Calculations of Bethe logarithm for hydrogen and helium using B-splines in different gauges

Yong-Hui Zhang, Lu-Jun Shen, Chang-Min Xiao, Jun-Yi Zhang, and Ting-Yun Shi

1 State Key Laboratory of Magnetic Resonance and Atomic and Molecular Physics, Wuhan Institute of Physics and Mathematics, Innovation Academy for Precision Measurement Science and Technology, Chinese Academy of Sciences, Wuhan 430071, People’s Republic of China
2 Department of Physics, Hunan Normal University, Changsha 410081, People’s Republic of China
E-mail: tyshi@wipm.ac.cn

Received 8 October 2019, revised 16 March 2020
Accepted for publication 20 April 2020
Published 4 June 2020

Abstract
The efficient and simple B-splines variational method is successfully used to calculate Bethe logarithm for the hydrogen atom in the velocity and length gauges. The ground state Bethe logarithm of hydrogen with fourteen accurate figures is obtained in the velocity gauge, and in the length gauge the ground state value has eleven accurate figures. Present velocity- and length-gauge results for the ns, np, nd, and nf states up to n = 200 of hydrogen are above the $10^{-10}$ level of relative difference, which represent the successful variational attempt to calculate Bethe logarithm of hydrogen in the velocity and length gauges. In addition, the B-splines variational method is successfully extended to calculate Bethe logarithm for the helium atom combined with configuration interaction. Results of numerical calculations for $n^{1S}$ up to $n = 8$ states are presented in the acceleration gauge, the velocity gauge, and a hybrid of the velocity and acceleration gauges (also called pa-gauge). For the $2^3S$ state, the acceleration-gauge value of 4.3640367(2) a.u. and the pa-gauge value of 4.3640364(2) a.u. both have eight significant digits. For other triplet S states, present results in three different gauges all have five to seven accurate figures. While for the singlet S states, the best convergent values are obtained in the pa-gauge, of which the relative differences with the latest results are at the $10^{-6}$ to $10^{-8}$ orders of magnitude.

Keywords: Bethe logarithm, hydrogen, helium, B-splines, different gauges

(Some figures may appear in colour only in the online journal)

1. Introduction

The lamb shift between the $2s_1/2$ and $2p_1/2$ energy levels of hydrogen discovered by Lamb and Retherford [1], has laid the experimental foundation of the quantum electronic dynamics (QED). Then Bethe performed a nonrelativistic calculation and provided a satisfactory explanation to the lamb shift of hydrogen atom [2]. Now the experimental measurements and theoretical determinations of transition energies in atoms with one and more than one electron have advanced in accuracy to the point that they are sensitive to the QED contribution [3–6]. At the leading term in the QED correction to the energy levels based modern QED theory [7], one will encounter a quantity involving logarithm sum, which is called Bethe logarithm (BL from now on). BL determines the single most important part of the QED shift for the energy levels of atoms.

BL is one of the most complicated numerical evaluation quantities. Mainly due to the fact that the logarithmic term $\ln |E_n - E_0|$ exists, where $E_0$ and $E_n$ are energies for the initial and intermediate states. Moreover there is no way to...
avoid the explicit dependence of BL on \((E_n - E_0)\) in one pure gauge. It is explained in detail that, on the one hand there will be a large contribution to BL from highly excited states, on the other hand, the negative contribution of the intermediate bound states will be cancelled by contributions from continuum states with energies \(E_n \geq 1 + E_0\), and this large cancellation requires an accurate representation of both the low- and high-energy regions of the spectrum [8, 9], which certainly leads to the general variational techniques to collapse.

A variety of nonvariational methods [10–14] and variational methods of calculating the hydrogen atom BL in the acceleration or velocity gauge [8, 9, 15–18] have been proposed, and results with high accuracy have been achieved. In addition, the Gaussian basis set has been used in calculating the hydrogen atom BL as well [19], although giving a little poorer results than such as that obtained by the modified Slater–Laguerre radial functions [18]. It must be noted that the spectral representation method in references [13, 14] are successfully finished in the length gauge, and abundant BL have been given for the ground state, low-lying and Rydberg states.

For the case of helium, in 1961 Schwartz first developed an integration representation to evaluate BL for the ground state of helium [20], and his result has been the most accurate for more than 30 years [8, 21, 22]. In 1999, Drake and Goldman suggested a direct variational method [17] to estimate BL for helium, in which the expression of BL was represented in terms of the acceleration gauge dipole operator. This method has been used to calculate BL for the ground and some low-lying states of helium [17, 23], and the estimated accuracy is about nine to twelve significant digits. The same year, Korobov [24] carried out the Schwartz-type expansion to compute BL for the \(1\)S and \(2\)S states of helium to a precision of \(10^{-6}\) to \(10^{-7}\). Korobov also has developed the Schwartz approach to deal with BL for a general three-body system such as helium [25], in which the dipole matrix elements are expressed in the velocity gauge. There have been other reports on the calculations of BL for the ground state and low-lying S states of helium as well [22, 26–29].

