
p_a^4	628.449 022(4)	622.859 40(2)	620.044 977(8)
$[p_a^4]_{\rm mp}$	41.176 62(5)	40.628 83(7)	40.628 87(6)
$p_a^i(\frac{\delta^{ij}}{r_{ab}}+\frac{r_{ab}^i r_{ab}^j}{r_{ab}^3})p_b^j$	0.871 195 809(9)	0.859 817 43(18)	0.792 851 59(4)
$[p_a^i(\frac{\delta^{ij}}{r_{ab}}+\frac{r_{ab}^i r_{ab}^j}{r_{ab}^3})p_b^j]_{\rm mp}$	6.154 303 2(3)	5.844 828 2(5)	6.002 973(11)
$\delta^3(r_a)$	13.842 610 787(6)	13.736 502 84(7)	13.676 197 06(7)
$[\delta^3(r_a)]_{\rm mp}$	0.484 589 3(6)	0.487 894 7(6)	0.647 914(5)
$\delta^3(r_{ab})$	0.544 324 632 0(7)	0.536 168 418 9(4)	0.532 274 098 9(3)
$[\delta^3(r_{ab})]_{\rm mp}$	−0.082 009 7(4)	−0.078 406(2)	−0.066 725(2)
$p_N^i(\frac{\delta^{ij}}{r_a}+\frac{r_a^i r_a^j}{r_a^3})p_a^j$	87.276 740 9(3)	86.289 222 5(7)	85.743 261 2(7)
$1/r_{ab}^3$	0.273 413(5)	0.198 05(8)	0.289 57(5)
$[1/r_{ab}^3]_{\rm mp}$	−1.627 46(5)	−1.645 4(2)	−1.892(5)
$1/r_a^3$	−308.314 23(6)	−305.939 0(2)	−304.517 7(2)
$\ln(k_0)-2\ln Z$	2.981 06(1)	2.982 36(6)	2.982 57(6)
$[\ln(k_0)]_{\rm mp}$	−0.113 05(5)	−0.110 5(3)	−0.111 2(5)
$\vec{r}_a/r_a^3\times\vec{p}_a\cdot\vec{\sigma}_a$			−0.125 946 352(50)
$[\vec{r}_a/r_a^3\times\vec{p}_a\cdot\vec{\sigma}_a]_{\rm mp}$			0.376 388(3)
$\vec{r}_{ab}/r_{ab}^3\times\vec{p}_a\cdot\vec{\sigma}_a$			−0.224 640 70(5)
$[\vec{r}_{ab}/r_{ab}^3\times\vec{p}_a\cdot\vec{\sigma}_a]_{\rm mp}$			0.570 585(4)
$\vec{r}_{ab}/r_{ab}^3\times\vec{p}_b\cdot\vec{\sigma}_a$			0.038 473 60(6)
$[\vec{r}_{ab}/r_{ab}^3\times\vec{p}_b\cdot\vec{\sigma}_a]_{\rm mp}$			−0.213 52(3)
$\vec{r}_a/r_a^3\times\vec{p}_N\cdot\vec{\sigma}_a$			0.022 524 93(9)

