Application of the correlated *B*-spline basis functions to the leading relativistic and QED corrections of helium

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B-spline functions have been widely used in computational atomic physics. Recently, correlated *B*-spline basis functions (C-BSBFs), where the interelectronic coordinate r_{12} is explicitly incorporated, have greatly improved the computational accuracy in determining polarizability for helium's singlet states [S. J. Yang, X. S. Mei, T. Y. Shi, and H. X. Qiao, Phys. Rev. A **95**, 062505 (2017)] and Bethe logarithm [S. J. Yang, Y. B. Tang, Y. H. Zhao, T. Y. Shi, and H. X. Qiao, Phys. Rev. A **100**, 042509 (2019)]. This represents a significant advancement over the traditional *B*-spline basis, which comprises a straightforward product of two *B* splines. In this paper, we detail the extension of C-BSBFs towards calculating leading relativistic and quantum electrodynamics (QED) corrections for energy levels of the $1\,^1S$, $2\,^1S$, $2\,^3S$, and $3\,^3S$ states in helium. To accomplish this, the relativistic kinetic term p_1^4, contact potentials $\delta^3(r_1)$ and $\delta^3(r_{12})$, and Araki-Sucher correction $\langle 1/r_{12}^3\rangle$ were calculated via the global operator method, wherein r_{12}^n and $r_{12}^n \ln r_{12}$ were derived from the generalized Laplace's expansions. Our computations yielded values for the ground state of $\delta E_{\rm rel}/\alpha^2 = -1.951\,754\,76(6)$ and $\delta E_{\rm QED}/\alpha^3 = 57.288\,164\,8(5)$, aligning well with previous results. These results illustrate the potential of the C-BSBFs for computing higher-order relativistic and QED effects.

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I. INTRODUCTION

Recent advances in atomic spectroscopy, reaching part-per-trillion precision for helium, have provided strong experimental support for testing quantum electrodynamics (QED) and determining the fine-structure constant α as well as the nuclear charge radius [1–7]. These measurements, when paired with high-accuracy atomic structure calculations, present a robust platform for understanding atomic structure [8–11]. In particular, helium, the simplest many-electron system, offers an exemplary testing ground for exploring different methodologies to describe atomic structures.

Finite basis set variational calculations have emerged as a potent tool for solving the Coulomb three-body bound-state problem. This technique, when applied to helium, is particularly effective when basis functions incorporate explicitly the interelectron separation. The effectiveness of this technique is exemplified by Patkóš *et al.*; they employed the explicitly correlated exponential basis with nonlinear parameters and completed the $\alpha^7 m$ Lamb shift of helium triplet states, improving the theoretical accuracy of ionization energies by over an order of magnitude [8]. Nevertheless, to circumvent the loss of stability accompanying an increase in the number of basis functions, the employment of multiprecision packages and variational optimization of nonlinear parameters is essential.

In computational atomic physics, *B* splines enjoy popularity due to their complete-enough nature and linear independence for large basis sets [12–21]. However, systems with strong electron correlations challenge the generation of high-accuracy computational results using traditional *B*-spline basis functions. An imperative need arises, therefore, to incorporate the interelectronic coordinate into these basis functions.

Tang *et al.* [17] and Zhang *et al.* [21] have developed a method to compute Bethe logarithms, the dominant part of QED, of hydrogen and helium atoms, respectively, using *B*-spline basis sets. However, the precision of these methods is somewhat constrained for the singlet states, which lack the electron correlation effect in the basis set. To address this, Yang *et al.* developed the explicitly correlated *B*-spline basis method, demonstrating its applicability in the computation of energy levels, static dipole polarizabilities [22], and Bethe logarithms [23] for the helium atom singlet states. The success of the correlated *B*-spline basis functions (C-BSBFs) in describing electronic correlation and improving numerical convergence rates is indeed remarkable.

In this paper, we exploit the C-BSBF method to compute the leading relativistic and QED corrections to helium atom energy levels. We utilize the global operator method to enhance the numerical convergence for the relativistic kinetic term p_1^4, the contact potentials $\delta^3(r_1)$ and $\delta^3(r_{12})$, and the Araki-Sucher correction $\langle 1/r_{12}^3\rangle$. This endeavor extends the applicability of the C-BSBF method, demonstrating its efficacy in numerical calculations of the expectation values of singular operators.

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The remainder of this paper is structured as follows. Section II provides an overview of the theoretical formulas and methodologies employed in our calculations. Section III presents calculations of the leading relativistic and QED corrections to energy levels for the $1\,^1S$, $2\,^1S$, $2\,^3S$, and $3\,^3S$ states of helium, in comparison with the available literature. We conclude and offer potential directions for future work in Sec. IV. All computations throughout this paper use atomic units (a.u.).

II. THEORY AND METHOD

A. C-BSBFs

The nonrelativistic Hamiltonian for a two-electron atom with an infinite mass nucleus has the form of

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

where $\mathbf{p}_i = -i\nabla_i$ is the momentum operator of the ith electron, r_i is the coordinate of the ith electron to the atomic nucleus, r_{12} is the interelectronic coordinate, and the nuclear charge $Z = 2$ for the helium atom.

