Application of the Hylleraas-*B*-spline basis set: Nonrelativistic Bethe logarithm of helium

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In this paper, we report an application of the Hylleraas-*B*-spline basis to the calculation of the nonrelativistic Bethe logarithm of helium. The Bethe logarithms for the $n\,^1S$ states of helium, where n is up to 10, are calculated precisely in the acceleration and the velocity-acceleration gauges, which greatly improves the accuracy of the traditional B-spline basis. In addition, to overcome numerical instability problem emerging from the use of this basis, a multiple-precision generalized symmetric eigenvalue problem solver is developed.

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I. INTRODUCTION

For few-electron atomic systems, an atomic energy level can be calculated to high precision using the theory of nonrelativistic quantum electrodynamics [1], which provides a series expansion of the energy level in terms of $Z\alpha$ and α, with Z being the nuclear charge and α the fine-structure constant. The leading-order relativistic correction is scaled as $m\alpha^4$, and the leading-order radiative correction is scaled as $m\alpha^5$, which contains the so-called Bethe logarithm. The Bethe logarithm can be expressed as an infinite sum over a complete set of intermediate states. Since the Bethe logarithm involves the factor $\ln|E_m - E_0|$ that makes the summation extremely slowly converge, precise evaluation of the Bethe logarithm is a very challenging task.

For helium and heliumlike ions, Drake and Goldman [2] developed an approach for calculating the Bethe logarithm. In their approach, it requires only a single matrix diagonalization with respect to a carefully constructed basis set in Hylleraas coordinates that can reflect a huge range of distance scales. For highly excited Rydberg states, they established the $1/n$ expansion formula [3,4] that contains the Rydberg electron hydrogenic Bethe logarithm and the correction due to the higher multipole moments. The Drake-Goldman's method has also been successfully applied to helium using different basis sets [5] and to other few-body systems, including hydrogen [6,7], the hydrogen molecular ion [8], and lithium [9]. Another independent approach of calculating the Bethe logarithm is the integral representation method of Schwartz [10], which has been further developed by Korobov [11,12] and Pachucki and Komasa [13,14] and applied to few-electron atomic and molecular systems.

By building Hylleraas coordinates into the *B*-spline functions, we have recently proposed the Hylleraas-*B*-spline basis and used this type of basis to calculate static dipole polarizabilities, dynamic dipole polarizabilities and dynamic hyperpolarizabilities of helium [15,16]. This method has significantly improved the traditional *B*-spline basis in the sense that it is capable of generating a wider range of energy spectrum of the Hamiltonian. In this work, we will extend the Hylleraas-*B*-spline basis to the calculations of the Bethe logarithm of helium. Tang *et al*. [7] performed a calculation of the Bethe logarithm for atomic hydrogen using the traditional *B*-spline basis set and found that the first nonzero knot of *B*-splines is closely related to the range of the intermediate energy spectrum generated by the *B*-spline basis. For the case of helium, however, the knot sequence of *B*-splines that are situated very near the origin could result in a numerical degeneracy problem. To overcome this problem, based on Message Passing Interface and the software ARPREC [17], we have developed a parallel program, the Multiple-precision Generalized Symmetric Eigenvalue Problem Solver (MGSEPS), which can solve a generalized symmetric matrix eigenvalue problem efficiently with great stability. With this program, we will calculate the Bethe logarithm for the $n\,^1S$ states of helium with n up to 10, in both the acceleration gauge and the velocity-acceleration gauge. Comparisons with previous *B*-spline results and with results from other methods will be made.

The article is organized as follows. In Sec. II we briefly introduce the Hylleraas-*B*-spline basis and the basic formulas for the Bethe logarithm in two gauges. Numerical results are presented in Sec. III, together with comparisons with available theoretical results. Finally, a summary is given in Sec. IV. Atomic units are used throughout.

