Nonrelativistic energies and fine-structure splittings for the Rydberg *P* states of lithium

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The Schrödinger equation for the nP $(4 \leqslant n \leqslant 10)$ states of lithium is solved using the Rayleigh-Ritz variational method in Hylleraas coordinates, where the asymptotic behavior of the wave function that is specific to a Rydberg state is built in explicitly to improve the accuracy of the solution. The nonrelativistic variational energies of the nP $(4 \leqslant n \leqslant 10)$ states reach an accuracy of 10^{-13} to 10^{-14}. In addition, the fine-structure splittings of these states are also calculated and compared with experimental results.

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I. INTRODUCTION

In the past two decades, significant progress has been made in high-precision spectroscopy of atomic lithium, both experimentally [1–7] and theoretically [8–14]. For the first three lowest states of lithium, i.e., the $2S$, $3S$, and $2P$ states, the nonrelativistic energies have been calculated to an accuracy of 10^{-14} to 10^{-15} [11,13,14]. The leading-order relativistic and QED corrections of α^2 and α^3 (in a.u. units), respectively, have been evaulated precisely [10,11,13,14]. The higher-order relativistic and QED corrections can only be evaluated approximately at present time. However, the α^4 order correction to the fine-structure splitting of the $2P$ state has been calculated rigorously by Puchalski and Pachucki [12]. The theoretical fine-structure splittings between $2P_{1/2}$ and $2P_{3/2}$ for both ^{6}Li and ^{7}Li agree very well with the most accurate measurements [6,7]. The theoretical transition frequencies between the $2\ ^2S_{1/2}$ and $3\ ^2S_{1/2}$ states in ^{6}Li and ^{7}Li [10,13] also agree with the best measurements, but less accurate than the measured values by two orders of magnitude [3,4]. To further improve the theoretical accuracy, one has to treat the higher-order relativistic and QED corrections of orders α^4 and α^5 rigorously, which will be very challenging for theorists [15].

In addition to these lowest-lying states, highly excited Rydberg states of lithium have also been studied both experimentally [16–22] and theoretically [11,14,23–28]. The energies of the $4S$ to $9S$ states and transition frequencies between $2S$ and nS $(4 \leqslant n \leqslant 9)$ states were calculated in Hylleraas coordinates by Puchalski and Pachucki [11], including the relativistic and QED corrections, and compared with available experimental values. These calculations were repeated and extended up to the $13S$ state very recently by Bralin *et al.* [14] with explicitly correlated Gaussian (ECG) bases. The nonrelativistic energies of the nP $(2 \leqslant n \leqslant 10)$ and nD $(3 \leqslant n \leqslant 11)$ states were also evaluated by Adamowicz's group using ECG bases [26–28]. Although the Schrödinger equation for low-lying states of Li can be solved variationally with high precision, as n increases, the accuracy of the result gradually decreases. In order to overcome this drawback, Drake [29,30] introduced a "zero-order" term in his variational basis set of helium in a Rydberg state, which reflects explicitly the asymptotic behavior of the wave function, and demonstrated its effectiveness of dealing with highly excited states. This method was also extended to the calculations of the $2S$ and $2P$ states of lithium-like ions by Yan *et al.* [31]. However, the advantage of including the zero-order wave function is to deal with high-lying states rather than low-lying ones.

The main purpose of the present paper is to extend this "zero-order" strategy to three-electron atomic lithium in Rydberg states and provide benchmark results for further studies. Specifically, we focus on the nP $(4 \leqslant n \leqslant 10)$ states of lithium and demonstrate that the zero-order wave function is essential in maintaining the stability of the algorithm and the accuracy of the nonrelativistic variational energies, as the principal quantum number increases. The nonrelativistic energies of these states are calculated to an accuracy of 10^{-13} to 10^{-14}, which are the most precise results so far. In addition, the fine-structure splittings of these states are also calculated and compared with available experimental values.

The physical constants used here are as follows. The fine-structure constant is $\alpha = 1/137.035\,999\,046(31)$ [32], the Rydberg constant is $R_\infty = 10\,973\,731.568\,508(65)$ m^{-1} [33], and the atomic masses of ^{6}Li and ^{7}Li are, respectively, 6.015 122 8874(15) u and 7.016 003 437(5) u [34].