The two-electron wave function is expanded by the following C-BSBFs in which the interelectronic coordinate r_{12} is included explicitly:

$$\phi_{ij,c,\ell_1\ell_2} = \mathcal{A}\big[r_{12}^c B_i^k(r_1) B_j^k(r_2)\mathcal{Y}_{\ell_1\ell_2}^{LM}(\hat{\mathbf{r}}_1, \hat{\mathbf{r}}_2)\big], \tag{2}$$

where the operator $\mathcal{A}$ ensures the antisymmetry of the basis function with respect to the exchange of the two electrons. c is the power of the r_{12} coordinate. The coupled spherical harmonic function is given by

$$\mathcal{Y}_{\ell_1\ell_2}^{LM}(\hat{\mathbf{r}}_1, \hat{\mathbf{r}}_2) = \sum_{m_1 m_2} \langle \ell_1\ell_2 m_1 m_2 \mid LM\rangle \times Y_{\ell_1 m_1}(\hat{\mathbf{r}}_1) Y_{\ell_2 m_2}(\hat{\mathbf{r}}_2), \tag{3}$$

with $\langle \ell_1\ell_2 m_1 m_2 \mid LM\rangle$ being the Clebsch-Gordan coefficient, and the orbital angular momentum ℓ_1 and ℓ_2 are less than the maximum partial wave $\ell_{\max}$. $B_i^k(r)$ is the ith of N B-spline functions with the order of k and constrained to a spherical cavity [13]; the exponential knots sequence is used to define B splines:

$$\begin{cases} t_i = 0, & i = 1, 2, \ldots, k-1, \\ t_{i+k-1} = R_0 \frac{\exp\left(\tau R_0 \frac{i-1}{N-2}\right)-1}{\exp(\tau R_0)-1}, & i = 1, 2, \ldots, N-1, \\ t_i = R_0, & i = N+k-1, N+k, \end{cases} \tag{4}$$

where τ represents an adjustable knot parameter utilized to modify the knot sequence; R_0 is the cavity radius. In the present calculations, c is restricted to be 0 and 1 without making integral evaluations overly complicated; R_0 is chosen appropriately and set large enough to accommodate the bound state of interest. The final convergent results will be obtained by increasing the number of B splines N and the partial wave $\ell_{\max}$.

B. Leading relativistic and QED corrections

The leading relativistic correction to the nonrelativistic energy of the two-electron atom is given by the expectation value of the Breit-Pauli Hamiltonian with the nonrelativistic wave function ψ:

$$\delta E_{\rm rel} = \langle\psi|H_{\rm BP}|\psi\rangle, \tag{5}$$

where

$$H_{\rm BP} = \alpha^2\left\{-\frac{1}{8}\left(p_1^4 + p_2^4\right) + \pi\delta^3(r_{12}) + \frac{Z\pi}{2}[\delta^3(r_1) + \delta^3(r_2)] - \frac{1}{2r_{12}}\left(\mathbf{p}_1\cdot\mathbf{p}_2 + \frac{\mathbf{r}_{12}\cdot(\mathbf{r}_{12}\cdot\mathbf{p}_1)\mathbf{p}_2}{r_{12}^2}\right)\right\}, \tag{6}$$

for the S state [11,24,25], where $\alpha = 7.297\,352\,569\,3(11)\times 10^{-3}$ [26] is the fine-structure constant; $\delta^3(r_{12})$, $\delta^3(r_1)$, and $\delta^3(r_2)$ represent the Dirac delta functions. The last term of Eq. (6) is a retardation term, since this correction is due to the retardation of the electromagnetic field produced by an electron [27], and $-[\mathbf{p}_1\cdot\mathbf{p}_2 + \mathbf{r}_{12}\cdot(\mathbf{r}_{12}\cdot\mathbf{p}_1)\mathbf{p}_2/r_{12}^2]/2r_{12}$ is labeled as H_2.

The leading QED correction can be expressed as an expectation value of the following effective operators [11,28,29]:

$$\delta E_{\rm QED} = \alpha^3\left\{\frac{4Z}{3}\left[\frac{19}{30} - 2\ln\alpha - \ln k_0\right]\langle\psi|\delta^3(r_1) + \delta^3(r_2)|\psi\rangle + \left[\frac{164}{15} + \frac{14}{3}\ln\alpha\right]\langle\psi|\delta^3(r_{12})|\psi\rangle - \frac{7}{6\pi}\langle\psi|r_{12}^{-3}|\psi\rangle\right\}. \tag{7}$$

Here $\ln k_0$ is the Bethe logarithm, and the last term in Eq. (7) is usually called Araki-Sucher correction [28,31,32], and the expectation of $\langle\psi|r_{12}^{-3}|\psi\rangle$ is defined as

$$\langle\psi|r_{12}^{-3}|\psi\rangle = \lim_{a\to 0}\langle r_{12}^{-3}\Theta(r_{12}-a) + 4\pi(\gamma + \ln a)\delta^3(r_{12})\rangle, \tag{8}$$

where $\Theta(x)$ and γ are the step function and the Euler constant, respectively. Compared with the relativistic correction, the more difficult to calculate in the leading QED correction are the Bethe logarithm and Araki-Sucher correction. The Bethe logarithms for the $1\,^1S$, $2\,^1S$, $2\,^3S$, and $3\,^3S$ state of the helium atom are summarized in Table I calculated by Zhang *et al.* [21] using the traditional B-spline functions and Yang *et al.* [23] using the C-BSBFs, respectively, based on the Drake-Goldman method. Korobov's results listed in the last column of Table I based on the integral representation method of Schwartz are the benchmarks. The value of the Bethe logarithms from Zhang *et al.* and Yang *et al.* are used in this paper, which will achieve the complete calculation of

TABLE I. Bethe logarithm for the $1\,^1S$, $2\,^1S$, $2\,^3S$, and $3\,^3S$ states of helium.

State	Zhang *et al.* [21] and Yang *et al.* [23]	Korobov [30]
$1\,^1S$	4.370 160 22(5)	4.370 160 223 070 3(3)
$2\,^1S$	4.366 412 71(1)	4.366 412 726 417(1)
$2\,^3S$	4.364 036 7(2)	4.364 036 820 476(1)
$3\,^3S$	4.368 666 7(1)	4.368 666 996 159(2)

the leading relativistic and QED correction using the B-spline function.

