RAPID COMMUNICATION

Transition frequencies between 2S and 2P states of lithium-like ions

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(Received 13 November 2022; revised manuscript received 7 December 2022; accepted manuscript online 21 December 2022)

The Schrödinger equation for the 2S and 2P states of the lithium-like ions $Z = 5$–7, 9–10 is solved by using the Rayleigh-Ritz variational method in Hylleraas coordinates. The leading-order relativistic and QED corrections are calculated perturbatively and higher-order corrections are estimated. The transition frequencies between the $2S_{1/2}$ and $2P_J$ ($J = 1/2,\ 3/2$) states are determined and compared with experimental and other theoretical results. Specifically, isotope shifts are also calculated for B^{2+}.

Keywords: Li-like ions, transition frequency, relativistic corrections, QED corrections

PACS: 31.30.jc, 31.30.jf, 31.15.xt **DOI:** 10.1088/1674-1056/acad6f

1. Introduction

For atomic systems with low nuclear charge numbers, such as $Z = 1, 2, 3, \ldots$, energy levels and other properties can be calculated to high precision in the NRQED framework,[1,2] in which the nonrelativistic Schrödinger equation is solved to high precision using variational method first, then other small effects, such as relativistic corrections and QED corrections, are taken into consideration order by order with perturbation theory. The correlation effects between electrons can be fully treated by using explicit correlated basis functions in the NRQED framework. However, for atoms with large Z, say $Z > 30$, the NRQED method is inadequate because of the slow convergence of the perturbation series, methods which are relativistic from the beginning should be adopted. Many such methods have been developed, such as the relativistic many-body perturbation theory (RMBPT)[3,4] and its variant the coupled cluster method (CC),[5,6] the relativistic configuration interaction method (RCI),[7] and the multiconfiguration Dirac–Fock method (MCDF).[8] For convenience in phrase, from now on, we call all of these methods the relativistic many-body methods (RMB). The electron correlation effect and the inadequate treatment of QED effect are the two main factors that limit the accuracy of RMB methods. Though the traditional application field of RMB methods is the high Z domain, they have been extended to the low Z domain for Li-like ions with $Z < 10$ since 1990s, such as in Refs. [9–11]. A unified theory which combined the merits of NRQED method and RMB methods was developed by Drake several decades ago,[12] and developed by Yerokhin *et al.* very recently.[13] However, this unified theory is only applied to the calculations of energy levels of helium-like ions and the fine structure splittings of lithium-like ions at present.

In the side of experiment, the lithium atom and lithium-like ions have attracted a lot of interest of researchers, especially the transition frequencies between 2S and $2P_J$ ($J = 1/2, 3/2$) states, and the fine structure of 2P state, see Refs. [14,15] and references therein. Very high accurate experimental data exists for neutral lithium atom and Be^+,[15–17] and equal or less accurate theoretical results can be gotten by NRQED calculations.[18,19] For other lithium-like ions with $Z > 4$, the energy levels are usually calculated by RMB methods and the accuracy of results is lower than the experiment in general, except for the fine structure splittings calculated by Yerokhin *et al.* using the unified theory,[13] and the ionization energies calculated by Earwood and Davis by using explicit correlated Gaussian wave functions in NRQED framework.[20] In our recent work,[21,22] referred to hereafter as paper I, we applied the NRQED method to the calculations of transition frequencies between 2S and $2P_J$ ($J = 1/2, 3/2$) states of lithium-like ion O^{5+}, including the nonrelativistic contribution, leading order relativistic correction ($O(\alpha^2)$), leading order QED correction ($O(\alpha^3)$) and the estimation of higher orders of relativistic and QED corrections. The results gotten by us are in agreement with experiment and more accurate then RMB calculations by one order of magnitude.

The purpose of the present paper is to extend the NRQED calculations to the transition frequencies between 2S and $2P_J$ ($J = 1/2, 3/2$) states of lithium-like ions with $Z = 5$–7, 9–10. By comparing with the experimental results given by Edlén in Ref. [14], we find that our results are in agreement with the experimental ones very well but more accurate than the former by a factor of 4–26 for $Z = 5$–7. More accurate experimental results have also been given in Refs. [23–25] for $Z = 5$–6, and we find that our theoretical results agree with these experimental results within 1σ or 2σ. For $Z = 9$–10, a systematic deviation with 1σ between our results and Edlén's experimental

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results[14] is found. This indicates the present "boundary" of the NRQED method in applying to three-electron atomic systems. For further improving the theoretical results, accurate calculations of α^4 a.u. order relativistic and QED corrections are needed. However this will be a very challenging task.[26] Additionally, the isotope shifts are also calculated for B^{2+} and compared with available experimental and theoretical results.