The present paper is organized as follows. Section II discusses the construction of the variational wave functions. Section III presents the calculated nonrelativistic energy eigenvalues and a comparison with other literature values. In Sec. IV the Hamiltonian responsible for the fine structure is introduced and the fine-structure splittings are evaluated. Finally, a summary is given in Sec. V.

II. HAMILTONIAN AND VARIATIONAL BASIS SETS

After separating out the center of mass motion, the nonrelativistic energy eigenvalue problem for a three-electron atomic system is [35] (in atomic units throughout, unless otherwise stated)

$$H\Psi = E\Psi, \tag{1}$$

where

$$H = -\frac{1}{2}\sum_{i=1}^{3}\nabla_i^2 - Z\sum_{i=1}^{3}\frac{1}{r_i} + \sum_{i<j}^{3}\frac{1}{r_{ij}} - \frac{\mu}{M}\sum_{i<j}^{3}\nabla_i\cdot\nabla_j, \tag{2}$$

in units of $2R_M$ with $R_M = (1-\frac{\mu}{M})R_\infty$, μ is the reduced mass of electron, M is the nuclear mass, Z is the nuclear charge, r_i denotes the distance between electron i and the nucleus, and r_{ij} is the distance between electron i and electron j. Since $\mu/M \sim 10^{-4}$ for light atoms, the last term in Eq. (2) may be treated as a perturbation. Alternatively, one can diagonalize the full Hamiltonian H in Eq. (2). In the limit of infinite nuclear mass, Eq. (2) becomes

$$H = -\frac{1}{2}\sum_{i=1}^{3}\nabla_i^2 - Z\sum_{i=1}^{3}\frac{1}{r_i} + \sum_{i<j}^{3}\frac{1}{r_{ij}}, \tag{3}$$

in units of $2R_\infty$. Following Ref. [31], we repartition the Hamiltonian in Eq. (3) into

$$H = H_S + V_I, \tag{4}$$

where H_S is the Hamiltonian describing the core, which consists of the nucleus and two $1s$ electrons, and the valence electron

$$H_S = \left(-\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 - \frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{r_{12}}\right) + \left(-\frac{1}{2}\nabla_3^2 - \frac{Z-2}{r_3}\right), \tag{5}$$

and V_I describes the interaction between the core and the valence electron

$$V_I = \frac{1}{r_{23}} + \frac{1}{r_{31}} - \frac{2}{r_3}. \tag{6}$$

When the atom is in a Rydberg state, the valence electron will be far away from the core, so that r_{23}, r_{31}, and r_3 will be large. As a result, the interaction V_I will be small compared to H_S, and so H_S could be considered as a good approximation to the full Hamiltonian. Thus, the solution to the zero-order eigenequation

$$H_S\psi_0 = E_0\psi_0 \tag{7}$$

can be written as the following direct product:

$$\psi_0 = \phi_c(1s^2\ {}^1S)\phi(nl, Z-2). \tag{8}$$

In the above, $\phi_c(1s^2\ {}^1S)$ is the ground-state eigenfunction of the helium-like ion with the nuclear charge Z, which can be easily constructed variationally using Hylleraas coordinates [30]; and $\phi(nl, Z-2)$ is the nl-state eigenfunction of the hydrogen-like ion with the core charge $Z-2$, which has an analytical expression.

The variational wave function for the full Hamiltonian in Eq. (3) is expanded in the form

$$\Psi = \mathcal{A}\left(a_0\psi_0\chi_1 + \sum_{i=1}^{N}a_i\psi_i(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)\chi_1\right), \tag{9}$$

where

$$\psi_i(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3) = r_1^{j_1}r_2^{j_2}r_3^{j_3}r_{12}^{j_{12}}r_{23}^{j_{23}}r_{31}^{j_{31}}e^{-\alpha r_1-\beta r_2-\gamma r_3} \times \mathcal{Y}^{LM}_{(\ell_1\ell_2)\ell_{12},\ell_3}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3) \tag{10}$$

is a basis function with

$$\mathcal{Y}^{LM}_{(\ell_1\ell_2)\ell_{12},\ell_3}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3) = r_1^{\ell_1}r_2^{\ell_2}r_3^{\ell_3}\sum_{m_i}\langle\ell_1m_1;\ell_2m_2|\ell_1\ell_2;\ell_{12}m_{12}\rangle \times\langle\ell_{12}m_{12};\ell_3m_3|\ell_{12}\ell_3;LM\rangle Y_{\ell_1m_1}(\mathbf{r}_1)Y_{\ell_2m_2}(\mathbf{r}_2)Y_{\ell_3m_3}(\mathbf{r}_3) \tag{11}$$