Drachman proposed the global operator method to evaluate the two-particle contact potentials $\delta^3(r_1)$ and $\delta^3(r_{12})$, which achieved significant improvements over the direct evaluations [33]. We employ the equivalent form containing global operators given by Drachman to calculate the expectation value of $\delta^3(r_1)$ and $\delta^3(r_{12})$:

$$4\pi\langle\psi|\delta^3(r_i)|\psi\rangle = 4\langle\psi|r_i^{-1}(E_\psi - V)|\psi\rangle - 2\sum_{s=1}^{2}\langle\nabla_s\psi|r_i^{-1}|\nabla_s\psi\rangle, \tag{9}$$

$$4\pi\langle\psi|\delta^3(r_{12})|\psi\rangle = 2\langle\psi|r_{12}^{-1}(E_\psi - V)|\psi\rangle - \sum_{s=1}^{2}\langle\nabla_s\psi|r_{12}^{-1}|\nabla_s\psi\rangle, \tag{10}$$

where E_ψ is the corresponding eigenvalue of the two-electron wave function ψ, and $V = -Z/r_1 - Z/r_2 + 1/r_{12}$. It will result in a slow convergence for the kinetic term $p_1^4 + p_2^4$ in the relativistic correction if we calculate its expectation value directly in the C-BSBFs. Pachucki and Komasa also used a similar way to transform both the kinetic term and the Araki-Sucher correction to much more regular forms and obtained much better numerical convergence on that account [34]. In the present calculations, as Pachucki and Komasa have done, we use the following expression to evaluate $\langle p_1^4 + p_2^4\rangle$:

$$\sum_{i=1}^{2}\langle\psi|p_i^4|\psi\rangle = 4\langle\psi|(E_\psi - V)^2|\psi\rangle - 2\langle\nabla_1^2\psi|\nabla_2^2\psi\rangle. \tag{11}$$

The integration of $\langle\psi|r_{12}^{-2}|\psi\rangle$ will be involved in Eq. (11), and it is also evaluated to be as follows by using the global operator method:

$$\langle\psi|r_{12}^{-2}|\psi\rangle = 2\langle\psi|\ln r_{12}(V - E_\psi)|\psi\rangle + \sum_{i=1}^{2}\langle\nabla_i\psi|\ln r_{12}|\nabla_i\psi\rangle, \tag{12}$$

since we find that $\nabla_1^2 \ln r_{12} = \nabla_2^2 \ln r_{12} = r_{12}^{-2}$. The complete expansion of Eq. (11) is written as

$$\sum_{i=1}^{2}\langle\psi|p_i^4|\psi\rangle = 4E_\psi^2 + 8E_\psi\left\langle\psi\left|\frac{2Z}{r_1} - \frac{1}{r_{12}}\right|\psi\right\rangle + 4\left\langle\psi\left|\frac{2Z^2}{r_1^2} - \frac{2Z^2}{r_1 r_2} - \frac{2Z}{r_1 r_{12}} + \frac{1}{r_{12}^2}\right|\psi\right\rangle - 2\langle\nabla_1^2\psi|\nabla_2^2\psi\rangle. \tag{13}$$

The Araki-Sucher correction is converted to the regular form as well to facilitate the present numerical evaluations:

$$\langle\psi|r_{12}^{-3}|\psi\rangle = -\sum_{i=1}^{2}\langle\nabla_i\psi|r_{12}^{-1}\ln r_{12}|\nabla_i\psi\rangle + \langle\psi|2(E_\psi - V)\frac{\ln r_{12}}{r_{12}} + 4\pi(1+\gamma)\delta^3(r_{12})|\psi\rangle, \tag{14}$$

where $r_{12}^n \ln r_{12}$ $(n = -2, -1, 0, 1)$ will be involved in integration. In addition to the above three terms, the expectation values of other operators appearing in Eqs. (6) and (7) will be calculated in the C-BSBFs directly.

C. Laplace's expansion of r_{12}^n and $r_{12}^n \ln r_{12}$

The integrations of r_{12}^n and $r_{12}^n \ln r_{12}$ are involved in the computation of Breit-Pauli operators and Araki-Sucher corrections. It is crucial to process this type of integration in spherical coordinates, which requires separating their radial and angular dimensions. The generalization of Laplace's expansion to arbitrary powers and functions of r_{12} given by Sack [35] is used to calculate the integration in which different powers of r_{12} are involved. r_{12}^n can be expanded in the form

$$r_{12}^n = \sum_{\ell=0}^{\infty} R_{n\ell}(r_1, r_2)P_\ell(\cos\theta_{12}), \tag{15}$$

where the Legendre polynomials of $\cos\theta_{12}$ are expressed by using the identity as $P_\ell(\cos\theta_{12}) = 4\pi/(2\ell+1)\sum_{m=-\ell}^{m=\ell} Y_{\ell m}^*(\hat{r}_1)Y_{\ell m}(\hat{r}_2)$, and the radial function $R_{n\ell}(r_1, r_2)$ has been formulated by Sack [35] as follows:

$$R_{n\ell}(r_1, r_2) = \frac{\left(-\frac{1}{2}n\right)_\ell}{\left(\frac{1}{2}\right)_\ell} r_>^n \left(\frac{r_<}{r_>}\right)^\ell \times {}_2F_1\left(\ell - \frac{1}{2}n, -\frac{1}{2} - \frac{1}{2}n; \ell + \frac{3}{2}; \frac{r_<^2}{r_>^2}\right). \tag{16}$$