2. Theory and methods

2.1. Nonrelativistic energies and wavefunctions

The theory and method used here have been described in detail in paper I,[21,22] and else where,[27,28] here we just recapitulate them briefly for completeness. The essential points of the present paper are the data given in following paragraphs. Atomic units are used through out unless otherwise stated.

The nonrelativistic Schrödinger equation describing the internal motion of a three-electron atomic system can be written as

$$H_0\Psi_0 = E_0\Psi_0, \tag{1}$$

where

$$H_0 = -\frac{1}{2}\sum_{i=1}^{3}\nabla_i^2 - Z\sum_{i=1}^{3}\frac{1}{r_i} + \sum_{i<j}^{3}\frac{1}{r_{ij}} - \frac{\mu}{M}\sum_{i<j}^{3}\boldsymbol{\nabla}_i\cdot\boldsymbol{\nabla}_j, \tag{2}$$

in units of $2R_M$ with $R_M = (1-\frac{\mu}{M})R_\infty$, μ is the reduced mass of electron, and M is the nuclear mass.

The Rayleigh–Ritz variational method is used to solve Eq. (1), and the variational wave function is constructed by a superposition of the Hylleraas-type basis functions

$$\{\mathcal{A}\phi(\boldsymbol{r}_1,\boldsymbol{r}_2,\boldsymbol{r}_3)\}, \tag{3}$$

where

$$\phi(\boldsymbol{r}_1,\boldsymbol{r}_2,\boldsymbol{r}_3) = r_1^{j_1}r_2^{j_2}r_3^{j_3}r_{12}^{j_{12}}r_{23}^{j_{23}}r_{31}^{j_{31}}\,\mathrm{e}^{-\alpha r_1-\beta r_2-\gamma r_3} \times\mathcal{Y}^{LM}_{(\ell_1\ell_2)\ell_{12},\ell_3}(\boldsymbol{r}_1,\boldsymbol{r}_2,\boldsymbol{r}_3)\chi_1, \tag{4}$$

and

$$\mathcal{Y}^{LM}_{(\ell_1\ell_2)\ell_{12},\ell_3}(\boldsymbol{r}_1,\boldsymbol{r}_2,\boldsymbol{r}_3) = r_1^{\ell_1}r_2^{\ell_2}r_3^{\ell_3}\sum_{m_i}\langle\ell_1m_1;\ell_2m_2|\ell_1\ell_2;\ell_{12}m_{12}\rangle \times\langle\ell_{12}m_{12};\ell_3m_3|\ell_{12}\ell_3;LM\rangle Y_{\ell_1m_1}(\boldsymbol{r}_1)Y_{\ell_2m_2}(\boldsymbol{r}_2)Y_{\ell_3m_3}(\boldsymbol{r}_3) \tag{5}$$

is the vector-coupled product of spherical harmonics for the three electrons to form a state of total angular momentum L and z-component M. Also in the above, χ_1 is the spin wave function and $\mathcal{A}$ the three-particle anti-symmetrizer.

The largest number of basis functions used by us is in the range 13000–26000. The nonrelativistic energies of 2S and 2P states of all ions with $Z = 5$–7, 9–10 converge to an accuracy of 10^{-13} or better. For convenience, we write the nonrelativistic energy of any isotope of a Li-like ion as (in atomic units)

$$E = \varepsilon_0 + \lambda(\varepsilon_0+\varepsilon_1) + \lambda^2(\varepsilon_1+\varepsilon_2) + \lambda^3(\varepsilon_2+\varepsilon_3) + O(\lambda^4), \tag{6}$$

where $\lambda = -\mu/M$, ε_0 denotes the energy calculated in the assumption of infinite nuclear mass, ε_i, $i = 1,2,3$, the ith mass polarization coefficient. The values of ε_i, $i = 0,1,2,3$ are listed in Table 1. ε_1 and ε_2 are calculated by perturbation method, ε_3 is calculated by finite difference method and it has three or four accurate digits.

Table 1. Nonrelativistic energies and mass polarization coefficients of 2S and 2P states of Li-like ions, in a.u.. The data for $Z = 8$ are cited from Refs. [21,22].