B-splines are piecewise polynomials defined in a finite interval, which have much good mathematical properties, such as localization, approximation completeness, and the feasible adjustment of knots [30, 31]. B-splines have been successfully used to compute the hydrogen atom BL in the acceleration gauge [32], which largely simplify the calculations and give high-accuracy results. This mainly due to that B-splines can give good approximations to the bound and continuum states at the same time. As a follow-up to this work, in the present paper, we will calculate the hydrogen atom BL in the velocity and length gauges with the B-splines variational method. Moreover, we will extend B-splines variational method to compute BL for the helium atom combined with configuration interaction [33, 34], and calculations of BL for the S states are carried out in the acceleration, velocity-acceleration and velocity gauges. Atomic units are used throughout this paper, and all calculations are finished in quadruple precision except special indications.

2. Formulations

BL is responsible for the nonrelativistic part of the self-energy of an electron in a quantum state interacting with transverse photons, and can be evaluated using nonrelativistic quantum mechanics. BL is defined by a sum over intermediate states [8]

\[
\beta = \frac{B}{C},
\]

where

\[
B^{(A)} = \sum_n \int |\langle \psi_0 | Zr \rangle_{\psi_n}|^2 (E_n - E_0)^{-1} \ln |E_n - E_0|, \tag{2}
\]

and

\[
C^{(A)} = \begin{cases} \sum_n \int |\langle \psi_0 | Zr \rangle_{\psi_n}|^2 (E_n - E_0)^{-1}, & \text{for s state,} \\ \frac{2Z^4}{n_0^6}, & \text{otherwise,} \end{cases} \tag{3}
\]

are expressed in the dipole acceleration gauge. In equations (2) and (3), \(Z\) is the nuclear charge, \(r\) represents the position vector of the electron relative to the nucleus, the operator \(\hat{Zr}\) will becomes \(\sum Zn\) if there is more than one electron, \(\psi_0\) and \(E_0\) are the wavefunction and energy of the initial state with \(n_0\) being the principal quantum number, and similarly \(\psi_n\) and \(E_n\) label the wavefunction and energy for one of a complete set of intermediate states. The summation integration over intermediate states includes the bound states as well as the continuum.

Based on the equivalent forms for the dipole transition matrix element [35], the expressions in the velocity and length gauges can be obtained respectively, where

\[
B^{(V)} = \sum_n \int \left| \langle \psi_0 | p | \psi_n \rangle \right|^2 (E_n - E_0) \ln |E_n - E_0|, \tag{4}
\]

is in the velocity gauge with \(p\) being the momentum operator, and

\[
B^{(L)} = \sum_n \int \left| \langle \psi_0 | r | \psi_n \rangle \right|^2 (E_n - E_0)^3 \ln |E_n - E_0|, \tag{5}
\]

is in the length gauge. Expressions for \(C^{(V)}\) and \(C^{(L)}\) can be obtained according to equations (4) and (5) by removing the logarithm term \(\ln |E_n - E_0|\). In addition, another expressions for BL in the other gauge which is called the pa-gauge are as following [9, 18],

\[
B^{(PA)} = \sum_n \int \left| \langle \psi_0 | Zr \rangle_{\psi_n} \langle p | \psi_n \rangle \right| \ln \left| \frac{\langle \psi_0 | Zr | \psi_n \rangle}{\langle \psi_n | p | \psi_n \rangle} \right| \tag{6}
\]

\[
C^{(PA)} = \sum_n \int \left| \langle \psi_0 | Zr \rangle_{\psi_n} \langle p | \psi_n \rangle \right|^2. \tag{6}
\]

The pa-gauge is a hybrid of the velocity and acceleration gauges, and can avoid the explicit inclusion of energies of the intermediate states. Different gauges can be used to monitor the calculations.
In order to calculate BL, we must obtain energies and wavefunctions firstly. In present calculations, the Hamiltonian of hydrogen is expressed as

$$H = \frac{p^2}{2} - \frac{Z}{r},$$

(7)

and the hydrogen atom wavefunction is written as

$$\psi_{n\ell m}(r) = |n\ell m\rangle = \sum_i c_i B_i^{\ell}(r) Y_{\ell m}(\hat{r}),$$