In Eq. (16), $r_< = \min(r_1, r_2)$, $r_> = \max(r_1, r_2)$, and the hypergeometric function has the form of

$${}_2F_1(\alpha, \beta; \gamma; x) = 1 + \sum_{s=1}^{\infty}\frac{(\alpha)_s(\beta)_s}{(\gamma)_s s!}x^s, \tag{17}$$

where the Pochhammer symbol is defined as

$$(\alpha)_s = \begin{cases} 1 & if\ s = 0 \\ \alpha(\alpha+1)\cdots(\alpha+s-1) & if\ s > 0 \end{cases}. \tag{18}$$

The hypergeometric function is a finite series if either α or β is zero or a negative integer, which implies that for all positive odd integer values of n, the series of $R_{n\ell}$ break off; and for $n = -1$, they consist of the leading term only. For positive even n, the summation is truncated to $\ell = \frac{n}{2}$, since the factor $(-\frac{1}{2}n)_\ell$ ensures that $R_{n\ell}$ vanishes when $\ell > \frac{n}{2}$. In addition, the individual functions $R_{n\ell}$ are divergent for $n \leqslant -2$, but they remain integrable as long as $n > -3$ [32,36]. Present calculations involve the integrations of $\langle\psi|r_{12}^{-2}|\psi\rangle$ and $\langle\psi|r_{12}^{-3}|\psi\rangle$. So giving appropriate radial expansions of r_{12}^{-2} and r_{12}^{-3} is important in the computation of radial and angular integrations. Substituting $n = -2, \ell = 0$ and $n = -2, \ell = 1$ separately into Eq. (16), and performing a summation of the series, as a result the following specific expressions in terms of reverse hyperbolic tangent function $\tanh^{-1}(x)$ are achieved:

$$R_{-2,0}(r_1, r_2) = \frac{\tanh^{-1}(x)}{x r_>^2}, \tag{19}$$

$$R_{-2,1}(r_1, r_2) = \frac{3}{2x^2 r_>^2}[(x^2+1)\tanh^{-1}(x) - 1], \tag{20}$$

TABLE II. The convergence of energies for the ground state with the number of B splines increased under different cavity radii. The order of B splines is $k = 7$ and the partial wave is $\ell_{\max} = 4$.

N	$R_0 = 10$ a.u.	$R_0 = 20$ a.u.	$R_0 = 40$ a.u.
50	−2.903 724 375 350 18	−2.903 724 377 034 14	−2.903 724 377 034 03
60	−2.903 724 375 412 40	−2.903 724 377 034 12	−2.903 724 377 034 10
70	−2.903 724 375 455 99	−2.903 724 377 034 10	−2.903 724 377 034 12
Extrap.	−2.903 724 375 5(2)	−2.903 724 377 034 0(2)	−2.903 724 377 034 1(1)

where $x = r_</r_>$; then the recurrence relation

$$\frac{r_1^2 + r_2^2}{r_1 r_2} R_{n,\ell} - \frac{\ell + 2 + \frac{1}{2}n}{\ell + \frac{3}{2}} R_{n,\ell+1} - \frac{\ell - 1 - \frac{1}{2}n}{\ell - \frac{1}{2}} R_{n,\ell-1} = 0 \tag{21}$$

can be used to calculate the radial functions for other values of ℓ. For $n = -3$, the expansion coefficients of the hypergeometric functions are canceled, and the hypergeometric functions are reduced to a series summation of x^n. The hypergeometric function can be expressed as an analytic function that is independent of ℓ; correspondingly the radial expansion of $R_{-3,\ell}$ can be written as [37]

$$R_{-3,\ell}(r_1, r_2) = \frac{(2\ell + 1)x^\ell}{(1 - x^2)r_>^3}. \tag{22}$$

Next we will give the explicit formula for the product of r_{12} with different powers and $\ln r_{12}$. With differentiation of Eq. (15), the expansion for $r_{12}^n \ln r_{12}$ can be expressed as

$$r_{12}^n \ln r_{12} = \sum_\ell R_{n\ln,\ell}(r_1, r_2) P_\ell(\cos\theta_{12}), \tag{23}$$

where $R_{n\ln,\ell}(r_1, r_2)$ represents the radial function of $r_{12}^n \ln r_{12}$, and $R_{n\ln,\ell}(r_1, r_2) = \frac{\partial R_{n\ell}(r_1,r_2)}{\partial n}$. Similarly, the following recurrence relation for $R_{n\ln,\ell}(r_1, r_2)$ can be derived by taking the derivative of Eq. (21):

$$\begin{aligned}\frac{1}{2\ell + 3} R_{n,\ell+1} - \frac{1}{2\ell - 1} R_{n,\ell-1} &= \frac{r_1^2 + r_2^2}{r_1 r_2} R_{n\ln,\ell} - \frac{2\ell + 4 + n}{2\ell + 3} R_{n\ln,\ell+1} \\ &\quad - \frac{2\ell - 2 - n}{2\ell - 1} R_{n\ln,\ell-1}.\end{aligned} \tag{24}$$

Then we can calculate the integration with the $r_{12}^n \ln r_{12}$ ($n \geqslant -2$) operator in the present paper. For example, for $n = -2$, $\ell = 0$ and $n = -2$, $\ell = 1$,

$$R_{-2\ln,0} = \frac{\tanh^{-1}(x) \ln(r_>^2 - r_<^2)}{2r_>^2 x}, \tag{25}$$

$$\begin{aligned}R_{-2\ln,1} = &\frac{3[\ln(r_>^2 - r_<^2) - 1]}{4r_>^2 x^2} \\ &\times [(x^2 + 1)\tanh^{-1}(x) - x],\end{aligned} \tag{26}$$

and the estimations of $R_{-2\ln,\ell}$ for other values of $\ell > 1$ can be obtained according to the recurrence relation of Eq. (24).