Z	ε_0	ε_1	ε_2	ε_3
		$1s^22s\ ^2S$		
5	–23.424 605 721 377 08(3)	–0.606 077 703 780 98(6)	–5.497 770 853 157(6)	–1.3078
6	–34.775 511 275 996 14(3)	–0.760 164 226 592 7(2)	–8.449 207 327 94(2)	–1.9463
7	–48.376 898 319 457 78(8)	–0.914 754 296 746(1)	–12.035 468 163 3(2)	–2.7007
8	–64.228 542 083 020 7(2)	–1.069 650 001 42(3)	–16.256 605 445 2(3)	–3.5705
9	–82.330 338 097 648 0(3)	–1.224 745 660 357(3)	–21.112 659 769(2)	–4.5557
10	–102.682 231 482 659 0(2)	–1.379 979 461 553(3)	–26.603 659 624(2)	–5.6561
		$1s^22p\ ^2P$		
5	–23.204 441 193 523(3)	0.083 496 995 13(2)	–6.365 397 27(3)	–0.5382
6	–34.482 103 180 524 37(4)	0.493 997 589 7(1)	–9.946 861(2)	–0.7505
7	–48.011 054 283 019 2(2)	1.062 618 779 94(2)	–14.304 515(2)	–0.9958
8	–63.790 739 580 558(3)	1.788 338 363 60(1)	–19.438 334(2)	–1.2692
9	–81.820 880 914 764(1)	2.670 704 576 8(6)	–25.348 588 9(2)	–1.5683
10	–102.101 324 296 493(3)	3.709 492 168(1)	–32.035 533(1)	–1.8921

2.2. Leading-order relativistic corrections

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

$$\Delta E_{\mathrm{rel}} = \langle\Psi_0|H_{\mathrm{rel}}|\Psi_0\rangle, \tag{7}$$

where Ψ_0 is the nonrelativistic wave function calculated by variational method and $H_{\rm rel}$ denotes the Breit–Pauli operators for three-electron atomic systems

$$\begin{aligned} H_{\rm rel} &= B_1 + B_2 + B_{3z} + B_{3e} + B_5 \\ &\quad - \pi\alpha^2 \sum_{i<j}^{3} \left(1 + \frac{8}{3}\boldsymbol{s}_i \cdot \boldsymbol{s}_j\right) \delta(\boldsymbol{r}_{ij}) \\ &\quad + \frac{1}{2} Z\pi\alpha^2 \sum_{i=1}^{3} \delta(\boldsymbol{r}_i) + \frac{m_{\rm e}}{M}\left(\tilde{\Delta}_2 + \tilde{\Delta}_{3z}\right) \\ &\quad + \gamma\left(2B_{3z} + \frac{4}{3}B_{3e} + \frac{2}{3}B_{3e}^{(1)} + 2B_5\right) + \gamma\frac{m_{\rm e}}{M}\tilde{\Delta}_{3z}. \end{aligned} \tag{8}$$

The explicit expressions of B_1, B_2, etc in the above equation are given in paper I. The terms containing γ are spin-dependent QED corrections due to the electron anomalous magnetic moment, which are discussed here for convenience. The expectation values of these relativistic correction operators are listed in Tables 2 and 3.

Table 2. Expectation values of spin-independent relativistic correction operators, in a.u. The masses of nuclei are assumed to be infinite, the symbol [x] in each entry means 10^x, and the data for $Z = 8$ are cited from Refs. [21,22].

Z	B_1	B_2	$\sum_i \delta(\boldsymbol{r}_i)$	$\sum_{i<j} \delta(\boldsymbol{r}_{ij})$	$\tilde{\Delta}_2$
			$1s^2 2s\ ^2S$		
5	–3.661 996 841 8(5)[–2]	–8.317 930 500 4(4)[–5]	7.146 106 958 07(7)[1]	3.476 708 402 6(1)	–6.055 976 771 2(2)[–2]
6	–7.849 169 663(2)[–2]	–1.273 805 783(1)[–4]	1.269 682 468 394(4)[2]	6.495 022 263 9(2)	–1.294 527 852 78(2)[–1]
7	–1.489 437 330 19(4)[–1]	–1.810 613 101 2(1)[–4]	2.056 847 845 39(2)[2]	1.089 774 647 41(1)[1]	–2.451 191 794 56(3)[–1]
8	–2.587 438 417(1)[–1]	–2.442 236 651(2)[–4]	3.116 690 319(2)[2]	1.694 717 141 7(3)[1]	–4.250 842 824(4)[–1]
9	–4.203 871 340(2)[–1]	–3.168 689 02(1)[–4]	4.489 793 906 3(6)[2]	2.490 559 715 7(2)[1]	–6.896 691 391(2)[–1]
10	–6.480 960 642 8(3)[–1]	–3.989 977 928(6)[–4]	6.216 742 867(3)[2]	3.503 532 833 5(2)[1]	–1.061 990 500 3(3)
			$1s^2 2p\ ^2P$		
5	–3.532 992 494(3)[–2]	–3.369 786 46(3)[–5]	6.915 849 885 6(6)[1]	3.313 549 34(1)	–5.763 719 491(2)[–2]
6	–7.531 420 47(3)[–2]	–1.651 351 69(1)[–5]	1.222 406 986 27(2)[2]	6.162 932 638(1)	–1.221 728 092 5(2)[–1]
7	–1.423 820 367(1)[–1]	2.662 698 30(4)[–5]	1.973 142 874 5(1)[2]	1.031 383 721 95(1)[1]	–2.299 605 481 1(2)[–1]
8	–2.466 802 874(1)[–1]	1.034 902 018(2)[–4]	2.981 998 14(1)[2]	1.601 288 946(2)[1]	–3.970 384 215(4)[–1]
9	–3.999 765 787 2(6)[–1]	2.218 548 60(3)[–4]	4.287 173 729(6)[2]	2.350 669 463(3)[1]	–6.419 804 87(1)[–1]
10	–6.156 593 336 0(6)[–1]	3.895 053 581(5)[–4]	5.926 868 798 6(4)[2]	3.304 185 035(1)[1]	–9.858 969 483(2)[–1]