(8)

where \(c_i\) is the expansion coefficient, the radial component of the wavefunction is expanded with \(N\) B-splines with the order of \(k = 11\), and the angular component is a spherical harmonic function. The Hamiltonian of helium can be written as

$$H = \frac{p_1^2}{2} - \frac{Z}{r_1} + \frac{p_2^2}{2} - \frac{Z}{r_2} + \frac{1}{r_{12}},$$

(9)

and the helium atom wavefunction will be expanded as following,

$$\psi_{LM}(r_1, r_2) = \sum_{i,j,\ell_1,\ell_2} c_{i,j,\ell_1,\ell_2}(r_1, r_2)$$

(10)

with \(L\) being the orbital angular quantum number with the projection of \(M_L\), \(c_{i,j,\ell_1,\ell_2}\) being the expansion coefficient, and the configuration wavefunction \(\phi_{i,j,\ell_1,\ell_2}(r_1, r_2)\) taking the form

$$\phi_{i,j,\ell_1,\ell_2}(r_1, r_2) = B_i^{\ell_1}(r_1) B_j^{\ell_2}(r_2) Y_{\ell_1,\ell_2}^{LM}(\hat{r}_1, \hat{r}_2) + (-1)^{\ell_1+\ell_2+L} B_j^{\ell_1}(r_1) B_i^{\ell_2}(r_2) Y_{\ell_2,\ell_1}^{LM}(\hat{r}_1, \hat{r}_2),$$

(11)

where the radial components are constructed in terms of B-splines of order \(k = 7\), and \(Y_{\ell_1,\ell_2}^{LM}(\hat{r}_1, \hat{r}_2)\) is a coupled spherical harmonic which takes the form

$$Y_{\ell_1,\ell_2}^{LM}(\hat{r}_1, \hat{r}_2) = \sum_{m_1m_2} \langle \ell_1 m_1, \ell_2 m_2 | LM \rangle Y_{\ell_1 m_1}(\hat{r}_1) Y_{\ell_2 m_2}(\hat{r}_2).$$

(12)

The angular quantum numbers \(\ell_1\) and \(\ell_2\) in equations (11) and (12) will be chosen as the number of partial wave \(\ell_{\text{max}}\). The full-configuration-interaction calculations are performed for helium.

B-splines used to expand radial wavefunctions are defined by the exponential knots. The exponential knots \(\{t_i\}\) with the exponential parameter \(\gamma\) employed here will be the same with that used in reference [36],

$$t_i = \begin{cases} 0, & i = 1, 2, \ldots, k - 1; \\ R_0 \exp\left[\frac{\gamma}{R_0}\left(\frac{i-k}{k}^k\right) - 1\right], & i = 1, 2, \ldots, N - 1; \\ R_0, & i = N + k - 1, N + k; \end{cases}$$

(13)

here \(R_0\) represents the radius of the box where the hydrogen or helium atom is placed in. All matrix elements, including the Hamiltonian and the overlap matrices, are evaluated using Gaussian–Legendre quadrature, which are near the machine precision. By full diagonalization of the Hamiltonian matrix with the subroutine of RSG from LAPACK, we will obtain the quasi eigenspectrum for hydrogen or helium atom, including the bound states and quasi-continuum states, i.e. energies and normalized wavefunctions for the initial and intermediate states to calculate BL.

3. The hydrogen atom BL

To begin with, we carry out a calculation of BL for the ground state of hydrogen as a test and demonstration case in the velocity and length gauges. Results of BL for the ground state of hydrogen of \(\beta^{(V)}(1s)\) and \(\beta^{(L)}(1s)\), separately in the velocity and length gauges, with the numbers of B-splines, \(N\), and the exponential parameter of \(\gamma\) changing, are presented in table 1, where the order of B-splines is \(k = 11\) and the radius of the box is \(R_0 = 50\) a.u. The values of \(B^{(V)}(1s)\), \(C^{(V)}(1s)\), \(B^{(L)}(1s)\) and \(C^{(L)}(1s)\) are also listed. \(\delta C^{(V)}(1s) = |C^{(V)}(1s) - C^{\text{exact}}|\) and \(\delta C^{(L)}(1s) = |C^{(L)}(1s) - C^{\text{exact}}|\), of which \(C^{\text{exact}}\) is equal to 2. \(C\) can be used to monitor the completeness of present B-splines basis and the convergence rate. Convergence studies of \(C^{(V)}(1s)\) and \(C^{(L)}(1s)\) as the changing of \(N\) and \(\gamma\) are displayed in figure 1. Calculations in table 1 and figure 1 are finished in the double precision.