II. THEORETICAL METHOD

A. Hylleraas-*B*-spline basis set

The Hamiltonian of helium for the case of infinite nuclear mass is

$$H = \sum_{i=1}^{2}\left(-\frac{1}{2m_e}\vec{\nabla}_i^2 - \frac{Z}{r_i}\right) + \frac{1}{r_{12}}, \tag{1}$$

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where $Z = 2$ is the nuclear charge, m_e is the electron mass, r_i is the distance between ith electron and the nucleus, and r_{12} is the distance between the two electrons. Considering the wave function behavior at the two electron coalescences, the wave function of helium can be expanded using the following basis:

$$\left\{\Phi_{ijcl_1l_2} = B_{i,k}(r_1)B_{j,k}(r_2)r_{12}^c \mathbf{\Lambda}_{l_1l_2}^{LM}(\hat{r}_1, \hat{r}_2) \pm \text{exchange}\right\}, \quad (2)$$

where r_{12}^c is a Hylleraas factor, $\mathbf{\Lambda}_{l_1l_2}^{LM}$ is the vector coupled product of angular momenta l_1 and l_2 for the two electrons to form the eigenstate of $L(L+1)$ and M, respectively, and $B_{i,k}(r)$ is the ith B-spline function of order k defined in the finite domain $(0, r_{\max})$ [18]. The shape of $B_{i,k}(r)$ depends on the nondecreasing knot sequence $\{t_i\}$ and the spline order k, as defined as

$$\begin{cases} t_i = 0 & i = 1, 2, \ldots, k-1, \\ t_i = r_{\max}\dfrac{e^{\gamma\left(\frac{i-k}{N-k+1}\right)} - 1}{e^{\gamma} - 1} & i = k, k+1, \ldots, N, \\ t_i = r_{\max} & i = N+1, \ldots, N+k-1, \end{cases} \quad (3)$$

where N is the total number of B-splines, $k = 7$, and $\gamma = \tau \times r_{\max}$, with τ being an adjustable parameter.

In this article, we restrict c in Eq. (2) to be less than 2. The parameters i, j, c, l_1, l_2 are arranged according as follows:

$$\begin{aligned} &i = 1, 2, \ldots, j, \quad j = 1, 2, \ldots, N, \quad c = 0, 1, \\ &l_1 = 0, 1, \ldots, l_{\max}, \quad l_2 = 0, 1, \ldots, l_{\max}, \end{aligned} \quad (4)$$

where $l_{\max}$ is the partial-wave expansion length. The terms which make the norm of $\Phi_{ijcl_1l_2}$ be zero must be eliminated.

B. Nonrelativistic Bethe logarithm

The definition of the nonrelativistic Bethe logarithm in the acceleration gauge is

$$\beta(n, L, S) = \frac{\mathcal{N}^{(A)}(n, L, S)}{\mathcal{D}^{(A)}(n, L, S)}. \quad (5)$$

In the above, n, L, S are the principal, total angular momentum, and total electron spin quantum numbers, respectively, for the state of interest Ψ_0. $\mathcal{N}^{(A)}$ and $\mathcal{D}^{(A)}$ are defined by

$$\begin{aligned} \mathcal{N}^{(A)}(n, L, S) = &\sum_{m,i} \left| \langle \Psi_0 | \frac{Z\vec{r}_i}{r_i^3} | \Psi_m \rangle \right|^2 \\ &\times (E_m - E_0)^{-1} \ln |E_m - E_0| \end{aligned} \quad (6)$$

and

$$\mathcal{D}^{(A)}(n, L, S) = \sum_{m,i} \left| \langle \Psi_0 | \frac{Z\vec{r}_i}{r_i^3} | \Psi_m \rangle \right|^2 (E_m - E_0)^{-1}, \quad (7)$$

where the summation over m is carried out for all intermediate states Ψ_m.