III. RESULTS AND DISCUSSIONS

The C-BSBFs on an exponential grid are constructed using B splines confined to a spherical cavity [13]. The accurate computation of energy levels and wave functions depends on the appropriate selection of the cavity radius. Taking the ground state as an example, Table II illustrates the convergence behavior of energy with an increasing number of B splines in different cavity radii. At a cavity radius of $R_0 = 10$ a.u., the energy converges to −2.903 724 375 5(2) a.u.. For $R_0 = 20$ and 40 a.u., the convergence results are consistent with the range of uncertainties, yielding −2.903 724 377 034 0(2) and −2.903 724 377 034 1(1) a.u., respectively. This consistency indicates that a cavity radius of $R_0 = 20$ a.u. is sufficient for calculating the ground-state properties. The same test calculations have been done for other states, establishing the cavity radius of $R_0 = 40$ a.u. for the $2\,^1S$ state and $R_0 = 70$ a.u. for both the $2\,^3S$ and $3\,^3S$ states. Furthermore, the effect of the order of B splines, k, on the energy was examined. At $k = 5$, the energy was calculated to be −2.903 724 376 920 87 a.u., whereas at $k = 7$ and 9, the results were consistent within double precision, being −2.903 724 377 034 14 and −2.903 724 377 034 11 a.u., respectively. In light of the fact that higher orders of B splines significantly increase computational complexity and resource consumption, $k = 7$ is deemed sufficient. After a comprehensive evaluation of the convergence behavior with respect to N and $\ell_{\max}$, we fix the maximum partial wave to be $\ell_{\max} = 4$. The final convergent result is extrapolated based on the outcomes obtained at the last three larger numbers of B splines, N, and the error margin is determined by the difference between the extrapolated result and the result of the maximum deviation from the extrapolated result in the last three larger B-splines' numbers.

Employing C-BSBFs, Yang *et al.* [22] calculated the helium atomic energy levels, obtaining a nonrelativistic ground-state energy of −2.903 724 377 1(2) a.u.. An optimization of the knot distribution was carried out for each state, yielding the energy values for the $1\,^1S$, $2\,^1S$, $2\,^3S$, and $3\,^3S$ states, which are detailed in Table III. For the ground state, the convergence result of −2.903 724 377 034 0(2) a.u. was achieved, yielding 13 significant digits, matching Drake's results [38]. For the $2\,^1S$, $2\,^3S$, and $3\,^3S$ states, 14 significant digits consistent with Drake's results [38] were also attained. It becomes apparent from Eq. (13) that the computation of $\langle p_1^4 \rangle$ entails numerous operators, which we subsequently partition into two distinct categories. The first category encompasses general operators like $1/r_1$, $1/r_1^2$, $1/r_1 r_2$, $1/r_{12}$, and $1/r_1 r_{12}$. These operators, due to their relative computational simplicity, provide the final convergence values directly

TABLE III. Energies for the $1\,^1S$, $2\,^1S$, $2\,^3S$, and $3\,^3S$ states of helium.

State	This paper	Ref. [38]
$1\,^1S$	−2.903 724 377 034 0(2)	−2.903 724 377 034 119 5
$2\,^1S$	−2.145 974 046 054 4(2)	−2.145 974 046 054 419(6)
$2\,^3S$	−2.175 229 378 236 7(2)	−2.175 229 378 236 791 30
$3\,^3S$	−2.068 689 067 472 4(2)	−2.068 689 067 472 457 19

tabulated in Table IV. Notably, our results exhibit an alignment with Drake's work up to at least ten significant digits, confirming the high accuracy of the wave function obtained by C-BSBFs. The second category includes the operators $1/r_{12}^2$ and $\nabla_1^2\nabla_2^2$, which pose a higher level of computational complexity. The numerical results of $\langle 1/r_{12}^2\rangle$, $\langle\nabla_1^2\nabla_2^2\rangle$, and $\langle p_1^4\rangle$ as the number of B splines N increased are given in the last three columns of Table V. Under the application of the global operator method, our C-BSBF based calculations deliver excellent convergent values for $\langle 1/r_{12}^2\rangle$. In the ground state, a value of 1.464 770 923 3(5) is procured, bearing 11 significant figures, harmonizing with reference values using the explicitly correlated exponential basis [10] and the Hylleraas basis [38]. The expectation values of $1/r_{12}^2$ for the $2\,^1S$, $2\,^3S$, and $3\,^3S$ states of the helium atom have, at a minimum, eight convergent digits, resonating well with the values reported in the available literature [9,10,39]. However, for the $\langle\nabla_1^2\nabla_2^2\rangle$ operator, no effective strategy for expedited convergence could be identified, necessitating direct calculation. Consequently, the convergence accuracy of $\langle\nabla_1^2\nabla_2^2\rangle$ is relatively diminished, primarily limiting the numerical precision of $\langle p_1^4\rangle$. Nonetheless, the derived value for $\langle p_1^4\rangle$ for the $1\,^1S$ state from the C-BSBFs exhibits nine digits, being consistent with Drake's Hylleraas results [38,39]. The numerical convergence for triplet states demonstrates superior performance compared to singlet states, by one to two significant figures, corroborating well with Hylleraas results [39].

Employing the traditional B-spline basis set, we computed $\langle 1/r_{12}^2\rangle$ and $\langle\nabla_1^2\nabla_2^2\rangle$, yielding the ground-state results of 1.463 697 and 7.079, respectively. Given the singularity of these operators, they offer a mere one to three significant digits, posing a challenge for high-precision atomic energy-level computations. It becomes discernible that the primary hindrance stems from the traditional B-spline basis set, which struggles to precisely characterize the local properties of the wave function without incorporating the electron correlation effect. The expectation values for the remaining three components from $H_{\rm BP}$, along with the singular electron-electron term $\langle 1/r_{12}^3\rangle$ from the leading QED corrections, are elucidated in Table VI. The expectation values of $\delta^3(r_{12})$ for the triplet states are zero, and hence omitted from Table VI. Comparisons with results obtained in available literatures are also made.