In figure 1, only the number of B-splines \(N\) are marked on the abscissa, and the corresponding \(\gamma\) parameter can be found in the table 1. We can see that the convergent rate of \(C^{(V)}(1s)\) is better than that of \(C^{(L)}(1s)\), which indicates that BL in the velocity gauge converges better than in the length gauge when calculations are performed in the pure gauge. In addition, the convergence of BL for hydrogen in the acceleration gauge has been studied by Tang et al [32]. Moreover, previous calculations [8, 9, 18] have presented that the best convergence of BL is obtained in the acceleration gauge. It is concluded that, for hydrogen, BL in the acceleration gauge gives the best convergent result, convergence rate in the velocity gauge is the second, and results in these two gauges are better than the length gauge.
the double precision.

The relationships between the first non-zero inner knot, \( t_{12} \), the energy of the highest intermediate state, \( E_{\text{max}} \), BL for the ground state of hydrogen in the velocity and length gauges with the highest energy in the intermediate states and the first non-zero inner knot, will be investigated by changing the exponential parameter \( \gamma \) at a large range. Here the box size is \( R_0 = 200 \) a.u., and the number of B-splines is \( N = 300 \) with the order of \( k = 11 \). \( \gamma \) will be determined by changing the value of itself from small to large. In present calculations, the first nonzero inner knot is \( t_{12} \), and \( E_{\text{max}} \) represents the highest energy value in the intermediate energy spectrum.

From the top half of the table 1, it can be seen that with increasing \( N \) and changing \( \gamma \), the convergent rate of \( C^{(V)} \) is somewhat better than that of \( B^{(V)} \) because of the existence of the logarithm term, which limits largely the numerical precision of BL. The ground state BL of 2.290981(1) with six convergent figures are obtained easily in present velocity-gauge calculations for \( N = 50 \) and \( \gamma = 0.296 \).

At the bottom half of the table 1, the length-gauge result of \( \beta^{(L)}(1s) = 2.290981(1) \) with six convergent figures is obtained. Because of the numerical cancellations, the convergence of \( \beta^{(L)} \) is a little better than \( B^{(L)} \). In addition, it indicates that the value of BL is very sensitive to the exponential parameter \( \gamma \) for the relatively small dimension of B-splines basis in present length-gauge calculations of table 1.

Table 2 lists the comparison of present value of BL with those given with the same B-splines functions, and those obtained using approximately the same number of basis functions. All values are compared to the exact group-theoretical result [11]. For the sake of comparison, only some selected figures given by Huff are shown in the last row. Present calculations are finished in the double precision.

### Table 1. Results of BL (a.u.) for the ground state of hydrogen in the velocity and length gauges with the numbers of B-splines, \( N \), and the exponential parameter of \( \gamma \) changing. The order of B-splines is \( k = 11 \), and the radius of the box is \( R_0 = 50 \) a.u. Calculations are finished in the double precision.

| \((N, \gamma)\) | \(\beta^{(V)}(1s)\) | \(B^{(V)}(1s)\) | \(C^{(V)}(1s)\) | \(\delta C^{(V)}(1s)\) |
|-----------------|------------------|------------------|------------------|------------------|
| (20, 0.15)      | 2.288            | 4.576            | 1.99986          | 1.38 \times 10^{-4} |
| (35, 0.23)      | 2.290918         | 4.58183          | 1.999969718      | 3.03 \times 10^{-6} |
| (40, 0.249)     | 2.2909808        | 4.58196366       | 2.0000008956     | 8.96 \times 10^{-7} |
| (50, 0.296)     | 2.290981337      | 4.58196283       | 2.0000006603     | 6.60 \times 10^{-8} |

### Table 2. Comparisons of present value of BL (a.u.) with those given with the same B-splines functions, and those obtained using approximately the same number of basis functions. All values are compared to the exact group-theoretical result [11]. For the sake of comparison, only some selected figures given by Huff are shown in the last row. Present calculations are finished in the double precision.