Using the commutation relation

$$\begin{aligned} (E_m - E_0)\langle \Psi_0 | \vec{p} | \Psi_m \rangle &= \langle \Psi_0 | [\vec{p}, H] | \Psi_m \rangle \\ &= -iZ\langle \Psi_0 | \frac{\vec{r}}{r^3} | \Psi_m \rangle, \end{aligned} \quad (8)$$

one can recast the Bethe logarithm into the velocity-acceleration gauge,

$$\begin{aligned} \mathcal{N}^{(VA)}(n, L, S) = &\sum_{m,i} \langle \Psi_0 | \frac{Z\vec{r}_i}{r_i^3} | \Psi_m \rangle \langle \Psi_0 | \vec{p}_i | \Psi_m \rangle \\ &\times \ln |E_m - E_0| \end{aligned} \quad (9)$$

and

$$\mathcal{D}^{(VA)}(n, L, S) = \sum_{m,i} \langle \Psi_0 | \frac{Z\vec{r}_i}{r_i^3} | \Psi_m \rangle \langle \Psi_0 | \vec{p}_i | \Psi_m \rangle. \quad (10)$$

It is noted that the following expression is valid:

$$\mathcal{D}^{(A)}(n, L, S) = \sum_{m,i} |\langle \Psi_0 | \vec{p}_i | \Psi_m \rangle|^2 (E_m - E_0). \quad (11)$$

$\mathcal{D}^{(A)}(n, L, S)$ in the above is similar to the expression of the dipole polarizability in the velocity gauge if the factor $1/(E_m - E_0)^4$ were inserted. Because of the absence of this factor, contributions from high-energy intermediate states are significant. For the numerator $\mathcal{N}^{(A)}$, the existence of $\ln |E_m - E_0|$ makes high-energy intermediate states more important. Drake and Goldman [2] pointed out that, in order to obtain a converged value of the Bethe logarithm for helium, the maximum intermediate energy should exceed 10^6 to cover a huge range of distance scales.

III. RESULTS AND DISCUSSION

The maximum energy $E_{\max}$ of intermediate states is crucial to obtain a precise value of the Bethe logarithm. For the case of hydrogen, Ref. [7] shows that $E_{\max}$ generated by the B-spline basis is closely related to the first nonzero knot T_1. In the case of helium, first, we do the calculations with $r_{\max} = 200$, $\tau = 0.0875$ and $r_{\max} = 400$, $\tau = 0.0475$, respectively, letting the first nonzero knot in the range 10^{-5}–10^{-6}. In these two cases, under the total number of B-splines $N = 50$ and partial-wave expansion length $l_{\max} = 2$, the first nonzero knot $T_1 = 2.38 \times 10^{-6}$ and 1.17×10^{-6} and $E_{\max} = 1.85 \times 10^{15}$ and 7.50×10^{14}, respectively.

The extrapolated values of ground-state energy of helium under these parameters are $E = -2.903724(1)$ and $-2.903723(1)$, respectively. Table I shows a convergence

TABLE I. Convergence of the Bethe logarithm for the ground state of helium as the total number of B-splines N increases, where the partial-wave expansion length $l_{\max} = 2$. Numbers in parentheses are computational uncertainties.

N	$r_{\max} = 200$	$r_{\max} = 400$
20	4.378	4.37
25	4.371	4.369
30	4.3703	4.3705
35	4.37019	4.3702
40	4.370167	4.37017
45	4.370161	4.370164
50	4.3701599	4.370161
∞	4.3701596(3)	4.370160(1)
Ref. [2]	4.370160218(3)	
Ref. [21]	4.3701602229(1)	
Ref. [12]	4.3701602230703(3)	

TABLE II. Convergence study for the ground-state energy of helium as the total number of *B*-splines N and the partial-wave expansion length $l_{\max}$ increase. Numbers in parentheses are computational uncertainties.

$N\backslash l_{\max}$	1	2	3	4
40	–2.9035	–2.90363	–2.9036	–2.9036
45	–2.90366	–2.90369	–2.90370	–2.90371
50	–2.90370	–2.90371	–2.90371	–2.903720
55	–2.90371	–2.903721	–2.90372	–2.9037231
60	–2.903722	–2.9037231	–2.903723	–2.9037239
65	–2.9037235	–2.9037238	–2.9037241	–2.9037242
70	–2.9037239	–2.9037241	–2.9037242	–2.903724306
∞				–2.90372436(6)

TABLE IV. Convergence study of the Bethe logarithm for the ground state of helium in the acceleration gauge as the total number of *B*-splines N and the partial-wave expansion length $l_{\max}$ increase. Numbers in parentheses are computational uncertainties.