Operator	Be$^+$ $2S_{1/2}$	Be$^+$ $3S_{1/2}$	Be$^+$ $2P_{1/2}$
$p_a p_b$	0.452 919 136 1(7)	0.429 051 623 1(7)	0.166 174 23(2)
$p_a p_b/(E-H)' p_c p_d$	−3.181 137 97(3)	−2.865 022 8(3)	−3.562 60(5)
p_a^4	2146.520 76(5)	2108.368 02(9)	2088.652 95(4)
$[p_a^4]_{\rm mp}$	115.923 1(2)	112.589 8(3)	154.322 2(4)
$p_a^i(\frac{\delta^{ij}}{r_{ab}}+\frac{r_{ab}^i r_{ab}^j}{r_{ab}^3})p_b^j$	1.819 804 86(12)	1.774 364 56(14)	1.226 817 28(11)
$[p_a^i(\frac{\delta^{ij}}{r_{ab}}+\frac{r_{ab}^i r_{ab}^j}{r_{ab}^3})p_b^j]_{\rm mp}$	17.854 151(2)	16.414 367(3)	17.777 145(11)
$\delta^3(r_a)$	35.105 055 72(8)	34.577 877 6(1)	34.245 820 96(5)
$[\delta^3(r_a)]_{\rm mp}$	0.927 607 3(4)	0.932 129 (2)	1.831 450(7)
$\delta^3(r_{ab})$	1.580 538 588(3)	1.537 328 373(1)	1.518 990 086(6)
$[\delta^3(r_{ab})]_{\rm mp}$	−0.431 732(2)	−0.409 936 9(9)	−0.351 752(3)
$p_N^i(\frac{\delta^{ij}}{r_a}+\frac{r_a^i r_a^j}{r_a^3})p_a^j$	222.628 511 9(4)	217.799 579 5(7)	214.562 695 2(8)
$1/r_{ab}^3$	−7.514 6(1)	−7.579 45(7)	−6.794 2(2)
$[1/r_{ab}^3]_{\rm mp}$	−7.514 6(1)	−7.579 45(7)	−6.794 2(2)
$1/r_a^3$	−910.919 4(1)	−897.084 8(3)	−887.841 7(3)
$\ln(k_0)-2\ln Z$	2.979 26(2)	2.981 62(1)	2.982 27(6)
$[\ln(k_0)]_{\rm mp}$	−0.125 58 4	−0.117 1(1)	−0.121 7(6)

TABLE II. (*Continued.*)

Operator	Be^+ $2S_{1/2}$	Be^+ $S_{1/2}$	Be^+ $2P_{1/2}$
$\vec{r}_a/r_a^3\times\vec{p}_a\cdot\vec{\sigma}_a$			−0.969 131 7(11)
$[\vec{r}_a/r_a^3\times\vec{p}_a\cdot\vec{\sigma}_a]_{\rm mp}$			3.043 394(15)
$\vec{r}_{ab}/r_{ab}^3\times\vec{p}_a\cdot\vec{\sigma}_a$			−1.659 492 5(3)
$[\vec{r}_{ab}/r_{ab}^3\times\vec{p}_a\cdot\vec{\sigma}_a]_{\rm mp}$			4.532 68(9)
$\vec{r}_{ab}/r_{ab}^3\times\vec{p}_b\cdot\vec{\sigma}_a$			0.360 851 6(2)
$[\vec{r}_{ab}/r_{ab}^3\times\vec{p}_b\cdot\vec{\sigma}_a]_{\rm mp}$			−1.549 82(10)
$\vec{r}_a/r_a^3\times\vec{p}_N\cdot\vec{\sigma}_a$			0.339 008 2(2)

of Li and Be^+ for various sizes of basis sets are presented in Table I. The results for the ground state of Li are in agreement with our previous evaluation [22]. Results denoted by ∞ are obtained by extrapolation to the infinitely large (complete) basis set, by fitting the function $X(\Omega)=X_0+X_1/\Omega^n$ with some integer n. The similar fit is used for all other matrix elements, presented in the following tables.

Calculation of relativistic corrections, which are given by Eqs. (5)–(9), involve spin-independent and spin-dependent terms. The matrix element of spin-independent terms are calculated according to Eq. (23), while spin-orbit terms are obtained for the $P_{1/2}$ state by using

$$\begin{aligned}\langle\psi_a|\sum_{c=1}^{3}\vec{Q}_c\cdot\vec{\sigma}_c|\psi_b\rangle_{J=1/2}\\ &= i\langle\vec{\phi}_a(r_1,r_2,r_3)|-2\vec{Q}_3\times[\vec{\phi}_b(r_1,r_2,r_3)+\vec{\phi}_b(r_2,r_1,r_3)]\\ &\quad+(\vec{Q}_1-\vec{Q}_2+\vec{Q}_3)\times[\vec{\phi}_b(r_2,r_3,r_1)+\vec{\phi}_b(r_3,r_2,r_1)]\\ &\quad+(-\vec{Q}_1+\vec{Q}_2+\vec{Q}_3)\times[\vec{\phi}_b(r_1,r_3,r_2)+\vec{\phi}_b(r_3,r_1,r_2)]\rangle,\end{aligned} \tag{27}$$

and the result for $P_{3/2}$ is equal to $-1/2$ of that for $P_{1/2}$. The tensor spin-spin interaction vanishes for both the $P_{1/2}$ and