| Term   | \(N\) | Basis set | \(\beta(1s)\) |
|--------|------|-----------|---------------|
| \(\beta^{(L)}\) | 50   | B-spline  | 2.29098143    |
| \(\beta^{(V)}\) | 50   | B-spline  | 2.290981337   |
| \(\beta^{(V)}\) [16] | 102  | B-spline  | 2.290981277   |
| \(\beta^{(V)}\) [18] | 54   | Slater–Laguerre | 2.290945 |
| \(\beta^{(V)}\) [19] | 45   | Gaussian  | 2.2908556864  |
| \(\beta_{\text{max}}\) [11] | 2.290981375 |               |
Table 3. Results of BL (a.u.) in the velocity and length gauges for the ground state of hydrogen using different exponential parameter, $\gamma$, $t_{12}$ represents the first non-zero inner knot, $E_{\text{max}}$ represents the energy of the highest intermediate state. The number of B-splines is $N = 300$ with the order of $k = 11$, the radius of the box is $R_0 = 200$ a.u., and, $[a,b]$ represents $a \times 10^b$. The digits in italics do not converge. Too many non-convergent digits of BL are listed in order to show the difference between values in two different gauges.

| $\gamma$ | $t_{12}$ | $E_{\text{max}}$ | $\beta^{(V)}(1s)$ | $\beta^{(L)}(1s)$ |
|----------|----------|-----------------|-------------------|-------------------|
| 0.005    | 0.392    | 4.44 [3]        | 2.254 042 947     | 2.254 042 951     |
| 0.015    | 0.107    | 5.96 [4]        | 2.280 895 920 439 8 | 2.280 895 920 439 6 |
| 0.026    | 1.98 [−2] | 1.72 [6]        | 2.289 104 140 602 218 432 865 | 2.289 104 140 602 218 432 849 |
| 0.036    | 3.73 [−3] | 4.81 [7]        | 2.290 626 523 744 997 489 703 | 2.290 626 523 744 997 489 704 |
| 0.047    | 5.45 [−4] | 2.23 [9]        | 2.290 929 303 425 834 593 785 2 | 2.290 929 303 425 834 593 785 8 |
| 0.057    | 9.04 [−5] | 8.06 [10]       | 2.290 972 712 409 531 547 2 | 2.290 972 712 409 531 547 3 |
| 0.067    | 1.45 [−5] | 3.09 [12]       | 2.290 979 978 362 145 709 37 | 2.290 979 978 362 145 709 31 |
| 0.078    | 1.89 [−6] | 1.80 [14]       | 2.290 981 192 323 899 089 91 | 2.290 981 192 323 899 089 93 |
| 0.088    | 2.92 [−7] | 7.52 [15]       | 2.290 981 346 903 679 587 95 | 2.290 981 346 903 679 587 92 |
| 0.098    | 4.45 [−8] | 3.22 [17]       | 2.290 981 370 882 427 71 | 2.290 981 370 882 427 72 |
| 0.109    | 5.54 [−9] | 2.06 [19]       | 2.290 981 374 664 871 | 2.290 981 374 664 872 |
| 0.119    | 8.27 [−10] | 9.16 [20]      | 2.290 981 375 124 593 | 2.290 981 375 124 592 |
| 0.130    | 1.01 [−10] | 6.06 [22]      | 2.290 981 375 195 6 | 2.290 981 375 195 8 |
| 0.140    | 1.49 [−11] | 2.78 [24]      | 2.290 981 375 204 | 2.290 981 375 202 |
| 0.150    | 2.18 [−12] | 1.28 [26]      | 2.290 981 375 205 | 2.290 981 375 218 |
| 0.160    | 3.18 [−13] | 5.99 [27]      | 2.290 981 375 205 521 | — |
| 0.172    | 3.14 [−14] | 6.10 [29]      | 2.290 981 375 205 550 | — |

Term $\beta^{(1s)}$

- Present$^{(V)}$: 2.290 981 375 218
- Present$^{(L)}$: 2.290 981 375 205 550
- Reference [15]: 2.290 981 375 205 611
- Reference [18]: 2.290 981 375 205 552 301 342 514
- Reference [11]: 2.290 981 375 205 552 301 342 544 9686

Figure 3. The differences between results of BL for $n_s$ (up to $n = 200$) states of hydrogen in the velocity or length gauge and results in the acceleration gauge. $N = 3000$ B-splines with the order of $k = 11$ are used, the box radius is $R_0 = 110 000$ a.u., and, the exponential parameter is $\gamma = 0.000 27$.

Figure 4. The differences between results of BL for $n_p$ (up to $n = 200$) states of hydrogen in the velocity or length gauge and results in the acceleration gauge. $N = 3000$ B-splines with the order of $k = 11$ are used, the box radius is $R_0 = 110 000$ a.u., and, the exponential parameter is $\gamma = 0.000 2$.

obtained by full diagonalization. The relationship between $t_{12}$, $E_{\text{max}}$, $\beta^{(V)}(1s)$ and $\gamma$ are graphically shown in the figure 2. And numerical results are given in table 3. The digits in italics do not converge. Too many non-convergent digits of BL are listed in order to show the difference between values in two different gauges.