Table 3. Expectation values of spin-dependent relativistic correction operators of $2P_{1/2}$ states, in a.u. The masses of nuclei are assumed to be infinite, the symbol [x] in each entry means 10^x, and the data for $Z = 8$ are cited from Refs. [21,22].

Z	B_{3z}	B_{3e}	$B_{3e}^{(1)}$	$\tilde{\Delta}_{3z}$
5	–2.0440172(8)[–4]	1.011438082(3)[–4]	5.263832(4)[–5]	1.59385184(1)[–4]
6	–5.53511578(1)[–4]	2.28928955(1)[–4]	1.163176174(1)[–4]	4.46730803(3)[–4]
7	–1.215572609(3)[–3]	4.31645854(4)[–4]	2.16173716(1)[–4]	9.9455468(7)[–4]
8	–2.33384178(2)[–3]	7.25915890(5)[–4]	3.60077531(3)[–4]	1.9208178(2)[–3]
9	–4.07820363(3)[–3]	1.12837605(2)[–3]	5.5590923(2)[–4]	3.3650381(3)[–3]
10	–6.64516976(4)[–3]	1.65567094(2)[–3]	8.1155308(2)[–4]	5.4882916(6)[–3]

2.3. Leading-order QED corrections

The leading-order QED corrections of order α^3 can be expressed in the form

$$E_{\rm QED} = E_{\rm L,1} + E_{\rm M,1} + E_{\rm R,1} + E_{\rm L,2}, \tag{9}$$

where $E_{\rm L,1}$ denotes the mass-independent QED corrections to the electron–nucleus interaction, $E_{\rm M,1}$ the corrections due to finite nuclear mass, i.e., mass scaling and mass polarization effects, and $E_{\rm R,1}$ the QED recoil corrections. $E_{\rm L,2}$ denotes the QED corrections due to the interaction between a pair of electrons. These terms have the explicit expressions as follows:

$$\begin{aligned} E_{\rm L,1} &= \frac{4}{3} Z\alpha^3 \left\langle \sum_i \delta(\boldsymbol{r}_i) \right\rangle^{(0)} \\ &\quad \times \left[\ln(Z\alpha)^{-2} - \beta^{(0)}(1s^2 n\ell^2 L) + \frac{19}{30}\right], \end{aligned} \tag{10}$$

$$\begin{aligned} E_{\rm M,1} &= \frac{\mu}{M} \frac{\langle \sum_i \delta(\boldsymbol{r}_i)\rangle^{(1)}}{\langle \sum_i \delta(\boldsymbol{r}_i)\rangle^{(0)}} E_{\rm L,1} + \frac{\mu}{M}\frac{4}{3} Z\alpha^3 \left\langle \sum_i \delta(\boldsymbol{r}_i) \right\rangle^{(0)} \\ &\quad \times \left[1 - \Delta\beta_{\rm MP}(1s^2 n\ell^2 L)\right], \end{aligned} \tag{11}$$

$$\begin{aligned} E_{\rm R,1} &= \frac{\mu}{M}\frac{4}{3} Z^2\alpha^3 \left\langle \sum_i \delta(\boldsymbol{r}_i) \right\rangle^{(0)} \left[\frac{1}{4}\ln(Z\alpha)^{-2} \right. \\ &\quad \left. - 2\beta(1s^2 n\ell^2 L) - \frac{1}{12} - \frac{7}{4} a(1s^2 n\ell^2 L)\right], \end{aligned} \tag{12}$$

$$E_{\rm L,2} = E_{\rm L,2}^{(0)} + \frac{\mu}{M} E_{\rm L,2}^{(1)} + \cdots, \tag{13}$$