being the vector-coupled product of spherical harmonics for the three electrons to form the eigenstate of the total angular momentum squared L^2 and its z component M. Also in the above, χ_1 is the spin wave function and $\mathcal{A}$ the three-particle antisymmetrizer. With some truncations to avoid near linear dependence, all terms in Eq. (10) are included in the basis set such that

$$j_1 + j_2 + j_3 + j_{12} + j_{23} + j_{31} \leqslant \Omega, \tag{12}$$

where Ω is an integer. Further details about the construction of variational wave functions and matrix element evaluations can be found in Ref. [36].

III. NONRELATIVISTIC ENERGIES

In our calculations, when we enlarge the size of basis set N in Eq. (9) from 1870 to 22302 progressively, a smooth convergence pattern for the energy eigenvalues of the nP $(4 \leqslant n \leqslant 10)$ states can be formed, as shown in Table I, for the case of infinite nuclear mass, which indicates that these energy eigenvalues are converged to an accuracy of 10^{-13} to 10^{-14}. Also listed in the table are the energy eigenvalues calculated by Bubin and Adamowicz with ECG bases [27]. From the table one can see that the accuracy of their results becomes decreased from 4×10^{-10} to 1×10^{-7} as n increases from 4 to 10. This clearly demonstrates the importance of including the zero-order wave function in the variational wave function to maintain computational stability and accuracy. The energy levels for the ^{6}Li and ^{7}Li isotopes are also listed and compared with the values in Ref. [27].

IV. FINE-STRUCTURE SPLITTING

After obtaining the variational wave functions, the fine-structure splitting between the $nP_{1/2}$ and $nP_{3/2}$ states can be calculated using first-order perturbation theory. The fine-structure Hamiltonian can be written as

$$H_{\rm FS} = B_{3z} + B_{3e} + B_5 + \gamma\left(2B_{3z} + \frac{4}{3}B_{3e} + \frac{2}{3}B_{3e}^{(1)} + 2B_5\right) + \frac{m_e}{M}\tilde{\Delta}_{3z}, \tag{13}$$

TABLE I. Convergence study of the nonrelativistic energies for the $1s^2np\ ^2P$ $(4 \leqslant n \leqslant 10)$ states of lithium, where Ω is defined in Eq. (12) and N is the size of basis set, in atomic units.

Ω	N	$4P$	$5P$	$6P$	$7P$
9	1 870	−7.31188905957709	−7.30028816418607	−7.29402005312551	−7.29025490715296
10	3 300	−7.31188906045844	−7.30028816564631	−7.29402005506111	−7.29025491194212
11	5 600	−7.31188906073524	−7.30028816619148	−7.29402005531174	−7.29025491268719
12	9 160	−7.31188906075443	−7.30028816625896	−7.29402005536851	−7.29025491278110
13	13 230	−7.31188906075780	−7.30028816626384	−7.29402005537599	−7.29025491279438
14	17 094	−7.31188906075833	−7.30028816626470	−7.29402005537724	−7.29025491279614
15	22 302	−7.31188906075855	−7.30028816626505	−7.29402005537765	−7.29025491279716
	∞	−7.3118890607587(2)	−7.3002881662651(1)	−7.2940200553779(3)	−7.290254912799(2)
	$^{\infty}$Li[a]	−7.31188905938	−7.30028816488	−7.29402005293	−7.29025490809
	^{7}Li	−7.3112951016176(2)	−7.29969490233930(6)	−7.2934271878104(4)	−7.289662291990(2)
	^{7}Li[a]	−7.31129510065	−7.29969490106	−7.29342718542	−7.28966228734
	^{6}Li	−7.3111962542635(2)	−7.29959617066065(5)	−7.2933285220817(4)	−7.289563667321(2)
	^{6}Li[a]	−7.31119625321	−7.29959616923	−7.29332851960	−7.28956366258