The numerical results of $\delta^3(r_1)$ were also given by Yu *et al.* [40], applying the identical C-BSBFs via direct computation, with the r_{12} power raised to $c = 5$. The direct computation of $\delta^3(r_1)$ heavily depends on the origin value of the wave function. The implementation of the global operator method can significantly enhance calculation accuracy [33,34]. Our result of $\delta^3(r_1)$ for the ground state using the global operator method is obtained to be 1.810 429 318 50(6) with ten accurate figures; for other states, one can see that the numerical accuracy of $\delta^3(r_1)$ can reach a precision of at least ten accurate digits. All current calculations are carried out with the r_{12} power $c = 1$. This indicates that the numerical accuracy can be better in the global operator method with a smaller c than increasing the r_{12} power of the direct calculation. Especially for operators with stronger singularity, such as $\delta^3(r_{12})$, the global operator method remains imperative for efficient numerical convergence. For instance, Yu *et al.* strived to bolster the direct calculation accuracy by increasing the r_{12} power to $c = 5$, but with $c = 1$ and the global operator method, our present value of 0.106 345 370 66(4) for the ground state surpassed the accuracy of 0.106 346 068 obtained from Yu *et al.* [40] by five orders of magnitude, and aligns well with

TABLE IV. The expectation values of other operators needed for evaluating the relativistic kinetic terms for the $1\,^1S$, $2\,^1S$, $2\,^3S$, and $3\,^3S$ states of helium.

Operator	$1\,^1S$	$2\,^1S$	$2\,^3S$	$3\,^3S$
$\langle 1/r_1\rangle$	1.688 316 800 717 1(2)	1.135 407 686 126 1(2)	1.154 664 152 972 0(1)	1.063 674 075 760 7(2)
	1.688 316 800 717[a]	1.135 407 686 125 609(6)[b]	1.154 664 152 972 107 60(20)[b]	1.063 674 075 760 76(10)[b]
	1.688 316 800 635[c]	1.135 407 686[c]	1.154 664 152[c]	1.063 674 075 7[c]
$\langle 1/r_1^2\rangle$	6.017 408 867 0(3)	4.146 939 019 80(6)	4.170 445 551 31(2)	4.042 948 747 4(3)
	6.017 408 867 0(1)[a]	4.146 939 019 0(12)[b]	4.170 445 551 336 2(4)[b]	4.042 948 747 477(4)[b]
$\langle 1/r_1r_2\rangle$	2.708 655 474 480(4)	0.561 861 467 461(2)	0.560 729 635 682 9(3)	0.240 684 804 629 3(2)
	2.708 655 474 480[a]	0.561 861 467 459 6(7)[b]	0.560 729 635 682 926 40(20)[b]	0.240 684 804 629 353(11)[b]
$\langle 1/r_{12}\rangle$	0.945 818 448 799 95(5)	0.249 682 652 394 3(6)	0.268 197 855 414 82(5)	0.117 318 168 097 65(4)
	0.945 818 448 800[a]	0.249 682 652 393 566 7(19)[b]	0.268 197 855 414 847 80(20)[b]	0.117 318 168 097 636(6)[b]
	0.945 818 448 705 9[c]	0.249 682 652 3[c]	0.268 197 855 3[c]	0.117 318 168 0[c]
$\langle 1/r_1r_{12}\rangle$	1.920 943 921 900 0(5)	0.340 633 845 861 2(8)	0.322 696 221 719 8(2)	0.131 426 560 051 19(5)
	1.920 943 921 900[a]	0.340 633 845 861 0(19)[b]	0.322 696 221 719 854 32(8)[b]	0.131 426 560 051 184(5)[b]

[a]Drake [38].
[b]Drake [39].
[c]Yu *et al.* [40].

TABLE V. Convergence of the relativistic kinetic terms for the $1\ ^1S$, $2\ ^1S$, $2\ ^3S$, and $3\ ^3S$ states of helium as the number of B splines N increased. The expectation values of $1/r_{12}^2$ and $\nabla_1^2\nabla_2^2$ are also listed in the second and third columns. The partial wave is $\ell_{\max} = 4$.

N	$\langle 1/r_{12}^2\rangle$	$\langle \nabla_1^2\nabla_2^2\rangle$	$\langle p_1^4\rangle$
		$1\ ^1S$	
50	1.464 770 923 579	7.133 709 835	54.088 067 177
60	1.464 770 923 463	7.133 709 771	54.088 067 242
70	1.464 770 923 406	7.133 709 763	54.088 067 251
Extrap.	1.464 770 923 3(5)	7.133 709 7(2)	54.088 067 2(2)
Ref. [10]	1.464 771	7.133 710	
Ref. [38]	1.464 770 923 350(1)		54.088 067 230(2)
		$2\ ^1S$	
50	0.143 724 814 027	1.428 212 689 1	41.118 675 563 8
60	0.143 724 814 013	1.428 212 706 4	41.118 675 546 0
70	0.143 724 814 008	1.428 212 705 8	41.118 675 546 6
Extrap.	0.143 724 814 00(5)	1.428 212 70(4)	41.118 675 54(4)
Ref. [10]	0.143 725	1.428 213	
Ref. [39]	0.143 724 814 00(7)		41.118 675 544(19)
		$2\ ^3S$	
50	0.088 906 004 870	0.488 197 568 41	41.835 540 798 28
60	0.088 906 004 913	0.488 197 569 31	41.835 540 797 46
70	0.088 906 004 921	0.488 197 569 91	41.835 540 796 85
Extrap.	0.088 906 004 9(2)	0.488 197 570(4)	41.835 540 796(4)
Ref. [9]	0.088 906	0.488 198	
Ref. [39]	0.088 906 004 932 625(5)		41.835 540 797 348(6)
		$3\ ^3S$	
50	0.023 097 669 645	0.329 220 596 46	40.475 439 870 27
60	0.023 097 669 653	0.329 220 596 68	40.475 439 868 42
70	0.023 097 669 655	0.329 220 596 89	40.475 439 868 25
Extrap.	0.023 097 669 65(3)	0.329 220 597(2)	40.475 439 868(5)
Ref. [39]	0.023 097 669 656 893(13)		40.475 439 868 127 2(3)