TABLE III. Expansion of energy in powers of α and η in Li. The last column presents values in units cm^{-1} for the ground state ionization energy for ^{7}Li and $^9Be^+$ with atomic masses from Table V. $\mathcal{E}^{(4,0)}_{\rm fs}$ is the finite size correction with $r_{\rm ch}(^7{\rm Li})=2.39(3)$ fm [41] and $r_{\rm ch}(^9{\rm Be})=2.519(12)$ fm [43].

Energy	$3S_{1/2}-2S_{1/2}$	$2P_{1/2}-2S_{1/2}$	I.P. $2S_{1/2}$	I.P. $2S_{1/2}[\mathrm{cm}^{-1}]$
		Li		
$\mathcal{E}^{(2,0)}$	0.123 961 902 48(2)	0.067 903 791 24(2)	0.198 146 911 238(12)	43 488.220 301(6)
$\mathcal{E}^{(2,1)}$	0.133 764 841 8(7)	0.123 007 928(10)	0.211 013 905 1(6)	−3.621 708
$\mathcal{E}^{(2,2)}$	0.123 659 827(11)	−0.004 88(7)	0.235 270 010(19)	0.000 316
$\mathcal{E}^{(4,0)}$	0.178 745(2)	0.248 551 4(10)	0.240 540 1(4)	2.811 269(5)
$\mathcal{E}^{(4,0)}_{\rm fs}$	$-0.666\,695\langle r_{\rm ch}^2\rangle$	$-1.045608\langle r_{\rm ch}^2\rangle$	$-0.870\,799\langle r_{\rm ch}^2\rangle$	−0.000 390
$\mathcal{E}^{(4,1)}$	0.003 78(4)	−0.325 44(11)	0.013 50(3)	−0.000 012
$\mathcal{E}^{(5,0)}$	−2.193(3)	−3.478(3)	−2.860 8(6)	−0.243 99(5)
$\mathcal{E}^{(5,1)}$	−1.46(2)	1.30(3)	−1.889(3)	0.000 013
$\mathcal{E}^{(6,0)}$	−9.2(9)	−14.4(1.4)	−12.0(1.2)	−0.007 5(7)
$\mathcal{E}^{(6,1)}$	−38.(10)	−46.(12)	−49.(12)	0.000 002
$\mathcal{E}^{(7,0)}$	115.(29)	215.(54)	147.(37)	0.000 67(17)
		Be^+		
$\mathcal{E}^{(2,0)}$	0.401 973 908 21(2)	0.145 429 883 35(5)	0.669 196 938 370(19)	146 871.751 363(4)
$\mathcal{E}^{(2,1)}$	0.425 841 421 2(13)	0.432 174 796(11)	0.701 595 771 3(4)	−9.374 767
$\mathcal{E}^{(2,2)}$	0.339 982 7(3)	−0.094 72(3)	0.721 945 175(15)	0.000 587
$\mathcal{E}^{(4,0)}$	1.343 705(3)	1.564 047(3)	1.892 557(3)	22.118 92(4)
$\mathcal{E}^{(4,0)}_{\rm fs}$	$-4.416\,477(1)\langle r_{\rm ch}^2\rangle$	$-7.198\,308(1)\langle r_{\rm ch}^2\rangle$	$-5.937\,280(1)\langle r_{\rm ch}^2\rangle$	−0.002 955
$\mathcal{E}^{(4,1)}$	0.375 84(2)	−2.579 82(5)	0.620 19(3)	−0.000 441
$\mathcal{E}^{(5,0)}$	−13.168(2)	−21.864(11)	−17.742(4)	−1.513 1(3)
$\mathcal{E}^{(5,1)}$	3.19(2)	30.92(13)	28.75(8)	−0.000 149
$\mathcal{E}^{(6,0)}$	−81.(8)	−132.(13)	−109.(11)	−0.068(7)
$\mathcal{E}^{(6,1)}$	−361.(90)	−442.(111)	−477.(119)	0.000 018(5)
$\mathcal{E}^{(7,0)}$	1036.(259)	1787.(447)	1360.(340)	0.006 2(15)

TABLE IV. Atomic masses of Lithium and Beryllium isotopes and the atomic binding energy.