$$\begin{aligned} E_{\rm L,2}^{(0)} &= \alpha^3 \left(\frac{14}{3}\ln\alpha + \frac{164}{15}\right) \sum_{i<j} \langle \delta(\boldsymbol{r}_{ij})\rangle^{(0)} \\ &\quad - \frac{14}{3}\alpha^3 Q^{(0)}, \end{aligned} \tag{14}$$

$$\begin{aligned} E_{\rm L,2}^{(1)} &= \alpha^3 \left(\frac{14}{3}\ln\alpha + \frac{164}{15}\right) \sum_{i<j} \langle \delta(\boldsymbol{r}_{ij})\rangle^{(1)} \\ &\quad - \frac{14}{3}\alpha^3 \left(Q^{(1)} + \sum_{i<j} \langle \delta(\boldsymbol{r}_{ij})\rangle^{(0)}\right), \end{aligned} \tag{15}$$

$$a(1s^2 n\ell^2 L) = \frac{2Q_1^{(0)}}{\left\langle \sum_i \delta(\boldsymbol{r}_i) \right\rangle^{(0)}} + 2\ln Z - 3. \tag{16}$$

Table 4. Expectation values of QED operators, in a.u. The data for $Z = 8$ are cited from Refs. [21,22].

Z	$Q_1^{(0)}$	$Q^{(0)}$	$Q^{(1)}$	$\beta^{(0)}$	$\Delta\beta_{\rm MP}$
			$1s^22s\ ^2S$		
5	–163.734 317 1(3)	–2.348 785 0(3)	6.357 657(2)	2.977 981(6)	0.133 08(3)
6	–314.348 152(2)	–5.882 004 7(4)	15.297 81(2)	2.977 250(4)	0.138 25(2)
7	–541.281 658(5)	–11.911 917(3)	30.299 87(3)	2.976 739(2)	0.142 01(2)
8	–862.204 17(2)	–21.203 37(2)	53.166 39(2)[a]	2.976 364(2)	0.144 86(1)
9	–1 295.394 01(5)	–34.563 43(3)	85.798 3(1)	2.976 077(1)	0.147 10(1)
10	–1 859.658 72(3)	–52.835 63(3)	130.181 86(1)	2.975 851(1)	0.148 91(1)
			$1s^22p\ ^2P$		
5	–158.257 907(4)	–2.120 358(3)	6.281 36(6)	2.982 122(5)	0.128 56(6)
6	–302.188 595(3)	–5.307 829(2)	14.930 92(2)	2.982 067(6)	0.133 50(6)
7	–518.395 797(7)	–10.754 51(3)	29.344 2(5)	2.982 041(6)	0.137 07(6)
8	–823.500 85(7)	–19.159 51(1)	51.212 9(5)[a]	2.982 030(6)	0.140 2(5)
9	–1 234.694 6(5)	–31.261 72(2)	82.320 0(2)	2.982 026(6)	0.141 90(6)
10	–1 769.662 7(2)	–47.834 4(1)	124.529 4(3)	2.982 027(6)	0.143 60(6)

[a]The figure in Refs. [21,22] contains a mass-scaling contribution, here this contribution is subtracted.

Since the expectation values of $\delta(r_i)$ and $\delta(r_{ij})$ have been calculated in the leading-order relativistic corrections, only the operators $Q_1^{(0)}$, $Q^{(0)}$, $Q^{(1)}$, $\beta^{(0)}$ and $\Delta\beta_{\rm MP}$ need to be calculated. We listed the expectation values of these operators in Table 4.

2.4. Higher order corrections

Though the α^4 order effective relativistic and QED correction operators for a general N-electron atom have been derived by V. Patkóš, *et al.*,[26] the numerical computations of the expectation values of these operators are very complicated for Li-like ions and have never been completed up to now. So we use the following formulas to estimate the α^4 order contribution and α^5 order contribution:

$$\begin{aligned} E_{\rm H} = & \frac{4}{3}Z\alpha^3\left\langle\sum_i\delta(r_i)\right\rangle^{(0)}\{(3\pi\alpha Z)\,0.765\,405\,577 \\ & +\frac{\alpha}{\pi}\,[0.404\,206-(3\alpha Z/4)21.556\,85] \\ & +(Z\alpha)^2\big[-(3/4)\ln^2(Z\alpha)^{-2} \\ & +C_{61}(1s^2n\ell^2L)\ln(Z\alpha)^{-2}+C_{60}(1s^2n\ell^2L)\big]\}. \quad (17) \end{aligned}$$

The above equation is a generalization of the hydrogenic Lamb shift to three-electron atomic systems. It dominates the α^4 order and α^5 order contributions for light atomic systems and gives the main uncertainty of the theoretical results. For $Z = 4$–7, we take 10% of α^4 order contribution as its uncertainty, and take 25% of α^5 order contribution as its uncertainty. For $Z = 9$–10, the percentages are increased to 20% and 50%, respectively. For more details about the theory and method, please refer to Refs. [19,27,28].