$N\backslash l_{\max}$	1	2	3	4
40	4.3704	4.3702	4.3702	4.37019
45	4.3690	4.37018	4.37017	4.370170
50	4.370336	4.370168	4.370165	4.370163
55	4.370330	4.370162	4.370161	4.3701613
60	4.370328	4.370161	4.3701608	4.3701606
65	4.3703275	4.3701606	4.3701604	4.3701603
70	4.3703272	4.3701604	4.3701603	4.37016027
∞				4.37016022(5)

study for the ground-state Bethe logarithm. The extrapolated values of Bethe logarithm are 4.3701596(3) and 4.370160(1). In comparison with the highly precise value 4.3701602230703(3) of Korobov [12], our first extrapolated value is not so well converged, which could be caused by the lack of sufficient accuracy of our initial state. However, our calculations imply that the intermediate states, generated in two different boxes, are reliable, and further improvement could be made once we have a more accurate initial state. In the following calculations we set $r_{\max} = 400$ and $\tau = 0.056$ and increase N up to 70 and $l_{\max}$ up to 4. The corresponding values for T_1 and $E_{\max}$ are, respectively, 6.7×10^{-8}–3.0×10^{-8} and 10^{16}–10^{18}.

A. Energy levels

Table II shows a convergence study of the ground-state energy of helium as N and $l_{\max}$ increase. The extrapolated value for the ground state is $-2.90372436(6)$, which has eight significant digits in comparison with the benchmark value of Schwartz [19]. Table III displays a comparison of the energy levels for the $n\,^1S$ states with n up to 10, from which one can see that our values have eight significant digits in comparison with Drake's tabulation in Ref. [20]. These results provide suitable initial states for our Bethe logarithm calculations.

TABLE III. Comparison of the energies for the $n\,^1S$ states of helium, where n is up to 10. Numbers in parentheses of the extrapolated values are computational uncertainties.

n	^1S	Ref. [20]
1	–2.90372436(6)	–2.9037243770341195
2	–2.14597403(3)	–2.1459740460544l9(6)
3	–2.06127197(3)	–2.061271989740911(5)
4	–2.03358670(4)	–2.03358671703072(1)
5	–2.02117684(4)	–2.021176851574363(5)
6	–2.01456308(4)	–2.01456309844660(1)
7	–2.01062575(3)	–2.01062577621087(2)
8	–2.00809359(3)	–2.00809362210561(4)
9	–2.00636952(4)	–2.00636955310785(3)
10	–2.00514299(9)	–2.00514299174800(8)

B. Bethe logarithm

Convergence studies for the ground-state Bethe logarithm in the acceleration and velocity-acceleration gauges are given in Tables IV and Tables V, respectively, where the values in these two gauges gradually approach each other as N and $l_{\max}$ increase, as indicated in Fig. 1. The extrapolated values of the Bethe logarithm are 4.37016022(5) and 4.3701601(1), respectively, which have nine and seven significant digits. It is noted that the current results in the acceleration gauge have greatly improved the values from the traditional *B*-spline basis; for example, for the ground state, the present value has five more significant digits than the corresponding pure *B*-spline one (see Table VI).

For the $n\,^1S$ states of helium with n up to 10, our results of the Bethe logarithm in the two gauges are tabulated in Table VI, together with comparisons with other available data. One can see that our results in the two gauges are consistent with each other at the level of six or seven digits. In general, our results have also in good accord with other accurate values. It is noted that, in our calculations, most of the knot sequences of *B*-splines are concentrated in the first half of the box. Thus, further optimization of these knot sequences will improve the accuracy of our calculations.

TABLE V. Convergence study of the Bethe logarithm for the ground state of helium in the velocity-acceleration gauge as the total number of *B*-splines N and the partial-wave expansion length $l_{\max}$ increase. Numbers in parentheses are computational uncertainties.