Li isotope	Mass (u)	Ref.	Be isotope	Mass (u)	Ref.
^{6}Li	6.015122794(16)	[41]	^{7}Be	7.016 929 83(11)	[42]
^{7}Li	7.0160034256(45)	[43]	^{9}Be	9.012 182 20(43)	[42]
^{8}Li	8.02248624(12)	[41]	^{10}Be	10.013 533 82(43)	[42]
^{9}Li	9.02679020(21)	[41]	^{11}Be	11.021 661 55(63)	[44]
^{11}Li	11.04372361(69)	[41]	^{14}Be	14.042 890(140)	[42]
$E_{\rm Li}$	−7.281 au		$E_{\rm Be}$	−14.669 au	

$P_{3/2}$ states. All these matrix elements include Hylleraas integrals with $n_i=-1$, which are difficult to obtain accurately. We use the one-dimensional integral form for $f(-1,0,0;0,0,0)$ and $f(0,0,0;-1,n_5,n_6)$ and other f's with $n_i=-1$ are obtained by recursion relations [21,22]. Since these recursions are not stable numerically, we used quadruple, sextuple, and octuple precision arithmetic written by Korobov [38] to avoid loss of the numerical precision. It was especially important for excited states. Individual results for various operators are presented in Table II and the total relativistic correction in Table III. By the symbol $[\cdots]_{\rm mp}$ in these tables, we denote the mass polarization correction, namely,

$$[\cdots]_{\rm mp} = 2[\cdots]\frac{1}{(H-E)'}\sum_{a>b}\vec{p}_a\cdot\vec{p}_b. \tag{28}$$

QED corrections include two new terms, $1/r^3$ and the Bethe logarithm, see Eqs. (13) and (14). Matrix elements of the $1/r^3$ term involve Hylleraas integrals with $n_i=-2$. Their calculation using recursion relations was presented in Ref. [23], and numerical results are presented in Table II. We note a slow numerical convergence of $1/r^3$ terms and its mass polarization correction. Bethe logarithms are far the most difficult in accurate numerical evaluation and in this work we use the results obtained by Yan *et al.* in [7]. We note a weak dependence of Bethe logarithms on a state, all close to the 1S hydrogenic value.

IV. TRANSITION AND IONIZATION ENERGIES

Numerical values of all coefficients for relevant transition energies are presented for lithium and beryllium in Table III. $\mathcal{E}^{(5,0)}$ does not include there the nuclear polarizability contribution. It is a small correction, which results from modification of the nucleus by atomic electrons. The effect of nuclear polarizability in ^{11}Li was estimated in [16], and ^{11}Be^{+} is obtained here. While it does not affect, the absolute transition frequencies much, it is significant for the isotope shift and the corresponding determination of the charge radii difference, see the next section.

Obtained results for the energy expansion coefficients are in general in good agreement with the former calculation of Yan and Drake in [6,14,15], with corrections and improvements in [7]. We have not yet confirmed their results for the Bethe logarithms [7] and use them in our coefficients $\mathcal{E}^{(5,0)}$ and $\mathcal{E}^{(5,1)}$. We note that the present numerical precision of expansion coefficients is high enough, that the leading uncertainty of transition frequencies comes from $\mathcal{E}^{(6,0)}$, more precisely from the rough estimate of the relativistic (nonradiative) $m\alpha^6$ correction, which is about 10% of the leading radiative correction.

Using this expansion coefficients in Table III and atomic masses from Table IV, one obtains transition frequencies which are compared in Table V to the previous calculations of Yan *et al.* [7,14,15] and to the experimental results. Small differences with results of Drake and Yan are due to the better numerical accuracy of our results and the inclusion of

TABLE V. Comparison of our theoretical predictions with the previous theoretical and experimental values in units cm^{-1}.

