## Fine Structure and Ionization Energy of the 1s2s2p <sup>4</sup>P State of the Helium Negative Ion He<sup>-</sup>

Liming Wang,<sup>1</sup> Chun Li,<sup>2</sup> Zong-Chao Yan,<sup>3,4</sup> and G. W. F. Drake<sup>5</sup> <sup>1</sup>Department of Physics, Henan Normal University, Xinxiang, Henan, People's Republic of China 453007

<sup>2</sup>Department of Mathematics, Nanjing University, Nanjing, Jiangsu, People's Republic of China 210093

<sup>3</sup>Department of Physics, University of New Brunswick, Fredericton, New Brunswick, Canada E3B 5A3

<sup>4</sup> State Key Laboratory of Magnetic Resonance and Atomic and Molecular Physics,

Wuhan Institute of Physics and Mathematics, Chinese Academy of Sciences, Wuhan, People's Republic of China 430071

<sup>5</sup>Department of Physics, University of Windsor, Windsor, Ontario, Canada N9B 3P4

(Received 24 September 2014; published 31 December 2014)

The fine structure and ionization energy of the 1s2s2p <sup>4</sup>P state of the helium negative ion He<sup>-</sup> are calculated in Hylleraas coordinates, including relativistic and QED corrections up to  $O(\alpha^4 mc^2)$ ,  $O((\mu/M)\alpha^4 mc^2)$ ,  $O(\alpha^5 mc^2)$ , and  $O((\mu/M)\alpha^5 mc^2)$ . Higher order corrections are estimated for the ionization energy. A comparison is made with other calculations and experiments. We find that the present results for the fine structure splittings agree with experiment very well. However, the calculated ionization energy deviates from the experimental result by about 1 standard deviation. The estimated theoretical uncertainty in the ionization energy is much less than the experimental accuracy.

DOI: 10.1103/PhysRevLett.113.263007

PACS numbers: 32.10.Fn, 31.30.jf, 32.10.Hq

Because of its long lifetime and ease of production, the metastable 1s2s2p <sup>4</sup>P state of the helium negative ion He<sup>-</sup> has long been of interest to both experimentalists and theorists [1-4]. It provides an ideal testing ground to study strong electron-electron correlation effects in this fundamental atomic system, where high precision measurements are feasible. For example, White and Stillinger [5] have suggested that the exact wave function for the quartet states may contain higher-order logarithmic terms near the triple coalescence point. These strong electron-correlation effects have limited the accuracy of previous calculations of properties such as the energy level structure and lifetime. The nonrelativistic energy of this state was calculated to a relative accuracy of 1 part in 10<sup>7</sup> nearly two decades ago by Chung and co-workers by using the configuration interaction method [3], but subsequent work has not yielded significant improvements. The fine structure of this state was measured by Mader and Novick as early as 1972 [1] and the results were 825.23(83) MHz for J = 3/2 to 5/2 and 8663(56) MHz for J = 1/2 to 5/2, respectively. The corresponding theoretical fine structure was calculated by Chung and coworkers [3,6], but the accuracy was lower than that of the experiment. The ionization energy of the state was also measured and calculated in Ref. [3]. The experimental result 77.516(6) meV agrees with the less accurate theoretical result 77.518(11) meV and agrees with Bunge and Bunge's even less accurate theoretical result 77.51(4) meV [2], but differs slightly from the experimental result 77.67(12) meV of Walter et al. [7]. These accuracies fall far short of modern spectroscopic standards for fundamental atomic systems.

During the past two decades, high precision methods to calculate the properties of few-electron atoms in Hylleraas coordinates have been developed by Drake and Yan [8,9] and by Pachucki and Puchalski [10-12]. As a result, the nonrelativistic energy of the ground state of lithium has been calculated to a relative accuracy of  $10^{-15}$  [11,13] and its ionization energy to an accuracy of  $0.001 \text{ cm}^{-1}$  or better [11,14]. The agreement of theory with experiment demonstrates the power and utility of the methods developed by these authors.