Ω	N	$8P$	$9P$	$10P$
9	1 870	−7.28781807022726	−7.28615099205447	−7.28496059869027
10	3 300	−7.28781807924023	−7.28615101903177	−7.28496064365122
11	5 600	−7.28781808040483	−7.28615102681110	−7.28496065079984
12	9 160	−7.28781808055639	−7.28615102834520	−7.28496065283604
13	13 230	−7.28781808060789	−7.28615102840383	−7.28496065307241
14	17 094	−7.28781808061356	−7.28615102842079	−7.28496065310388
15	22 302	−7.28781808061515	−7.28615102842333	−7.28496065310864
	∞	−7.2878180806158(6)	−7.2861510284238(5)	−7.2849606531095(9)
	$^{\infty}$Li[a]	−7.28781806801	−7.28615097321	−7.28496052960
	^{7}Li	−7.2872256236354(6)	−7.2855586856755(5)	−7.2843683931451(9)
	^{7}Li[a]	−7.28722561109	−7.28555863054	−7.28436826971
	^{6}Li	−7.2871270262255(6)	−7.2854601072730(5)	−7.2842698285171(9)
	^{6}Li[a]	−7.28712701359	−7.28546005205	−7.28426970499

[a] Results from Ref. [27].

where

$$B_{3z} = \frac{Z\alpha^2}{2}\sum_{i=1}^{3}\frac{1}{r_i^3}\mathbf{r}_i \times \mathbf{p}_i \cdot \mathbf{s}_i, \tag{14}$$

$$B_{3e} = \frac{\alpha^2}{2}\sum_{i\neq j}^{3}\frac{1}{r_{ij}^3}\mathbf{r}_{ji} \times \mathbf{p}_i \cdot (\mathbf{s}_i + 2\mathbf{s}_j), \tag{15}$$

$$B_5 = \alpha^2\sum_{i>j}^{3}\left[\frac{1}{r_{ij}^3}(\mathbf{s}_i \cdot \mathbf{s}_j) - \frac{3}{r_{ij}^5}(\mathbf{r}_{ij} \cdot \mathbf{s}_i)(\mathbf{r}_{ij} \cdot \mathbf{s}_j)\right], \tag{16}$$

$$\tilde{\Delta}_{3z} = Z\alpha^2\sum_{i=1}^{3}\frac{1}{r_i^3}\mathbf{r}_i \times \mathbf{p} \cdot \mathbf{s}_i, \tag{17}$$

$$B_{3e}^{(1)} = \frac{\alpha^2}{2}\sum_{i\neq j}^{3}\frac{1}{r_{ij}^3}\mathbf{r}_{ji} \times \mathbf{p}_i \cdot (\mathbf{s}_i - \mathbf{s}_j), \tag{18}$$

and

$$\gamma \approx \frac{\alpha}{2\pi} + (-0.32847)\left(\frac{\alpha}{\pi}\right)^2. \tag{19}$$

In Eq. (13) the terms proportional to γ are the spin-dependent part of the electron anomalous magnetic moment corrections, and the last term is the relativistic recoil correction due to the finite nuclear mass. For a spin doublet state, the expectation value of the spin-spin term B_5 vanishes. Some singular integrals encountered in the calculations of B_{3e} and $B_{3e}^{(1)}$ can be handled by the special methods developed by Yan and Drake [36].

The next higher-order relativistic correction, not included in Eq. (13), is at the order of α^4. The theory of the α^4 correction has been established by Puchalski and Pachucki using nonrelativistic QED (NRQED) approach, and it has been applied to the fine-structure calculations of the $2P$ states of lithium and lithium-like beryllium ion [12,37]. Since a rigorous evaluation of this correction is very complicated, for a higher-n state, we use the following Dirac formula (in natural units) to make an estimation:

$$\begin{aligned} E_{nj} &= m\left\{1 + \frac{(Z\alpha)^2}{\left[\sqrt{(j+1/2)^2-(Z\alpha)^2}+n-(j+1/2)\right]^2}\right\}^{-1/2} \\ &= m\left\{1 - \frac{(Z\alpha)^2}{2n^2} - \frac{(Z\alpha)^4}{2n^3}\left(\frac{1}{j+1/2} - \frac{3}{4n}\right)\right. \\ &\quad - \frac{(Z\alpha)^6}{8n^3}\left[\frac{1}{(j+1/2)^3} + \frac{3}{n(j+1/2)^2}\right. \\ &\quad \left.\left. - \frac{6}{n^2(j+1/2)} + \frac{5}{2n^3}\right] + \cdots\right\}, \end{aligned} \tag{20}$$

where the terms proportional to $m(Z\alpha)^6$ (or $Z^6\alpha^4$ in a.u.) will give an approximate value of the α^4 order correction to the

TABLE II. Contributions to the fine-structure splittings of the $1s^2np\ ^2P_J$ $(4 \leqslant n \leqslant 10)$ states of lithium, in MHz.