	I.P. $2S_{1/2}$	$3S_{1/2}-2S_{1/2}$	$2P_{1/2}-2S_{1/2}$
^{7}Li (this work)	43 487.159 0(8)	27 206.093 7(6)	14 903.648 4(10)
^{7}Li (the)	43 487.158 3(10)[a]	27 206.093 0(10)[a]	14 903.647 9(10)[a]
^{7}Li (exp)	43 487.159 40(18)[b]	27 206.094 20(10)[c]	14 903.648 130(14)[d]
^{9}Be^{+} (this work)	146 882.918(7)	88 231.919(5)	31 928.734(8)
^{9}Be^{+} (the)	146 882.923(5)[a]	88 231.920(6)[a]	31 928.738(5)[a]
^{9}Be^{+} (exp)	146 882.86[e]	88 231.915[e]	31 928.744[e]

[a] Reference [7].
[b] Reference [25].
[c] Reference [26].
[d] Reference [24].
[e] Reference [27].

TABLE VI. Contributions to the ^{11}Li-^{7}Li isotope shift of $3S_{1/2}$-$2S_{1/2}$ transition, and to the ^{11}Be^{+9}Be^{+} shift of $2P_{1/2}$-$2S_{1/2}$ transition, with excluding the finite size correction. The second uncertainty of $\Delta\nu_{\rm the}$ is due to the atomic mass.

Correction	Li($3S_{1/2}$-$2S_{1/2}$) (MHz)	Be^{+}($2P_{1/2}$-$2S_{1/2}$) (MHz)
$\Delta\nu^{(2,1)}$	25 104.520 2(1)	31 568.577 3(8)
$\Delta\nu^{(2,2)}$	−2.967 9	0.765 7(2)
$\Delta\nu^{(4,1)}$	0.037 8(4)	−10.035 0(2)
$\Delta\nu^{(5,1)}$	−0.106 4(15)	0.877 7(36)
$\Delta\nu^{(6,1)}$	−0.020(5)	−0.092(23)
$\Delta\nu_{\rm pol}$	0.039(4)	0.208(21)
$\Delta\nu_{\rm the}$	25 101.502 8(64)(27)	31 560.302(31)(12)
$\Delta\nu_{\rm the}$ [7]	25 101.470(22)	31 560.01(6)

the finite nuclear size correction in transition and ionization energies for Be^{+}. In comparison to experimental values we observe an agreement for both the lithium atom and beryllium ion, with one exception. Namely, theoretical ionization energy is larger by 0.06 cm^{-1} than the experimental value, and this discrepancy was already pointed out in [7]. The relatively lower accuracy of theoretical results for the beryllium ion comes from the neglect of the nonradiative $m\alpha^{6}$ correction, which significantly grows with Z. The direct calculation of this correction for the three electron system is a challenge. A simpler approach would rely on matching the high Z results for lithiumlike systems [45] with the low Z results obtained by the expansion in α. We note that in spite of the relatively large uncertainties coming from $\mathcal{E}^{(6,0)}$ the obtained results for transition frequencies are the most accurate so far, and no other approach allows one for the systematic calculation of all corrections in the low Z atomic systems.

V. ISOTOPE SHIFT DETERMINATION OF NUCLEAR CHARGE RADII

The isotope shift in atomic transitions come mainly from different masses of nuclei. Much smaller effect of order $\sim 10^{-6}$ is due to different nuclear charge radii. Nevertheless, precision of isotope shift measurements and theoretical predictions is enough to derive charge radii from the comparison of the experimental and the theoretical data. Moreover, this determination of charge radii is far more accurate than the one obtained from electron scattering off nuclei and can be applied even to unstable nuclei such as ^{11}Li and ^{11}Be. From expansion coefficients for Li and Be^{+} in Table III, one obtains contributions to the isotope shift. The example for ^{11}Li-^{7}Li and ^{11}Be^{+}-^{9}Be^{+} is presented in Table VI. We observe that the leading nonrelativistic contribution gives at least 99.9% of the total isotope shift. The relativistic recoil corrections are small but still important, while the theoretical uncertainty is dominated by rough estimation of $\mathcal{E}^{(6,1)}$. The nuclear polarizability correction is significant for both ^{11}Li and ^{11}Be^{+}, and its value is presented in Table VI. Result from ^{11}Li was obtained in [16], while for ^{11}Be^{+} it is calculated here using both experimental [34] and theoretical data [35] for the so-called $B(E1)$ function which is the reduced line strength for the nuclear $E1$ excitation,