The purpose of this Letter is to report a dramatic advance in the accuracy that can be achieved for the nonrelativistic energy, fine structure splittings, and ionization energy of the 1s2s2p <sup>4</sup>P state of He<sup>-</sup>. The calculations are performed in Hylleraas coordinates by the method developed by Drake and Yan [8,9].

The nonrelativistic energy and wave function of the state are calculated by using the Rayleigh-Ritz variational method. The Hamiltonian of the system is

$$H = -\frac{1}{2}\sum_{i=1}^{3} \nabla_{i}^{2} - Z\sum_{i=1}^{3}\frac{1}{r_{i}} + \sum_{i>j}^{3}\frac{1}{r_{ij}} - \frac{\mu}{M}\sum_{i>j}^{3} \nabla_{i} \cdot \nabla_{j},$$
(1)

in units of  $2R_M$ , where the Rydberg constant for finite nuclear mass is defined by  $R_M = (1 - (\mu/M))R_{\infty}$ , and  $\mu$  is the reduced electron mass. The variational wave function is constructed from the basic correlated function

$$r_{1}^{j_{1}}r_{2}^{j_{2}}r_{3}^{j_{3}}r_{12}^{j_{12}}r_{23}^{j_{23}}r_{31}^{j_{31}}e^{-\alpha r_{1}-\beta r_{2}-\gamma r_{3}}\mathcal{Y}_{(\ell_{1}\ell_{2})\ell_{12},\ell_{3}}^{LM}(\mathbf{r}_{1},\mathbf{r}_{2},\mathbf{r}_{3})\chi, \quad (2)$$

where  $\mathcal{Y}_{(\ell_1 \ell_2) \ell_{12}, \ell_3}^{LM}$  is a vector-coupled product of spherical harmonics for the three electrons to form a state of total angular momentum L, and  $\chi$  is the spin function which can be chosen to be  $\alpha(1)\alpha(2)\alpha(3)$  for spin quartet states. See Ref. [13] for more detailed information about the construction of the variational wave function. We progressively enlarged the number of basis functions used in the variational procedure from 70 to 28 008. As shown in Table I, the extrapolated nonrelativistic energy has converged to approximately 13 significant figures with the result  $E_{\rm NR} = -2.178\,078\,044\,567\,6(3)$  a.u. for the 1s2s2p ${}^{4}P$  state of He<sup>-</sup>. This result is more accurate than the previous best values [3,15] by about 6 orders of magnitude. The high precision nonrelativistic energy and wave function provide the foundation for the calculation of relativistic and QED corrections to the energy. Considering that the 1s2s2p <sup>4</sup>P state is a doubly excited state, our calculation demonstrates the power of Hylleraas-type variational bases in dealing with doubly excited states of simple atomic systems.

The leading relativistic corrections of order  $\alpha^2$  Ry and the relativistic recoil corrections of order  $(\mu/M)\alpha^2$  Ry are calculated by first-order perturbation theory [for convenience the anomalous magnetic moment terms of order  $\alpha^3$ Ry and  $(\mu/M)\alpha^3$  Ry are included]

$$\Delta E_{\rm rel} = \langle \Psi_J | H_{\rm rel} | \Psi_J \rangle, \tag{3}$$

where  $\Psi_J$  is the nonrelativistic wave function and  $H_{\text{rel}}$  is defined by (in atomic units)

TABLE I. Convergence of the nonrelativistic energy for the 1s2s2p <sup>4</sup>*P* state of He<sup>-</sup> with infinite nuclear mass. The ratio of differences  $R(\Omega) = [E(\Omega - 1) - E(\Omega - 2)]/[E(\Omega) - E(\Omega - 1)]$  provides a measure of the rate of convergence to the extrapolated energy. Units are a.u.