$N\backslash l_{\max}$	1	2	3	4
40	4.369	4.3695	4.3697	4.3698
45	4.368	4.37002	4.37005	4.37008
50	4.37015	4.37012	4.37013	4.370138
55	4.370164	4.370152	4.370153	4.370154
60	4.370167	4.370158	4.3701584	4.3701585
65	4.3701682	4.370159	4.3701596	4.3701597
70	4.3701684	4.37016006	4.37016002	4.37016004
∞				4.3701601(1)

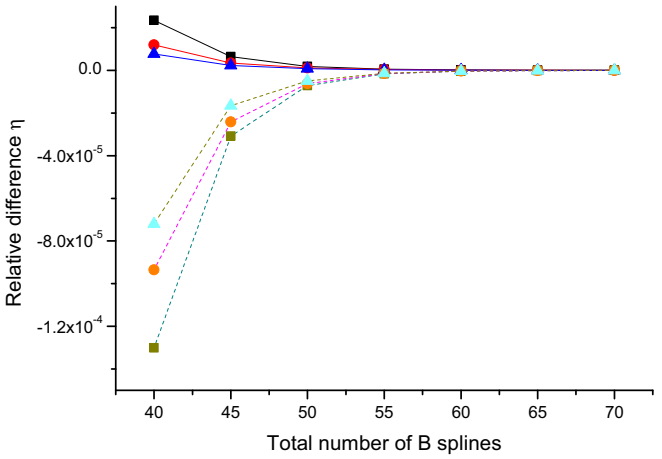

FIG. 1. Relative difference η against the total number of B-splines and the partial-wave expansion length $l_{\max}$. Points in solid lines and dash lines denote values in the acceleration and velocity-acceleration gauges, respectively. Square, circle, and triangle points denote the results under the conditions of $l_{\max} = 2, 3, 4$, respectively.

IV. SUMMARY

We have successfully applied the Hylleraas-B-spline basis to the calculations of the Bethe logarithm for various S states of helium. Agreement between the acceleration and the velocity-acceleration gauges has been achieved. Our results for the Bethe logarithm have significantly improved the results obtained from the traditional B-spline basis. The software MGSEPS that we have developed has helped us overcome numerical instability problem. It would be interesting to extend our Hylleraas-B-spline approach to atomic systems with more than two electrons.

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TABLE VI. Comparison of the Bethe logarithm for the $n\,^1S$ states of helium, where n is up to 10. The first entries in the second and third columns are from the acceleration gauge, and the second entries are from the velocity-acceleration gauge. Numbers in parentheses are computational uncertainties.

States	This work	B-spline [22]	References	Ssymptotic expansions
$1\,^1S$	4.37016022(5)	4.37034(2)	4.370160218(3)[a]	
	4.3701601(1)	4.37014(2)	4.3701602229(1)[b]	
			4.37016022307O3(3)[d]	
$2\,^1S$	4.36641271(1)	4.36643(1)	4.36641272(7)[a]	4.366412729[c]
	4.3664127(1)	4.366412(1)	4.3664127262(1)[b]	4.366378229[d]
			4.366412726417(1)[d]	
$3\,^1S$	4.36916480(6)	4.369170(1)	4.369164871(8)[a]	4.369164888[c]
	4.3691648(1)	4.3691643(2)	4.369164860824(2)[d]	4.369164809[d]
$4\,^1S$	4.36989065(5)	4.369893(1)	4.36989066(1)[a]	4.369890657[c]
	4.3698906(1)	4.3698903(5)	4.36989063236(1)[d]	4.369890661[d]
$5\,^1S$	4.3701520(1)	4.370152(3)	4.3701517(1)[a]	4.370152093[c]
	4.3701519(1)	4.3701511(2)	4.37015179631(1)[d]	4.370151761[d]
$6\,^1S$	4.370267(1)	4.37027(1)	4.37026697432(3)[d]	4.370267364[c]
	4.370267(1)	4.370266(2)		4.370266961[d]
$7\,^1S$	4.370326(1)	4.37033(1)	4.37032526176(2)[d]	4.370325649[c]
	4.370326(1)	4.37033(1)		4.370325274[d]
$8\,^1S$	4.370359(2)	4.37034(4)		4.370358160[c]
	4.370359(2)	4.37034(2)		4.370357839[d]
$9\,^1S$	4.370378(2)			4.370377682[c]
	4.370378(2)			4.370377414[d]
$10\,^1S$	4.370389(1)			4.370390095[c]
	4.370388(1)			4.370389875[d]

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