Term	$4P$	$5P$	$6P$	$7P$	$8P$	$9P$	$10P$
α^2	1194.9943(3)	606.9620(3)	349.4284(4)	219.2390(2)	146.4731(2)	102.6568(2)	74.71172(2)
$(\mu/M)\alpha^2$	−0.3721(2)	−0.1945(2)	−0.11315(5)	−0.07164(3)	−0.04835(5)	−0.03411(5)	−0.02479(2)
α^3	4.4342336(2)	2.266078(1)	1.3087766(3)	0.822722(2)	0.5503279(2)	0.3860191(2)	0.2811026(2)
$(\mu/M)\alpha^3$	−0.000350(1)	−0.0001917(3)	−0.0001149(3)	−0.0000743(1)	−0.0000507(1)	−0.0000365(3)	−0.0000266(1)
Subtotal	1199.0560(5)	609.0333(5)	350.62391(25)	219.99000(23)	146.97503(25)	103.00867(25)	74.96800(4)
α^4	0.045(45)	0.023(12)	0.013(3)	0.0077(19)	0.0051(13)	0.0035(9)	0.0025(6)
Total theory, ^{7}Li	1199.101(45)	609.056(12)	350.6369(35)	219.9977(22)	146.9810(15)	103.0121(11)	74.97050(66)
Total theory, ^{6}Li	1199.039(45)	609.023(12)	350.6180(35)	219.9857(22)	146.9721(20)	103.0064(12)	74.96637(66)
Experiment, ^{7}Li	1199.65(11)[a]						74.97(74)[b]

[a] From Ref. [16].

[b] From Ref. [22].

fine-structure splitting. For a Rydberg state of lithium atom, the valence electron can be seen as an independent electron moving in an approximate Coulomb field generated by the nucleus and the two inner electrons; so we expect that the Dirac formula can give a good approximation to the α^4 order contribution.

In Table II we list the various contributions to the fine-structure splittings of the nP $(4 \leqslant n \leqslant 10)$ states of ^{7}Li and the total contribution to ^{6}Li. Since the α^4 order contribution is estimated according to Eq. (20), we take the whole value of this contribution as its uncertainty for the $4P$ state, 50% of the value as its uncertainty for the $5P$ state, and 25% of the value as the uncertainty for any other state. One can see that, for all the states in Table II, the theoretical uncertainty mainly comes from the α^4 order contribution. At present, there are only two experimental measurements reported in the literature, which are 1199.65(11) MHz for the $4P$ state of ^{7}Li measured by Isler and co-workers in 1969 [16], and 74.97(74) MHz for the $10P$ state of ^{7}Li measured by Oxley and Collins in 2010 [22]. Our theoretical value 1199.101(45) MHz for the $4P$ state of ^{7}Li disagrees with the experimental value of Ref. [16] by 3.5σ standard deviations. For the $10P$ state, our theoretical value 74.97050(66) MHz is in agreement with the experimental value of Ref. [22] but is more accurate than the measured value by three orders of magnitude.

V. SUMMARY

We have solved the Schrödinger equation variationally for the nP $(4 \leqslant n \leqslant 10)$ states of lithium in Hylleraas coordinates. The zero-order wave function was included in the variational wave function, which has proven to be effective in maintaining numerical stability and accuracy of the energy eigenvalues as the principal quantum number increases. All the energy eigenvalues have been calculated to an accuracy of 10^{-13} to 10^{-14}, which represents the most accurate results so far. It is expected that our approach of including the zero-order wave function in the variational wave function will be even more powerful for other higher-lying Rydberg states, such as nD and nF states. The fine-structure splittings of the nP $(4 \leqslant n \leqslant 10)$ states have also been calculated for both ^{6}Li and ^{7}Li and compared with only a few available measured values. We hope to see that our work can stimulate more theoretical and experimental activities in this field, especially for high-(n, L) states [38], to understand more quantum behaviors of atomic Rydberg states, such as the Casimir-Polder effect [17,18].

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