$$|\langle\phi_N|\vec{d}|E\rangle|^2 = \frac{4\pi}{3}\frac{dB(E1)}{dE}, \tag{29}$$

in units e^2 fm^2 MeV^{-1}. The kets $|\varphi_N\rangle$ and $|E\rangle$ denote the ground state of the nucleus and the excited state with excitation energy E, respectively. The relevant formula relating electric dipole nuclear transition moment with the shift of atomic energy levels is [16]

$$\nu_{\rm pol} = -m\alpha^4\left\langle\sum_a \delta^3(r_a)\right\rangle(m^3\tilde{\alpha}_{\rm pol}), \tag{30}$$

where $\tilde{\alpha}_{\rm pol}$ is a *weighted* electric polarizability of the nucleus and is given by the following double integral:

$$\tilde{\alpha}_{\rm pol} = \frac{16\alpha}{3}\int dE\frac{1}{e^2}|\langle\phi_N|\vec{d}|E\rangle|^2\int_0^\infty\frac{dw}{w}\frac{E}{E^2+w^2}\times\frac{1}{(\kappa+\kappa^\star)}\left[1+\frac{1}{(\kappa+1)(\kappa^\star+1)}\left(\frac{1}{\kappa+1}+\frac{1}{\kappa^\star+1}\right)\right], \tag{31}$$

where $\kappa = \sqrt{1+2im/w}$. The first integral over the nuclear excitation spectrum may involve a sum over discreet levels, as it is the case of ^{11}Be. This nucleus has an excited state with $E=0.320$ MeV and $B(E1)=0.116e^2$ fm^2, and a continuum spectrum starts at $E_T=0.504$ MeV. The result for $\tilde{\alpha}_{\rm pol}$ using the experimental [34] or the theoretical data [35] is

$$\tilde{\alpha}_{\rm pol} = 39.7(40)\ {\rm fm}^3 = 6.90(69)10^{-7}m^{-3}, \tag{32}$$

and this value is used to obtain the shift of energy levels $\nu_{\rm pol}$ in Eq. (5) for Be^{+} in Table VI.

From the difference between experimental and theoretical isotope shift one determines nuclear charge radii by using

TABLE VII. Summary of isotope shift determination of Li charge radii from $3S_{1/2}$-$2S_{1/2}$ transition with respect to ^{7}Li, $r(^{7}{\rm Li})=2.39(3)$ fm [39]; the first uncertainty of $\nu_{\rm the}$ comes from unknown higher order terms, the second uncertainty is due to the atomic mass.

Isotope	$\nu_{\rm exp}$ (MHz) [13]	$\nu_{\rm the}$ (MHz)	C (MHz fm^{-2})	$\delta r^2_{\rm ch}$ (fm^2)	$r_{\rm ch}$ (fm)
^{6}Li	−11 453.983(20)	−11 452.820 5(23)(2)	−1.571 9(16)	0.740(13)	2.540(28)
^{8}Li	8 635.782(44)	8 634.981 2(17)(9)	−1.572 0(16)	−0.509(28)	2.281(32)
^{9}Li	15 333.272(39)	15 331.799 5(31)(12)	−1.572 1(16)	−0.937(25)	2.185(33)
^{11}Li	25 101.226(125)	25 101.502 8(64)(27)	−1.576 8(17)	0.176(79)	2.426(34)

TABLE VIII. Summary of isotope shift determination of Be^+ charge radii from $2P_{1/2}$-$2S_{1/2}$ transition with respect to $^9\mathrm{Be}^+$, $r(^9\mathrm{Be})=2.519(12)$ fm [40], the first uncertainty of ν_{the} comes from unknown higher order terms, the second uncertainty is due to the atomic mass.