	No. of		
Ω	terms	$E(\mathbf{\Omega})$	$R(\Omega)$
4	70	-2.177 521 110 364 780	
5	182	-2.178059296923302	
6	420	-2.178076202581397	31.8
7	880	-2.178077808759359	10.5
8	1710	-2.178078014352644	7.81
9	3130	-2.178078040867143	7.75
10	5430	-2.178078044036570	8.36
11	9000	-2.178078044498709	6.85
12	14 370	-2.178078044556858	7.94
13	22 202	-2.178078044565846	6.46
14	28 008	-2.178078044567332	6.05
Extrapolated		-2.1780780445676(3)	
Bunge and		-2.178 077 6(12)	
Bunge [2]			
Bylicki and		-2.17807767(5)	
Pestka [15]			
Kristensen et al. [3]		-2.17807785(32)	

$$H_{\rm rel} = \left(\frac{\mu}{m_e}\right)^4 B_1 + \left(\frac{\mu}{m_e}\right)^3 \\ \times \left[B_2 + B_4 + B_{\rm so} + B_{\rm soo} + B_{\rm ss} + \frac{m_e}{M}(\tilde{\Delta}_2 + \tilde{\Delta}_{3z}) \right. \\ \left. + \gamma \left(2B_{\rm so} + \frac{4}{3}B_{\rm soo} + \frac{2}{3}B_{3e}^{(1)} + 2B_{\rm ss}\right) + \gamma \frac{m_e}{M}\tilde{\Delta}_{3z}\right],$$

$$(4)$$

with  $\gamma = \alpha/(2\pi)$ . The factors of  $(\mu/m_e)^4$  and  $(\mu/m_e)^3$  arise from the mass scaling of each term in the Breit interaction. In the above equation,

$$B_1 = -\frac{\alpha^2}{8} (\nabla_1^4 + \nabla_2^4 + \nabla_3^4), \tag{5}$$

$$B_2 = \frac{\alpha^2}{2} \sum_{i>j}^3 \left[ \frac{1}{r_{ij}} \nabla_i \cdot \nabla_j + \frac{1}{r_{ij}^3} \mathbf{r}_{ij} \cdot (\mathbf{r}_{ij} \cdot \nabla_i) \nabla_j \right], \tag{6}$$

$$B_4 = \pi \alpha^2 \left[ \frac{Z}{2} \sum_{i=1}^3 \delta(\mathbf{r}_i) - \sum_{i>j}^3 \left( 1 + \frac{8}{3} \mathbf{s}_i \cdot \mathbf{s}_j \right) \delta(\mathbf{r}_{ij}) \right], \quad (7)$$

$$B_{\rm so} = \frac{Z\alpha^2}{2} \sum_{i=1}^{3} \frac{1}{r_i^3} \mathbf{r}_i \times \mathbf{p}_i \cdot \mathbf{s}_i, \qquad (8)$$

$$B_{\text{soo}} = \frac{\alpha^2}{2} \sum_{i \neq j}^3 \frac{1}{r_{ij}^3} \mathbf{r}_{ji} \times \mathbf{p}_i \cdot (\mathbf{s}_i + 2\mathbf{s}_j), \qquad (9)$$

$$B_{\rm ss} = \alpha^2 \sum_{i>j}^3 \left[ \frac{1}{r_{ij}^3} (\mathbf{s}_i \cdot \mathbf{s}_j) - \frac{3}{r_{ij}^5} (\mathbf{r}_{ij} \cdot \mathbf{s}_i) (\mathbf{r}_{ij} \cdot \mathbf{s}_j) \right], \qquad (10)$$

$$\tilde{\Delta}_2 = \frac{iZ\alpha^2}{2} \sum_{j=1}^3 \left[ \frac{1}{r_j} \mathbf{p} \cdot \nabla_j + \frac{1}{r_j^3} \mathbf{r}_j \cdot (\mathbf{r}_j \cdot \mathbf{p}) \nabla_j \right], \tag{11}$$

$$\tilde{\Delta}_{3z} = Z\alpha^2 \sum_{i=1}^{3} \frac{1}{r_i^3} \mathbf{r}_i \times \mathbf{p} \cdot \mathbf{s}_i,$$
(12)