At last, the correction due to nuclear finite size is calculated by the nonrelativistic approximation formula

$$\Delta E_{\rm nuc} = \frac{2}{3}\pi Z(r_{\rm c}/a_0)^2\left\langle\sum_i\delta(r_i)\right\rangle, \quad (18)$$

where $r_{\rm c}$ is the root-mean-square radius of the nuclear charge distribution and a_0 is the Bohr radius.

3. Transition energies and discussion

Based on the data listed in Tables 1–4, we finally get the transition energies between $2S_{1/2}$ and $2P_J, J = 1/2, 3/2$ states of Li-like ions with $Z = 5$–7, 9–10. We list the breakdown of various contributions to the transition energies in Tables 5 and 6. It is easy seen that, compared with the accuracy of available experimental results, the nonrelativistic contribution, leading-order relativistic contribution, leading-order QED contribution and the nuclear finite mass and nuclear finite size contributions are all calculated to sufficient accuracy, i.e., accurate to 10^{-7} eV or better. The major uncertainty comes from the higher order ($O(\alpha^4)$ and $O(\alpha^5)$) relativistic and QED contributions, which are calculated approximately.

For B^{2+}, high precision transition energies and isotope shifts have been measured by Litzén and Kling with a Fourier transform spectrometer and a Penning discharge source.[23] For isotope ^{11}B, their results are $\Delta E(2S_{1/2}-2P_{1/2}) = 5.995\,693\,2(12)$ eV and $\Delta E(2S_{1/2}-2P_{3/2}) = 5.999\,921\,1(12)$ eV. Ours theoretical results are $\Delta E(2S_{1/2}-2P_{1/2}) = 5.995\,690\,9(45)$ eV and $\Delta E(2S_{1/2}-2P_{3/2}) = 5.999\,916\,5(45)$ eV, which are in agreement with Litzén and Kling's experimental results within 1σ. For isotope ^{10}B, Litzén and Kling's experimental results are $\Delta E(2S_{1/2}-2P_{1/2}) = 5.995\,574\,4(25)$ eV and $\Delta E(2S_{1/2}-2P_{3/2}) = 5.999\,802\,3(25)$ eV. Ours theoretical results are $\Delta E(2S_{1/2}-2P_{1/2}) = 5.995\,568\,1(45)$ eV and $\Delta E(2S_{1/2}-2P_{3/2}) = 5.999\,793\,8(45)$ eV, which are in agreement with Litzén and Kling's experimental results within 2σ. The isotope shifts of ^{11}B relative to ^{10}B in the transitions $2S_{1/2}$–$2P_J$, $J = 1/2, 3/2$ are also measured by Litzén and Kling and the values are 0.958(22) cm^{-1} for both lines. Our theoretical results 0.99093(23) cm^{-1} for $2S_{1/2}$–$2P_{1/2}$ and 0.99119(23) cm^{-1} for $2S_{1/2}$–$2P_{3/2}$ are in agreement with Litzén and Kling's experimental results but more accurate by two orders of magnitude. Our results of isotope shifts are also in agreement with the nonrelativistic calculation of Godefroid

et al.[31] The breakdown of the isotope shifts are listed in Table 7. It is easy seen that the uncertainties of isotope shifts calculated by us are wholly due to the uncertainty of the nuclear charge radius difference.

Table 5. Transition energies between $2S_{1/2}$ and $2P_{1/2}$ states of Li-like ions, in eV. The data for $^{16}O^{5+}$ are cited from Refs. [21,22].