From the figure 2, we can see that as we gradually increase the value of $\gamma$, the first non-zero inner knot of $t_{12}$ correspondingly decreases. More and more higher $E_{\text{max}}$ of the largest energy in the intermediate states is achieved with using each new set of B-splines defined by each changing $\gamma$, as a result, $\beta^{(V)}(1s)$ is approaching the exact value of Huff’s [11], which indicates that the main contribution of BL come from high-energy region.

Table 3 shows that $\beta^{(V)}(1s)$ and $\beta^{(L)}(1s)$ have the same convergent results till $\gamma$ increased to 0.140, and achieve a value...
obtained by B-splines variational method both in the velocity and length gauges.

Then BL of ns, np, nd, and nf states up to n = 200 are calculated based on the velocity- and length-gauge formulations in this subsection. The acceleration-gauge results are taken as a benchmark. Quantities \( \delta^{(V)}(n\ell) = \left| \frac{\beta^{(V)}(n\ell) - \beta^{(A)}(n\ell)}{\beta^{(A)}(n\ell)} \right| \) and \( \delta^{(L)}(n\ell) = \left| \frac{\beta^{(L)}(n\ell) - \beta^{(A)}(n\ell)}{\beta^{(A)}(n\ell)} \right| \) are defined to analyze the agreement between different gauges. Results are graphically displayed in figures 3–6. For s and p states, \( \gamma = 0.00027 \), and the first nonzero inner knot is at \( 10^{-10} \) orders of magnitude, \( E_{\text{max}} \) is at the \( 10^{22} \) order of magnitude, correspondingly, energies for the 1s, 40s, 80s, 100s, and 200s, are respectively, \( -0.500000000000000003 \), \(-0.000312499999999999999 \), and \(-0.000012499999999999997 \) a.u. which shows that as the principal quantum number \( n \) increased, the numerical approximation precision is gradually decreasing. In order to reproduce much better d, f, and g states, \( \gamma = 0.0002 \), which makes the radial B-splines not much concentrated nearest the nuclei, and thus the first nonzero inner knot is at \( 10^{-7} \) orders of magnitude, \( E_{\text{max}} \) is at the \( 10^{17} \) order of magnitude, energy for the 200g state is \(-0.000012499999999999997 \) a.u. which approximates the exact energy \(-1/2 \times 200^2 = -0.0000125 \) a.u. very well. Present acceleration-gauge values have ten significant figures and can fully reproduce results shown in references [13, 14]. Figures 3–6 show that the agreement with the acceleration gauge is better in the velocity gauge than in the length. The bigger the value of \( \gamma \), such as \( \gamma = 0.00027 \) bigger than 0.0002, the much more radial B-splines concentrated nearest the nuclei, the numerical approximation precision of energies will fall relatively faster. Moreover, for s state in the length gauge, because of the term of \((E_n - E_0)^2\), so the accuracy of BL is relatively poor. For the same \( \gamma \), the numerical approximation precision of energies is gradually decreasing as \( n \) increased, and thus in the velocity and length gauges, computational accuracy of BL are correspondingly reduced. But results under different gauges agree with each other better than \( 10^{-10} \) orders of magnitude, which implies that B-splines variational method has succeed in calculating BL for Rydberg states of hydrogen in the velocity and length gauges, moreover has given high precision results with ten significant figures.

### 4. The helium atom BL

For helium, we will take the \( 2^3S \) state as an example to examine the convergence of BL with the increasing number of B-splines, \( N \), and the partial wave, \( \ell_{\text{max}} \). Previous calculations suggest that good computational values of BL can be obtained with the magnitude of the first nonzero inner knot equal to \( 10^{-6} \) to \( 10^{-7} \) [32]. In the present calculations, we will adjust the exponential parameter, \( \gamma \), to make the first nonzero inner knot of \( \delta_{\ell} \) at \( 10^{-6} \) to \( 10^{-7} \) orders of magnitude. Table 4 presents the convergence study of BL for the \( 2^3S \) state in the acceleration gauge. The helium atom is placed in a relative small box with \( R_0 = 20 \) a.u. because of only BL of the \( 2^3S \) state being considered. \( \gamma \) is adjusted to be 0.855, and values of \( \delta_{\ell} \) are listed in the second column of table 4. As is seen from table 4 the...
convergence rate is somewhat higher as $N$ increased than as $\ell_{\text{max}}$ increased. This convergence style suggests that we can fix the partial wave of $\ell_{\text{max}}$, then increase the number of B-splines of $N$ to obtain our final convergent result. The extrapolated convergent value is given as $4.364 \pm 0.007$ a.u., which has seven same figures with the best value given by Korobov and Yerokhin [23,28]. A conclusion can be drawn that B-splines have been used to calculate BL for the $2S$ state of He successfully, and also have given a result with high accuracy.