$$B_{3e}^{(1)} = \frac{\alpha^2}{2} \sum_{i \neq j}^3 \frac{1}{r_{ij}^3} \mathbf{r}_{ji} \times \mathbf{p}_i \cdot (\mathbf{s}_i - \mathbf{s}_j), \tag{13}$$

with  $\mathbf{p} = \mathbf{p}_1 + \mathbf{p}_2 + \mathbf{p}_3$ . In Eq. (4), only the terms which contain spin-dependent operators, i.e.,  $B_{so}$ ,  $B_{soo}$ ,  $B_{ss}$ , and  $\tilde{\Delta}_{3z}$ , contribute to the fine structure splittings (the expectation value of  $B_{3e}^{(1)}$  is zero for spin quartet states). The reduced matrix elements for these operators were calculated with the high precision nonrelativistic wave functions and the results are listed in Table II. Also listed in Table II are the matrix elements of the spin-independent Breit operators, which will be used in the determination of the ionization energy. All the matrix elements for these

TABLE II. Reduced matrix elements for the spin-dependent Breit operators and matrix elements for the spin-independent ones for the 1s2s2p <sup>4</sup>*P* state of He<sup>-</sup> with infinite nuclear mass. Units are a.u.

Operator	Value
$B_{\rm so} \times 10^6$	3.237 230 27(2)
$B_{\rm soo} \times 10^6$	-5.4729249(1)
$B_{\rm ss} \times 10^6$	-2.2678520(1)
$\tilde{\Delta}_{3_7} \times 10^6$	-2.578463(1)
$B_1 \times 10^4$	-5.483406606(4)
$B_2 \times 10^7$	5.148 246 185(14)
$\sum_{i=1}^{3} \delta(\mathbf{r}_i)$	2.605 303 906(2)
$\tilde{\Delta}_2  imes 10^4$	-8.823466952(8)
Q	0.003 664 529 86(3)
$Q, \text{He}(1s2s \ {}^{3}S)$	0.003 092 498 767 110(6) <sup>a</sup>
$Q_1$	-3.61184659(6)
$Q_1$ , He(1s2s <sup>3</sup> S)	$-3.6641502(2)^{b}$

<sup>a</sup>Drake and Yan [16].

<sup>b</sup>Pachucki and Sapirstein [17].

operators were calculated with wave functions containing up to 22 202 basis functions. The resulting fine structure splittings for the 1s2s2p <sup>4</sup>*P* state of He<sup>-</sup> (for isotopes <sup>3</sup>He and <sup>4</sup>He, respectively) are listed in Table III, which are accurate to  $\alpha^3$  Ry. A comparison of the theoretical results with the experimental ones shows that the two are in good agreement.

Following the formulation of Drake and Yan [18], the QED corrections to the energy levels of light atomic systems can be written in the form

$$\Delta E_{\text{OED}} = \Delta E_{L,1} + \Delta E_{L,2} + \Delta E_M + \Delta E_{\text{DK}}, \qquad (14)$$

where  $\Delta E_{L,1}$  denotes the QED correction to the electronnucleus interaction,  $\Delta E_{L,2}$  the correction to the electronelectron interaction,  $\Delta E_M$  the finite nuclear mass correction, and  $\Delta E_{\text{DK}}$  the Douglas and Kroll terms (including second-order Breit corrections). These terms have the following forms:

TABLE III. Contributions to the theoretical fine structure splittings for the 1s2s2p  ${}^{4}P_{J}$  states of  ${}^{3,4}\text{He}^{-}$  and comparison with other calculations and experiments. SIS denotes the splitting isotope shift. Units are MHz.