Term	$^{11}B^{2+}$	$^{12}C^{3+}$	$^{14}N^{4+}$	$^{16}O^{5+}$	$^{19}F^{6+}$	$^{20}Ne^{7+}$
E_{NR}	5.990 982 00	7.984 041 0	9.955 123 3	11.913 212 9	13.863 036 1	15.807 289 8
μ/M	–0.001 233 76	–0.001 925 5	–0.002 498 5	–0.003 076 6	–0.003 461 8	–0.004 234 9
$(\mu/M)^2$	–0.000 000 01	0.000 000 0	0.000 000 0	0.000 000 0	0.000 000 0	0.000 000 0
α^2	0.006 692 78	0.014 572 9	0.026 846 8	0.044 456 9	0.068 346 9	0.099 461 2
$(\mu/M)\alpha^2$	0.000 000 63	0.000 001 4	0.000 002 6	0.000 004 3	0.000 006 1	0.000 009 3
α^3	–0.000 712 50(1)	–0.001 623 6	–0.003 118 5	–0.005 354 0(2)	–0.008 485 9	–0.012 665 1(5)
$(\mu/M)\alpha^3$	–0.000 000 08	–0.000 000 2	–0.000 000 6	–0.000 001 2[a]	–0.000 001 9	–0.000 003 3
α^4	–0.000 042 9(43)	–0.000 126(13)	–0.000 305(31)	–0.000 640(64)	–0.001 22(24)	–0.002 15(43)
α^5	0.000 006 1(15)	0.000 020(5)	0.000 054(14)	0.000 130(40)	0.000 26(13)	0.000 49(25)
Nuclear size	–0.000 001 36(3)	–0.000 003 5	–0.000 007 8	–0.000 016 0	–0.000 031 1	-0.000 053 3
Total (theory)	5.995 690 9(45)	7.994 956(14)	9.976 096(33)	11.948 72(10)	13.918 44(28)	15.888 14(50)
Experiment	5.995 62(12)[b]	7.995 00(12)[b]	9.976 14(12)[b]	11.948 98(12)[b]	13.918 59(25)[b]	15.888 69(25)[b]
	5.995 693 2(12)[c]	7.994 954(11)[d]				
		7.994 962(62)[e]				
Other theory		7.994 7(14)[f]	9.975 7(16)[f]	11.948 2(16)[f]	13.917 8(16)[f]	15.887 4(19)[f]

[a]This figure in Refs. [21,22] is incorrect, here we modified it. [b]Ref. [14], [c]Ref. [23], [d]Ref. [24], [e]Ref. [25], [f]Ref. [11].

Table 6. Transition energies between $2S_{1/2}$ and $2P_{3/2}$ states of Li-like ions, in eV. The data for $^{16}O^{5+}$ are cited from Refs. [21,22].

Term	$^{11}B^{2+}$	$^{12}C^{3+}$	$^{14}N^{4+}$	$^{16}O^{5+}$	$^{19}F^{6+}$	$^{20}Ne^{7+}$
E_{NR}	5.990 982 00	7.984 041 0	9.955 123 3	11.913 212 9	13.863 036 1	15.807 289 8
μ/M	–0.001 233 76	–0.001 925 5	–0.002 498 5	–0.003 076 6	–0.003 461 8	–0.004 234 9
$(\mu/M)^2$	–0.000 000 01	0.000 000 0	0.000 000 0	0.000 000 0	0.000 000 0	0.000 000 0
α^2	0.010 907 47	0.027 821 5	0.058 844 4	0.110 087 7	0.188 750 3	0.303 117 9
$(\mu/M)\alpha^2$	0.000 000 31	0.000 000 5	0.000 000 8	0.000 001 2	0.000 001 4	0.000 001 8
α^3	–0.000 701 18(1)	–0.001 589 3	–0.003 037 3	–0.005 190 0(2)	–0.008 188 1(7)	–0.012 165 4(5)
$(\mu/M)\alpha^3$	–0.000 000 08	–0.000 000 2	–0.000 000 6	–0.000 001 2[a]	–0.000 001 9	–0.000 003 3
α^4	–0.000 042 9(43)	–0.000 126(13)	–0.000 305(31)	–0.000 64(6)	–0.001 22(24)	–0.002 15(43)
α^5	0.000 006 0(15)	0.000 020(5)	0.000 054(14)	0.000 13(4)	0.000 26(13)	0.000 49(25)
Nuclear size	–0.000 001 36(3)	–0.000 003 5	–0.000 007 8	–0.000 016 0	–0.000 031 1	–0.000 053 3
Total (theory)	5.999 916 5(45)	8.008 238(14)	10.008 173(33)	12.014 51(10)	14.039 14(28)	16.092 28(50)
Experiment	5.999 87(12)[b]	8.008 30(12)[b]	10.008 25(12)[b]	12.014 69(12)[b]	14.039 60(25)[b]	16.093 14(25)[b]
	5.999 921 1(12)[c]	8.008 262 1(50)[d]				
		8.008 224(62)[e]				
Other theory		8.007 8(14)[f]	10.007 6(16)[f]	12.013 8(16)[f]	14.038 4(16)[f]	16.092 2(19)[f]

[a]This figure in Refs. [21,22] is incorrect, here we modified it. [b]Ref. [14],[c]Ref. [23], [d]Ref. [24], [e]Ref. [25], [f]Ref. [11].

Table 7. Isotope shifts of $^{11}B^{2+}$ relative to $^{10}B^{2+}$ in the transitions between 2S and 2P states, in cm^{-1}.