Drake's Hylleraas value of 0.106 345 370 636 3(12) [39]. Similarly, for the $2\ ^1S$ state, the present value for $\delta^3(r_{12})$ obtained with $c = 1$ is also in good agreement with Drake's result [39], but much more accurate than the result of Yu *et al.* [40] by three orders of magnitude.

Results of the retardation term H_2 have ten convergent figures at least and are consistent with Drake's results [39]. The expectation of the singular electron-electron $\langle 1/r_{12}^3\rangle$ was computed using the global operator method by the C-BSBFs, and they coincided with previous results from different basis functions. We acquired the C-BSBF result of 0.989 273 55(1) with an accuracy of seven decimals for the ground state, which is on par with the results of 0.989 273 5 and 0.989 272 4(13) using explicitly correlated Gaussian functions [41] and exponential basis functions [42], respectively. An improved value with three additional exact digits is available at Drake's website [39] using the Hylleraas basis. For the $2\ ^1S$ and $2\ ^3S$ states, our values corroborate with prior values determined by the Hylleraas basis and the exponential basis [25]. The present result for $\langle 1/r_{12}^3\rangle$ of the $3\ ^3S$ state equals to 0.008 922 57(2), featuring five convergent figures; we have not found any available data to refer to yet.

The singular electron-electron $\langle 1/r_{12}^3\rangle$ expectation value was also calculated using the traditional B-spline basis set, yielding a ground-state result of $1.197(N = 70,\ \ell_{\max} = 4)$. The traditional B spline is profoundly inaccurate in computing $\langle 1/r_{12}^3\rangle$, demanding a more precise description of local properties of the wave function [41] than $1/r_{12}^2$ and $\nabla_1^2\nabla_2^2$. Hence, the incorporation of electron correlation in the B-spline basis set is indispensable.

The final relativistic corrections are depicted in the top half of Table VII, and are compared with results from the explicitly correlated exponential basis [11] and the Hylleraas basis [39]. Our relativistic corrections are wholly consistent with the most precise previous computations [11,39], achieving nine to ten significant figures. The leading QED corrections for the S states to energy levels are summarized in the bottom half of Table VII. These results are obtained utilizing Bethe logarithm values obtained from B splines [21,23] and given by Korobov [30], respectively. It can be seen that our calculated results are in good agreement with the significant figures listed by Yerokhin and Pachucki [11]. The overall computational accuracy of the leading QED correction is chiefly determined by the Bethe logarithms' contribution. The leading QED corrections results can reach at least seven significant digits, which already matches the accuracy level of the leading relativistic correction in this paper.

IV. SUMMARY AND OUTLOOK

In this paper, we employed the C-BSBFs to compute the leading relativistic and QED corrections to the energy levels of the helium atom. Challenging operators such as the relativistic kinetic term p_1^4, contact potentials $\delta^3(r_1)$ and $\delta^3(r_{12})$, and Araki-Sucher correction $\langle 1/r_{12}^3\rangle$, which typically pose significant calculation difficulties, were tackled via a global

TABLE VI. The expectation values of $\delta^3(r_1)$, $\delta^3(r_{12})$, H_2, and $1/r_{12}^3$ for the $1\,^1S$, $2\,^1S$, $2\,^3S$, and $3\,^3S$ states of helium. Comparisons with results obtained in available literatures are also made. The partial wave is $\ell_{\max} = 4$.