Term	$E_{3/2} - E_{5/2}$	$E_{1/2} - E_{5/2}$
$\alpha^2$	830.580(1)	8 639.061 4(5)
$\alpha^3$	-5.418176(2)	8.311 037(1)
$\alpha^2 \mu/M$ , <sup>3</sup> He	0.662 1(1)	1.027 8(1)
$\alpha^2 \mu/M$ , <sup>4</sup> He	0.498 8(1)	0.774 3(2)
$\alpha^3 \mu/M$ , <sup>3</sup> He	$-1.5341(1) \times 10^{-4}$	$-3.1871(1) \times 10^{-4}$
$\alpha^3 \mu/M$ , <sup>4</sup> He	$-1.1567(1) \times 10^{-4}$	$-2.4027(1) \times 10^{-4}$
Total, <sup>3</sup> He	825.824(1)	8 648.399 9(5)
Total, <sup>4</sup> He	825.661(1)	8 648.146 5(5)
SIS $({}^{3}\text{He} - {}^{4}\text{He})$	0.163 2(3)	0.253 4(3)
Theory <sup>a</sup>	836.4	7 857.5
Experiment <sup>b</sup>	825.23(83)	8 663(56)

<sup>a</sup>Kristensen *et al.* [3].

<sup>b</sup>Mader and Novick [1].

$$\begin{split} \Delta E_{L,1} &= Z \alpha^5 \mu c^2 \{ \ln(Z\alpha)^{-2} \mathcal{A}_{5,1} + \mathcal{A}_{5,0} + Z \alpha \mathcal{A}_{6,0} \\ &+ (Z\alpha)^2 [\ln^2(Z\alpha)^{-2} \mathcal{A}_{7,2} + \ln(Z\alpha)^{-2} \mathcal{A}_{7,1} + \mathcal{A}_{7,0}] \\ &+ (\alpha/\pi) [\mathcal{B}_{6,0} + Z \alpha \mathcal{B}_{7,0}] + O(Z\alpha)^3 + O(\alpha/\pi)^2 \}, \end{split}$$
(15)

$$\Delta E_{L,2} = \alpha^5 \mu c^2 [\ln(\alpha) C_{5,1} + C_{5,0} + \alpha \ln(\alpha) C_{6,1} + \alpha C_{6,0} + O(\alpha^2)],$$
(16)

$$\Delta E_{M} = \left(\frac{-2\mu}{M}\right) \left\{ \Delta E_{L,1} + \Delta E_{L,2} - \frac{1}{2} Z \alpha^{5} m c^{2} \left\langle \sum_{i} \delta(\mathbf{r}_{i}) \right\rangle \right\}$$
$$+ Z^{2} \alpha^{5} m_{e} c^{2} \frac{\mu}{M} \left\{ \left[\frac{1}{3} \ln(Z\alpha)^{-2} - \frac{8}{3} \ln(k_{0}) + \frac{62}{9}\right] \times \left\langle \sum_{i} \delta(\mathbf{r}_{i}) \right\rangle - \frac{14}{3} Q_{1} \right\}.$$
(17)

The expression for  $\Delta E_{\rm DK}$  is not written here explicitly, because we do not calculate it in this work. These terms

TABLE IV. Convergence study of the Bethe logarithm for the 1s2s2p <sup>4</sup>*P* state of He<sup>-</sup>. *N* is the total number of terms in the basis set and  $\ln(k_0) = \beta^{(0)} + (\mu/M)\beta^{(1)}$ .

Ω	Ν	$eta^{(0)}$	Ratio	$eta^{(1)}$
1	211 + 255 + 353	2.513 004		0.522 57
2	331 + 374 + 472	2.860 535		0.438 69
3	587 + 629 + 727	2.944 134	4.15	0.250 55
4	1089 + 1130 + 1228	2.966 138	3.80	0.146 32
5	2007 + 2047 + 2145	2.974 631	2.59	0.078 99
6	3596 + 3635 + 3733	2.977 419	3.04	0.046 66
7	6221 + 6259 + 6357	2.978 692	2.19	0.028 42
Extrap.		2.9797(11)		0.0048(48)
$He(1s2s^{-3}S)$		$2.977742^{\rm a}$		$0.004~78^{a}$
$\operatorname{He}^{+}(1s)$		$2.984\ 128\ 555^{a}$		

<sup>a</sup>Drake and Goldman [19].