In the following, B-splines will be used to calculate BL for the low-lying excited $S$ states. Based on the convergence examination of table 4, the number of the partial wave will be fixed as $\ell_{\text{max}} = 5$. Different from previous methods of optimizing all states individually, in order to give a series of low-lying excited states from one full diagonalization of Hamiltonian, a relative bigger box with the radius of $R_0 = 400$ a.u. will be chosen. We will firstly give the acceleration-gauge results. Calculations for the $n \ell S$ states will be carried out in other two gauges as well, which one is the velocity gauge, and the other is a hybrid of the velocity and acceleration gauges. This pa-gauge avoids the explicit inclusion of the energies of the intermediate states, and consequently reduces the numerical round-off error in the nth variational energy $E_n$.

Table 4 lists the convergence study of BL in three different gauges for the $3S$ state as the number of B-splines, $N$, increased. The corresponding configuration numbers $N_{3S}$ and $N_{3P}$ are listed in the second column of table 5 as well. It can be seen that the convergence in the acceleration and pa-gauges are one order of magnitude better than in the velocity gauge for the $3S$ state. Compared with the correlated Hylleraas value given based on the acceleration gauge dipole operator [9, 18], the $1/n$ expansion value in reference [37], and the $1/n$ expansion value in reference [38], present B-splines results in the acceleration and pa-gauges agree well with seven same figures for the $3S$ state. There is six same figures between present value and Korobov’s [38] in the velocity gauge.
Table 7. Results of BL (a.u.) for \( n^3S(n = 1–8) \) states of He obtained in the acceleration, pa- and velocity gauges. The numbers in parentheses give the computational uncertainties.

| State  | \( \beta(\alpha) \) | \( \beta(\text{VA}) \) | \( \beta(\text{V}) \) | Reference [37] | Reference [38] |
|--------|---------------------|---------------------|---------------------|----------------|----------------|
| \( 1^1S \) | 4.370 34(2)         | 4.370 14(2)         | 4.370 6(4)          | 4.370 160 223 070 3(3) |
| \( 2^1S \) | 4.366 43(1)         | 4.366 412(1)        | 4.366 5(2)          | 4.366 412 726 417(1) |
| \( 3^1S \) | 4.369 170(1)        | 4.369 164 3(2)      | 4.369 18(7)         | 4.369 164 888    |
| \( 4^1S \) | 4.369 893(1)        | 4.369 890 3(5)      | 4.369 90(2)         | 4.369 890 657    |
| \( 5^1S \) | 4.370 152(3)        | 4.370 151 1(2)      | 4.370 15(2)         | 4.370 152 093    |
| \( 6^1S \) | 4.370 27(1)         | 4.370 266(2)        | 4.370 26(2)         | 4.370 267 364    |
| \( 7^1S \) | 4.370 33(1)         | 4.370 33(1)         | 4.370 27(7)         | 4.370 325 649    |
| \( 8^1S \) | 4.370 34(4)         | 4.370 34(2)         | 4.370 34(2)         | 4.370 358 160    |

In the present paper, the hydrogenic ground and Rydberg states BL are calculated in the velocity and length gauges by using the B-splines variational method. We give a velocity-gauge result with fourteen accurate figures and a length-gauge value of eleven accurate figures for the 1s state of hydrogen. BL for Rydberg states in the velocity and length gauges are also achieved with high accuracy, which represents the successful variational attempt to calculate BL of the hydrogen atom in the velocity and length gauges.
values in three different gauges are at the $10^{-8}$ level of relative difference, while all other results given in present calculations also have at least five accurate figure. The best convergent results for the singlet states are achieved in the hybrid of the velocity and acceleration gauges, which have five to seven accurate figures as well.

Comprehensively compared present calculations of BL for hydrogen and helium, a conclusion also can be drawn that, for a enough large B-splines basis set, the acceleration, velocity, and length gauges all can give good convergent results, but the convergence rate in the acceleration gauge is better than in the velocity gauge, and these two gauges are both better than the length gauge. Otherwise, we had better perform calculations of BL in the acceleration gauge and the pa-gauge.

It is difficult and complex to overcome the linear dependence problem when the current existing correlated basis are largely expanded. B-spline method can avoid this problem and has the potential application in calculating BL for three-electron atoms or molecular systems, which will make contribution in evaluating QED effects in these complex systems.