N	$\langle\delta^3(r_1)\rangle$	$\langle\delta^3(r_{12})\rangle$	$\langle H_2\rangle$	$\langle 1/r_{12}^3\rangle$
		$1\,^1S$		
50	1.810 429 318 479 0	0.106 345 370 649 3	−0.139 094 690 900	0.989 273 549 0
60	1.810 429 318 502 1	0.106 345 370 658 3	−0.139 094 690 823	0.989 273 549 5
70	1.810 429 318 504 0	0.106 345 370 646 3	−0.139 094 690 720	0.989 273 548 4
Extrap.	1.810 429 318 50(6)	0.106 345 370 66(4)	−0.139 094 690 5(7)	0.989 273 55(1)
Ref. [40]	1.810 429 318 371 521 8	0.106 346 068		
Ref. [39]	1.810 429 318 499 0(6)	0.106 345 370 636 3(12)	−0.139 094 690 539 20(20)	0.989 273 544 768(13)
Ref. [41]				0.989 273 5
Ref. [42]				0.989 272 4(13)
		$2\,^1S$		
50	1.309 460 780 398 8	0.008 648 433 612 1	−0.009 253 046 273	0.067 946 580 5
60	1.309 460 780 376 2	0.008 648 433 588 4	−0.009 253 046 108	0.067 946 582 2
70	1.309 460 780 376 3	0.008 648 433 587 3	−0.009 253 046 092	0.067 946 578 8
Extrap.	1.309 460 780 37(5)	0.008 648 433 58(5)	−0.009 253 046 0(4)	0.067 946 58(2)
Ref. [40]	1.309 460 780 3	0.008 648 6		
Ref. [39]	1.309 460 780 1(4)	0.008 648 433 6(14)	−0.009 253 046 05(4)	
Ref. [43]				0.067 946 32
		$2\,^3S$		
50	1.320 355 082 933 78		−0.001 628 430 082 9	0.038 861 479 8
60	1.320 355 082 931 58		−0.001 628 430 067 4	0.038 861 479 6
70	1.320 355 082 931 10		−0.001.628 430 064 8	0.038 861 481 0
Extrap.	1.320 355 082 930(6)		−0.001 628 430 06(4)	0.038 861 46(3)
Ref. [40]	1.320 355 082 9			
Ref. [39]	1.320 355 082 934 92(9)		−0.001 628 430 061 553(3)	
Ref. [43]				0.038 861 485 631 95
		$3\,^3S$		
50	1.285 060 253 969 23		−0.000 504 504 232 33	0.008 922 569 5
60	1.285 060 253 936 06		−0.000 504 504 228 95	0.008 922 569 6
70	1.285 060 253 938 13		−0.000 504 504 228 33	0.008 922 569 9
Extrap.	1.285 060 253 93(7)		−0.000 504 504 228(9)	0.008 922 57(2)
Ref. [40]	1.285 060 253 9			
Ref. [39]	1.285 060 253 932 1(13)		−0.000 504 504 227 201(9)	

operator method to enhance their numerical convergence. Moreover, the Laplace expansion method as proposed by Sack [35] was introduced to handle the two-electron distance function. Combined with the high-precision calculation of the Bethe logarithms [23], the C-BSBF methodology facilitates high-precision computations of the leading relativistic and QED corrections for the energy levels of the helium atom. It is worth emphasizing that the inclusion of the correlated factor r_{12} in the C-BSBFs is vital to the calculations of p_1^4, $\delta^3(r_{12})$, and $\langle 1/r_{12}^3\rangle$; in the absence of this factor, these operators exhibit slow convergence. Thanks to its approximate linear independence and ample consideration of electronic correlation, the C-BSBF method provides stable numerical convergence. As evidenced in Table VIII, the C-BSBF methodology enables us to determine the accuracy of the $2\,^3S$-$2\,^1S$ transition frequency (including corrections up to the $m\alpha^5$ order) to a precision of kHz level. The fine-structure constant utilized in this paper is taken from CODATA 2018 [26]. It is noteworthy

TABLE VII. The leading relativistic and QED corrections to energy levels, $\delta E_{\rm rel}$ and $\delta E_{\rm QED}$ for the $1\,^1S$, $2\,^1S$, $2\,^3S$, and $3\,^3S$ states of helium. The corresponding comparison data given in available literatures are also listed.

	$1\,^1S$	$2\,^1S$	$2\,^3S$	$3\,^3S$
		The leading relativistic correction		
$\delta E_{\rm rel}/\alpha^2$	−1.951 754 76(6)	−2.034 167 34(2)	−2.164 477 971(2)	−2.045 092 764(2)
Ref. [39]	−1.951 754 767	−2.034 167 342	−2.164 477 972	−2.045 092 764
		The leading QED correction		
$\delta E_{\rm QED}/\alpha^3$(BL with B splines)	57.288 164 8(5)	42.523 605 15(8)	43.010 017(2)	41.839 303 4(7)
$\delta E_{\rm QED}/\alpha^3$(BL from Korobov)	57.288 164 808(6)	42.523 605 035(8)	43.010 017 06(2)	41.839 301 459(9)
Ref. [11]	57.288 165 2	42.523 605 1	43.010 016 8	

TABLE VIII. The $2\,^3S$-$2\,^1S$ transition frequency for the helium atom along the leading relativistic and QED corrections, in kHz.

	$\Delta E(2\,^3S$-$2\,^1S)$	Ref. [46]
NR	192 490 838 748(2)	192 490 838 756
$m\alpha^4$	45 657 858(8)	45 657 859
$m\alpha^5$	−1 243 670(6)	−1 243 671

that more recent and precise values of the fine-structure constant, α, have been reported [44,45], surpassing the accuracy of the value stipulated in CODATA 2018. However, given the current computational precision at the kHz level, variations in the values of α do not influence the final results of the present computations. This result aligns with the results of Pachucki *et al.* [46], and achieves a level of precision in the leading-order relativistic and QED correction to transition frequencies that is commensurate with the most recent experimental advancements [1]. These computations were accomplished using double precision alone, obviating the need for multiprecision calculations. Thus, this approach offers a pathway towards the calculation of atomic structure.

Given the inherent approximate completeness and substantial numerical stability of *B*-spline functions, they adeptly delineate both bound and continuum states, thereby finding extensive applicability in numerous problems necessitating state summation. The development of correlated *B*-spline basis sets, built upon the foundation of *B*-spline functions, meticulously incorporates electron correlation, facilitating a more accurate and encompassing representation of the eigenstates in two-electron systems. This approach holds promising potential for extensions to sophisticated calculations involving higher-order corrections, such as the second-order perturbations with the Breit-Pauli operator [47] and the relativistic corrections of the Bethe logarithm [48], and beyond. Moving forward, our ambition is to undertake the resolution of the Dirac-Coulomb-Breit equation, grounded on the foundation of correlated *B*-spline basis sets. This endeavor is projected to realize heightened precision in computations pertaining to atomic structures and to extend our reach to a more comprehensive array of atoms and ions with higher nuclear charge, particularly where the applicability of nonrelativistic QED theory is constrained.

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