TABLE V. Detailed breakdown of the QED contributions of order  $\mu c^2 \alpha^5$  and higher to the ionization energy of the  $1s2s2p \ ^4P$  state of  $^4$ He<sup>-</sup>. Units are MHz.

Term	Value
$\frac{1}{\mu c^2 \alpha^5 Z [\ln(Z\alpha)^{-2} \mathcal{A}_{5,1} + \mathcal{A}_{5,0}]}$	-1511(18)
$\mu c^2 \alpha^5 [\ln(\alpha) C_{5,1} + C_{5,0}]$	-6.830
$\Delta E_M$ (finite nuclear mass)	0.108(9)
$\mu c^2 \alpha^5$ (total)	-1518(18)
$\mu c^2 \alpha^6 Z^2 \mathcal{A}_{6,0}$	-25.421
$\mu c^2 \alpha^6 Z \mathcal{B}_{6,0}/\pi$	-0.227
$\mu c^2 \alpha^6 \ln(\alpha) \mathcal{C}_{6,1}$	0.000
$\Delta E_{\rm DK}$	0.0(2.0)
$\mu c^2 \alpha^6$ (total)	-25.6(2.0)
$\mu c^2 \alpha^7 Z^3 \ln^2 (Z\alpha)^{-2} A_{7,2}$	2.757
$\mu c^2 \alpha^7 Z^3 \ln(Z\alpha)^{-2} \mathcal{A}_{7,1}$	-1.697
$\mu c^2 \alpha^7 Z^3 \mathcal{A}_{7,0}$	1.192
$\mu c^2 \alpha^7 Z^2 \mathcal{B}_{7,0} / \pi$ (two-loop binding)	0.132
$\mu c^2 \alpha^7$ (total)	2.4(2.4)
Total	-1541(22)

were recently evaluated by Puchalski and Pachucki [12] for the  $1s^22p$  <sup>2</sup>*P* state of lithium, and will need to be included in future work. They can be expected to contribute at the  $\pm 1$  MHz level of accuracy. The expressions and meanings of the various coefficients  $\mathcal{A}_{m,n}$ ,  $\mathcal{B}_{m,n}$ , and  $\mathcal{C}_{m,n}$  are given in detail in Ref. [18], so we do not repeat the discussion of them (except for  $\mathcal{A}_{5,0}$ ). The coefficient  $\mathcal{A}_{5,0}$  has the form

$$\mathcal{A}_{5,0} = \frac{4}{3} [19/30 - \ln(k_0)] \left\langle \sum_i \delta(\mathbf{r}_i) \right\rangle, \qquad (18)$$

where  $\ln(k_0)$  is the Bethe logarithm of the state of interest and is defined by (with  $k_0$  in units of  $Z^2 R_M$ )

$$\ln(k_0) = \frac{\sum_n |\langle 0|\mathbf{p}|n\rangle|^2 (E_n - E_0) \ln |2(E_n - E_0)/Z^2|}{\sum_n |\langle 0|\mathbf{p}|n\rangle|^2 (E_n - E_0)}.$$
(19)

At present, there are two main methods to calculate nonrelativistic Bethe logarithms for light atomic systems. One is the variational pseudostate method of Drake and Goldman [19] and developed by Yan and Drake [20] for three-electron atoms. The other is the integral method developed by Puchalski *et al.* [21]. Both of these methods have been used in previous work to calculate Bethe logarithms for the low-lying states of lithium to about six or seven significant figures. The variational pseudostate method is used here to calculate the Bethe logarithm for the 1s2s2p <sup>4</sup>*P* state of He<sup>-</sup>. The results are listed in Table IV. Surprisingly, the numerical value converges very slowly and just three converged figures are obtained. The reason for the slow convergence is not yet known, but it may be attributed to the strongly correlated nature of the 1s2s2p <sup>4</sup>*P* 

TABLE VI. Contributions to the (negative) ionization energies of the 1s2s2p  ${}^{4}P_{J}$  states of  ${}^{4}\text{He}^{-}$  and comparison with other calculations and experiments. Units are MHz.