Isotope	ν_{exp} (MHz) [28]	ν_{the} (MHz)	C (MHz fm^{-2})	δr^2_{ch} (fm^2)	r_{ch} (fm)
$^7\mathrm{Be}^+$	−49 236.81(88)	−49 225.736(35)(9)	−17.021(31)	0.651(47)	2.645(14)
$^{10}\mathrm{Be}^+$	17 323.8(13)	17 310.437(13)(11)	−17.027(31)	−0.785(76)	2.358(21)
$^{11}\mathrm{Be}^+$	31 564.96(93)	31 560.302(31)(12)	−17.020(31)	−0.274(55)	2.464(16)

$$\Delta\nu_{\mathrm{exp}} - \Delta\nu_{\mathrm{the}} = C_{AB}(r^2_{\mathrm{ch}A} - r^2_{\mathrm{ch}B}), \tag{33}$$

with constant C obtained from Eq. (9) by including logarithmic relativistic corrections to the wave function at the origin

$$C = \frac{2\pi}{3} Z\alpha^4 \left\langle \sum_a \delta^{(3)}(r_a) \right\rangle [1 - (Z\alpha)^2 \ln(Z\alpha m r_{\mathrm{ch}})]. \tag{34}$$

Using isotope shifts as measured for Li in [12,13] and Be^+ in [28], we obtain nuclear charge radii for corresponding isotopes in Tables VII and VIII. Results for Li are slightly more accurate than our previous determination in [16] due to the more accurate ν_{the} and nuclear masses. Our results for Be isotopes agree with the recent determination presented in [28]. The uncertainty of our $\Delta\nu_{\mathrm{the}}$ comes mainly from 25% of $\Delta\nu^{(6,1)}$ and 10% of $\Delta\nu_{\mathrm{pol}}$. Non-negligible are numerical uncertainties of Bethe logarithms and their mass polarization corrections. The uncertainty of C coefficients comes from the estimation of relativistic correction to the wave function at origin, which is about 25% of the logarithmic part. Nevertheless, uncertainties in δr^2_{ch} come mainly from the experimental value for the isotope shift, and the uncertainty of the final r_{ch} comes mostly from the charge radius of the reference nucleus. As we have already mentioned, the direct determination of the charge radius from the absolute transition frequency is at present not possible for lithiumlike systems due to insufficient precision of theoretical predictions.

VI. SUMMARY

We have calculated nonrelativistic, relativistic, and QED contributions to low-lying energy levels of Li and Be^+ ions, including finite nuclear mass corrections. The computational method uses the Hylleraas basis set with the analytic integration technique. The obtained results are the most precise to date, with the accuracy limited mainly by higher order relativistic $m\alpha^6$ corrections. Using the experimental results for the isotope shift of $3S_{1/2}$-$2S_{1/2}$ transition in Li [12,13] and $2P_{1/2}$-$2S_{1/2}$ transition in Be^+ [28], we obtain improved charge radii for Li and Be isotopes. We note the significance of the nuclear polarizability effect in $^{11}\mathrm{Li}$ and $^{11}\mathrm{Be}^+$ and relativistic correction to the wave function at origin for the determination of charge radii.

The presented computational method is limited by unknown higher order relativistic and QED corrections, which become more significant for heavier nuclei. One possible solution for the charge radii determination for heavier nuclei is the spectroscopy of the four-electron ion, for which we think accurate calculations can be performed with the help of a Gaussian basis set with linear terms [46,47]. Apart from nuclear charge radii, precise atomic spectroscopy may bring information about the magnetic moment distribution within nuclei. Indeed a measurement of the hyperfine splitting in $^{11}\mathrm{Be}^+$ [48] may give the size of neutron halo, which cannot be probed by other means. However, the interpretation of the shift of the hyperfine splitting in terms of the Bohr-Weiskopf effect is not obvious, due to possible large nuclear polarizability effects [49].

The significant advantage of the presented computational approach with Hyllerras functions is the ability to calculate higher order relativistic [50] and QED corrections, although such a calculation is not simple. We aim to obtain $O(\alpha^2)$ and $O(\alpha^3)$ corrections to the hyperfine splitting in order to investigate nuclear structure correction with halo nuclei, and also to verify the accuracy of simplified approaches such as the relativistic configuration interaction or the multiconfiguration Dirac-Fock method.

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