Acknowledgments

This work is supported by the National Natural Science Foundation of China under Grants No. 11704386 and No. 11774386, by the Strategic Priority Research Program of the Chinese Academy of Sciences under Grant No. XDB21030300, and by the National Key Research and Development Program of China under Grant No. 2017YFA0304402. Jun-Yi Zhang is grateful for the support from the Hundred Talents program of the Chinese Academy of Sciences.

ORCID iDs

Yong-Hui Zhang https://orcid.org/0000-0002-9293-2037
Chang-Min Xiao https://orcid.org/0000-0003-1601-9358

References

[1] Lamb W E and Retherford R C 1947 Phys. Rev. 72 241
[2] Bethe H A 1947 Phys. Rev. 72 339
[3] Parthey C G et al 2011 Phys. Rev. Lett. 107 203001
[4] Yost D C et al 2016 Phys. Rev. A 93 042509
[5] Fleurban H, Galtier S, Thomas S, Bonnau M, Julien L, Biraben F, Nez F, Abgrall M and Guéna J 2018 Phys. Rev. Lett. 120 183001
[6] Pachucki K, Patkóš V and Yerokhin V A 2017 Phys. Rev. A 95 062510
[7] Bethe H A and Salpeter E E 1977 Quantum Mechanics of One- and Two-Electron Atoms (New York: Plenum)
[8] Goldman S P 1984 Phys. Rev. A 30 1219
[9] Goldman S P 1994 Phys. Rev. A 50 3039
[10] Lieber M 1968 Phys. Rev. 174 2037
[11] Huff R W 1969 Phys. Rev. 186 1367
[12] Drake G W F and Swaiss R A 1990 Phys. Rev. A 41 1243
[13] Jentschura U D and Mohr P J 2005 Phys. Rev. A 72 012110
[14] Jentschura U D and Mohr P J 2005 arXiv:quant-ph/0504002
[15] Haywood S E and Morgan J D 1985 Phys. Rev. A 32 3179
[16] Mallampalli S and Sapirstein J 1998 J. Phys. B 31 3779
[17] Drake G W F and Goldman S P 1999 Can. J. Phys. 77 835
[18] Goldman S P and Drake G W F 2000 Phys. Rev. A 61 052513
[19] Stanke M, Adamowicz L and Kedziera D 2013 Mol. Phys. 111 1063
[20] Schwartz C 1961 Phys. Rev. 123 1700
[21] Goldman S P and Drake G W F 1983 J. Phys. B: At. Mol. Phys. 16 L183
[22] Bhatia A K and Drachman R J 1998 Phys. Rev. A 57 4301
[23] Korobov V I 2004 Phys. Rev. A 69 054501
[24] Korobov V I and Korobov S V 1999 Phys. Rev. A 59 3394
[25] Korobov V I 2012 Phys. Rev. A 85 042514
[26] Baker J D, Forrey R C, Morgan III J D, Hill R N, Jeziorska M and Schertzer J 1993 Bull. Am. Phys. Soc. 38 1127
[27] Baker J D, Forrey R C, Jeziorska M and Morgan III J D 2000 Physics 99 1296
[28] Yerokhin V A and Pachucki K 2010 Phys. Rev. A 81 022507
[29] Yerokhin V A, Patkóš V and Pachucki K 2018 Phys. Rev. A 98 032503
[30] Bachau H, Cormier E, Decleva P, Hansen J E and Martin F 2001 Rep. Prog. Phys. 64 1815
[31] Fischer C F 2008 J. Phys. B: At. Mol. Opt. Phys. 55 235
[32] Tang Y B, Zhong Z X, Li C B, Qiao H X and Shi T Y 2013 Phys. Rev. A 87 022510
[33] Chen M K and Hsue C S 1992 J. Phys. B: At. Mol. Opt. Phys. 25 4059
[34] Chen M K 1993 J. Phys. B: At. Mol. Opt. Phys. 26 3025
[35] Cowan R D 1981 The Theory of Atomic Structure and Spectra (Berkeley, CA: University of California)
[36] Zhang Y H, Tang L Y, Zhang X Z and Shi T Y 2015 Phys. Rev. A 92 012515
[37] Drake G W F 2001 Phys. Scr. T95 22
[38] Korobov V I 2019 Phys. Rev. A 100 012517
[39] Yang S J, Mei X S, Shi T Y and Qiao H X 2017 Phys. Rev. A 95 062505
[40] Yang S J, Tang Y B, Zhao Y H, Shi T Y and Qiao H X 2019 Phys. Rev. A 100 042509