Term	Value
$\mu c^2 \alpha^2$	-18740754.820(2)
$\mu c^2 \alpha^2 (\mu/M)_{\rm mp}$	-23915.8256(1)
$\mu c^2 \alpha^2 (\mu/M)_{\rm mp}^2$	-9.542(1)
$\mu c^2 \alpha^4$	$28548.6745(7)_{1/2}$
	$20741.2616(7)_{3/2}$
	$19910.7972(7)_{5/2}$
$\mu c^2 \alpha^4 (\mu/M)$	$9.3602(2)_{1/2}$
	$8.0143(2)_{3/2}$
	$7.4017(2)_{5/2}$
$\mu c^2 \alpha^5$ : Breit $g-2$	$8.7317634(1)_{1/2}$
	$-4.9973306(4)_{3/2}$
	$0.42096572(1)_{5/2}$
E <sub>nuc</sub>	-0.985(3)
$E_{\rm QED}$	-1541(22)
Total (this work, MHz)	$-18737655(22)_{1/2}$
	$-18745478(22)_{3/2}$
	$-18746303(22)_{5/2}$
Total (this work, meV)	$-77.49271(9)_{1/2}$
	$-77.52507(9)_{3/2}$
	$-77.52848(9)_{5/2}$
Total (previous work, $J = 5/2$ , meV)	
Theory <sup>a</sup>	-77.51(4)
Theory <sup>b</sup>	-77.518(11)
Experiment <sup>b</sup>	-77.516(6)
Experiment <sup>c</sup>	-77.67(12)

<sup>a</sup>Bunge and Bunge [2]. <sup>b</sup>Kristensen *et al.* [3].

<sup>c</sup>Walter *et al.* [7].

Watter et al. [7].

state. This is the first application of variational pseudostate methods to calculate Bethe logarithms for doubly excited states. It is clear that further improvements are needed in the technology for these states. However, it is significant that, as found previously, the Bethe logarithm comes almost entirely from virtual excitations of the inner 1*s* electron, and the outer electrons are, to a good approximation, passive spectators. It seems likely that the Bethe logarithm for any atom up to moderately high *Z* can be predicted to about 0.2% accuracy from the hydrogenic value for a 1*s* electron.

For low-Z atoms and ions, the finite nuclear size correction to an energy level can be calculated according to

$$\Delta E_{\rm nuc} = \frac{2\pi Z (r_c/a_0)^2}{3} \left\langle \sum_i \delta(\mathbf{r}_i) \right\rangle, \tag{20}$$

where  $r_c$  is the root-mean-square radius of the nuclear charge distribution and  $a_0$  is the Bohr radius.

The results of various QED corrections to the ionization energy are listed in Table V. The main uncertainty of the QED contribution comes from the uncertainty in the value of  $\ln(k_0)$ , which gives an uncertainty of 18 MHz. Together with the nonrelativistic, relativistic, anomalous magnetic moment of the electron, and finite nuclear size corrections, we obtain the ionization energies (relative to the 1s2s <sup>3</sup>S state of He) of the three fine structure components (J = 1/2, 3/2, and 5/2) of the  $1s2s2p \ ^4P_J$  states of He<sup>-</sup>. These results are listed in Table VI. The ionization energy of the J = 5/2 component is usually defined in the literature as the electron affinity of the 1s2s <sup>3</sup>S state of He. So far there are two experimental results for this value: i.e., the relatively less accurate value 77.67(12) meV given by Ref. [7] and the relatively more accurate value 77.516(6) meV given by Ref. [3]. These two results do not agree with each other. On the theoretical side, our present result is 77.528 48(9) meV, which differs from the more accurate experimental value 77.516(6) meV by 1 standard deviation. Reference [2] and Ref. [15] give the same rough estimate value 77.51(4) meV. The error bar is large enough that it agrees with both the experimental ones.