Term	$2P_{1/2}-2S_{1/2}$	$2P_{3/2}-2S_{1/2}$
μ/M	0.990 424 3	0.990 424 3
$(\mu/M)^2$	0.000 020 2	0.000 020 2
$(\mu/M)^3$	0.000 000 0	0.000 000 0
$(\mu/M)\alpha^2$	–0.000 511 0	–0.000 256 0
$(\mu/M)\alpha^3$	0.000 070 2	0.000 070 4
$(\mu/M)\alpha^4$	–0.000 001 0(5)	–0.000 001 0(5)
Nuclear size	0.000 93(23)[a]	0.000 93(23)[a]
Total	0.990 93(23)	0.991 19(23)
Experiment	0.958(22)[b]	0.958(22)[b]
	0.813 1(834)[c]	0.841 0(626)[c]
Other theory	0.990 66[d]	0.990 66[d]

[a]The difference of mean-square charge radius $\langle r_c^2\rangle^{11} - \langle r_c^2\rangle^{10} = -0.49(12)\text{fm}^2$ is taken from Ref. [29].

[b]Ref. [23], [c]Ref. [30], [d]Ref. [31].

For C^{3+}, our theoretical result 7.994 956(14) eV for the $2S_{1/2}$–$2P_{1/2}$ transition agrees with the experimental result 7.994 954(11) eV measured by Griesmann and Kling with interferometry[24] very well, and also agrees with the recent experimental result 7.994 962(62) eV measured by Winzen *et al.* with laser spectroscopy.[25] For the transition $2S_{1/2}$–$2P_{3/2}$, our result 8.008 238(14) eV agrees with Griesmann and Kling's experimental result 8.008 262 1(50) eV[24] within 2σ, and agrees with the lower accurate experimental results 8.008 224(62) in Ref. [25].

For N^{4+}, F^{6+} and Ne^{7+}, we only find one set of experimental results, which are given by Edlén in 1983.[14] For N^{4+}, our results are in agreement with Edlén's experimental results but more accurate by a factor of 4. For F^{6+} and Ne^{7+}, the

uncertainties of our results increase very rapidly, and exceed the experimental ones. For the $2S_{1/2}$–$2P_{1/2}$ transition, our results are in agreement with the experimental ones within 1σ; for the $2S_{1/2}$–$2P_{3/2}$ transition, the agreement between theory and experiment is within 2σ. This phenomenon indicates the present "boundary" of the NRQED method in calculating the energy levels of three-electron atomic systems. It is worth to note that, for the $2S_{1/2}$–$2P_{3/2}$ transition in Ne^{7+}, our result calculated in NRQED framework is the same as the one calculated by Yerokhin *et al.* with RCI method.[11] For other lines, our results are systematically larger then the ones calculated by Yerokhin *et al.* but more accurate by a factor of 4–20.

The following physical constants are used: fine structure constant $\alpha = 1/137.035\,999\,084(21)$, 1 a.u. $= 27.211\,386\,245\,988(53)$ eV $= 2.194\,746\,313\,6320(43)$ cm^{-1}.[32] The masses of the atoms and the nuclear charge radii are listed in Table 8.

Table 8. Atomic masses and nuclear charge radii.

Z	Isotope	Mass (u)[a]	Charge radius (fm)[b]
5	^{10}B	10.012 936 862(016)	2.4278(0492)
	^{11}B	11.009 305 167(013)	2.4059(0291)
6	^{12}C	12.000 000 000	2.4703(0022)
7	^{14}N	14.003 074 004 251(241)	2.5037(0081)
9	^{19}F	18.998 403 162 067(883)	2.8976(0024)
10	^{20}Ne	19.992 440 175 3(16)	3.0053(0021)

[a] Ref. [33], [b] Ref. [34].

4. Conclusion

In the present paper, we calculate the nonrelativistic, leading-order relativistic, leading-order QED and nuclear finite mass and finite size contributions to the transition energies between $2S_{1/2}$ and $2P_J$, $J = 1/2, 3/2$ states of Li-like ions with $Z = 5$–7, 9–10 in the NRQED framework. Higher order relativistic and QED corrections are estimated. We find that all of our theoretical results are in agreement with the the available experimental results in literature within 2σ. Our results are also consistent with the theoretical results calculated by Yerokhin *et al.* with RCI method,[11] but more accurate than the latter by a factor of 4–20 in general. For further improving the theoretical results, rigorous treatment of the α^4 a.u. correction and even the α^5 a.u. correction are necessary. However, it will be a very challenging task.[26] Additionally, the isotope shifts are also calculated for B^{2+}, and our theoretical results are in agreement with the experimental results but more accurate.

Acknowledgements

Project supported by the National Natural Science Foundation of China (Grant No. 11774080). ZCY was supported by NSERC of Canada. The computing facility at SHARCnet of Canada is gratefully acknowledged. We thank Yongbo Tang for useful discussions.

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