The parameters used in the present work are [22]  $R_{\infty} = 3289841960.364(17)$  MHz,  $\alpha = 1/137.035999074(44)$ ,  $m_e/M(^3\text{He}) = 1.8195430761(16) \times 10^{-4}$ ,  $m_e/M(^4\text{He}) = 1.37093355578(55) \times 10^{-4}$ , and  $r_c(^4\text{He}) = 1.681(4)$  fm [23].

In summary, in this work we have obtained highly accurate nonrelativistic energies and wave functions for the 1s2s2p <sup>4</sup>P state of He<sup>-</sup> by solving the Schrödinger equation in Hylleraas coordinates. We have also obtained the fine structure splitting and ionization energy. The results for the fine structure agree with experiment very well. However, the theoretical ionization energy does not agree with either of the experimental values, and the two most precise experimental values do not agree with each other. Clearly, further experimental studies are needed to clarify the situation.

This work was supported by National Natural Science Foundation (NNSF) of China under Grants No. 11347116 and No. 91130003, and by Natural Sciences and Engineering Research Council (NSERC) of Canada. C. L. was also supported by the Priority Academic Program Development (PAPD) of Jiangsu Higher Education Institutions. Z.-C. Y. was also supported by the Chinese Academy of Sciences/State Administration of Foreign Experts Affairs (CAS/SAFEA) International Partnership Program for Creative Research Teams. Research support from the computing facilities of SHARCnet, ACEnet, and Wuhan University (No. TC5000) is gratefully acknowledged.

- [1] D. L. Mader and R. Novick, Phys. Rev. Lett. 29, 199 (1972).
- [2] A. V. Bunge and C. F. Bunge, Phys. Rev. A 30, 2179 (1984).
- [3] P. Kristensen, U. V. Pedersen, V. V. Petrunin, T. Andersen, and K. T. Chung, Phys. Rev. A 55, 978 (1997).
- [4] P. Reinhed et al., Phys. Rev. Lett. 103, 213002 (2009).
- [5] R. J. White and F. H. Stillinger, Phys. Rev. A 3, 1521 (1971).
- [6] K. T. Chung, Phys. Rev. A 29, 439 (1984).
- [7] C. W. Walter, J. A. Seifert, and J. R. Peterson, Phys. Rev. A 50, 2257 (1994).
- [8] Z.-C. Yan and G. W. F. Drake, Phys. Rev. A 52, 3711 (1995).
- [9] Z.-C. Yan and G. W. F. Drake, Phys. Rev. A 61, 022504 (2000).
- [10] M. Puchalski, D. Kedziera, and K. Pachucki, Phys. Rev. A 80, 032521 (2009).
- [11] M. Puchalski, D. Kedziera, and K. Pachucki, Phys. Rev. A 82, 062509 (2010).
- [12] M. Puchalski and K. Pachucki, Phys. Rev. Lett. 113, 073004 (2014).
- [13] L. M. Wang, Z.-C. Yan, H. X. Qiao, and G. W. F. Drake, Phys. Rev. A 85, 052513 (2012).
- [14] Z.-C. Yan, W. Nörtershäuser, and G. W. F. Drake, Phys. Rev. Lett. 100, 243002 (2008); 102, 249903(E) (2009).
- [15] M. Bylicki and G. Pestka, J. Phys. B 29, L353 (1996).
- [16] G. W. F. Drake and Z.-C. Yan, Phys. Rev. A 46, 2378 (1992).
- [17] K. Pachucki and J. Sapirstein, J. Phys. B 33, 455 (2000).
- [18] G. W. F. Drake and Z.-C. Yan, Can. J. Phys. 86, 45 (2008).
- [19] G. W. F. Drake and S. P. Goldman, Can. J. Phys. 77, 835 (1999).
- [20] Z.-C. Yan and G. W. F. Drake, Phys. Rev. Lett. 91, 113004 (2003).
- [21] M. Puchalski, D. Kedziera, and K. Pachucki, Phys. Rev. A 87, 032503 (2013).
- [22] P. J. Mohr, B. N. Taylor, and D. B. Newell, Rev. Mod. Phys. 84, 1527 (2012).
- [23] I. Sick, Phys. Rev. C 77, 041302(R) (2008).