Bethe logarithms for the $1^1S$, $2^1S$ and $2^3S$ states of helium and helium-like ions

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We have computed the Bethe logarithms for the $1^1S$, $2^1S$ and $2^3S$ states of the helium atom to about seven figure-accuracy using a generalization of a method first developed by Charles Schwartz. We have also calculated the Bethe logarithms for the helium-like ions Li$^+$, Be$^{++}$, O$^{6+}$ and Si$^{14+}$ for all three states to study the $1/Z$ behavior of the results. The Bethe logarithm of H$^-$ was also calculated with somewhat less accuracy. The use of our Bethe logarithms for the excited states of neutral helium, instead of those from Goldman and Drake’s first-order $1/Z$-expansion, reduces by several orders of magnitude the discrepancies between the theoretically calculated and experimentally measured ionization potentials of these states.

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Ever since the invention of quantum mechanics, the helium atom has served as an important testing-ground for our understanding of fundamental physics. In 1929 Hylleraas’ calculation of the binding energy of the non-relativistic helium atom Hamiltonian showed that Schrödinger’s formulation of quantum mechanics provided a quantitatively accurate description of not just two-body but three-body systems$^1$. During the 1950’s, with the advent of fast digital computers, calculations by Kinoshita$^2$ and Pekeris$^3$ of not only the non-relativistic binding energy but also of relativistic corrections of $O(\alpha^2)$ greatly improved the agreement between theory and experiment, and showed that the estimation of $O(\alpha^3)$ Rydberg effects arising from quantum electrodynamics was important for obtaining agreement between theory and experiment at the level of 1 part in $10^6$ or better. During the 1960’s and 1970’s the variational techniques employed by Pekeris on the lowest states of singlet and triplet symmetry were extended to a wide range of excited states of the helium atom$^4$$^5$. During the 1980’s, with the advent of two-photon spectroscopy with counterpropagating laser beams, which can be used to eliminate the 1st-order Doppler shift due to the thermal motion of the atoms, it became possible to measure the wavelengths for transitions between excited states of the helium atom with a precision of 1 part in $10^5$ or better$^6$. Though numerous examples of excellent agreement between theory and experiment in a wide variety of contexts leave no reasonable doubt that quantum electrodynamics is the correct theory for describing the interactions of charged particles at low energies, the extraordinary accuracy recently achieved in high-precision measurements on the helium atom poses a challenge to theorists to develop computational techniques capable of matching such accuracies. Since $\alpha^3$ is of order $10^{-10}$, it is clear that the coefficient of the lowest-order QED corrections needs to be evaluated with a relative accuracy of $10^{-3}$ or better, and the effects of contributions with higher powers of $\alpha$ must also be estimated, to match the experimental accuracy of 1 part in $10^9$ or better.

For a helium atom or helium-like ion of atomic number $Z$, the leading $O(\alpha^3)$ Rydberg contribution to the Lamb shift is given by the expression$^7$

$$E_{L,2} = \frac{8}{3} Z \alpha^3 \psi_0^2(0) \left[ 2 \ln \left( \frac{1}{\alpha} \right) - \ln \left( \frac{k_0}{\text{Ry}} \right) + \frac{19}{30} \right] \text{Ry},$$

where the so-called Bethe logarithm$^8$ is defined by an infinite and slowly-convergent sum over all bound and continuum eigenstates:

$$\ln(k_0/\text{Ry}) = \frac{\beta}{D} = \frac{\sum_n | \langle \psi_n | \mathbf{p} | \psi_0 \rangle |^2 (E_n - E_0) \ln |E_n - E_0|}{\sum_n | \langle \psi_n | \mathbf{p} | \psi_0 \rangle |^2 (E_n - E_0)},$$

Here $\mathbf{p}$ is the sum of single-particle momentum operators ($\mathbf{p} = \sum_i p_i$) and $\psi_0$ is an eigenfunction with eigenvalue $E_0$ of the Hamiltonian $H$ of the atom. For simplicity, we assume that $H$ is the nonrelativistic Hamiltonian of an atom with atomic number $Z$, with a point nucleus of infinite mass:

$$H = T + V = \sum_i \frac{p_i^2}{2} - Z \sum_i \frac{1}{r_i} + \sum_{i>j} \frac{1}{r_{ij}},$$
which has the important and useful property that it is unitarily equivalent to the scaled Hamiltonian

$$Z^2 \left( \sum_i p_i^2/2 - \sum_i 1/r_i + (1/Z) \sum_{i>j} 1/r_{ij} \right),$$

which after division by $Z^2$ tends to a well-defined limit as $Z \to \infty$. (The effects of the reduced mass $\mu = m_e M_N/(m_e + M_N)$ due to the finiteness of the nuclear mass $M_N$ are subsequently included by scaling by appropriate powers of $\mu/m_e$, and the negligible effect of the ‘mass-polarisation’ term $M_N^{-1} \sum_{i>j} p_i \cdot p_j$ on the Bethe logarithm is here ignored.) With the help of the closure relation $\sum_n |n\rangle \langle E_n - E_0|n\rangle = H - E_0$, the commutation relation $(H - E_0) p \psi_0 = i(\nabla V) \psi_0$, an integration by parts, and Gauss’ Law ($\nabla^2 V = 4\pi Z \sum_i \delta^{(3)}(r_i)$), the denominator $D$ is easily evaluated:

$$D = \langle \psi_0 | p \cdot (H - E_0) p | \psi_0 \rangle = 2\pi Z \psi_0^2(0),$$

but the logarithmic factor makes the numerator $\beta$ much harder to evaluate. Even for a very simple one-electron system such as the hydrogen atom, $\beta$ cannot be evaluated in closed form, though several rapidly convergent methods can be used to evaluate it to high accuracy [9], [10], [11], [12], and the Bethe logarithm of the electronic ground state of $\text{H}_2^+$ was recently evaluated numerically [13]. For a two-electron system such as the helium atom, whose unknown wavefunction $\psi_0$ must be represented by an expansion in a large basis set, the numerical challenges are even more daunting.

In the early 1960’s C. Schwartz recast the numerator as integral over the virtual photon energy $k$ [14],

$$\beta = \lim_{k \to \infty} \left( -K \langle \psi_0 | p \cdot p | \psi_0 \rangle + D \ln(K) + \int_0^k dk \langle \psi_0 | p \cdot (H - E_0 + k)^{-1} p | \psi_0 \rangle \right), \quad (1)$$

and thereby replaced the insuperable difficulties associated with accurately summing over an infinite number of bound and continuum eigenstates of $H$ with the more tractable difficulty of numerically integrating an accurate representation of the matrix element of the resolvent $(H - E_0 + k)^{-1}$ for small, intermediate and large values of $k$. When $k$ is very large, Schwartz found it sufficient to approximate the matrix element with a simple asymptotic formula. For smaller values of $k$, the action of the resolvent is solved explicitly as the solution of a system of linear equations in a suitable basis with $p$-wave symmetry. For intermediate $k$ the convergence was greatly improved by including a single function which has the same leading-order asymptotic behavior as the true solution as $k \to \infty$.

Despite growing problems with the numerical linear dependence of his basis as the number of basis functions was increased, Schwartz was able to compute for the $1S$ ground state of the neutral helium atom a Bethe logarithm of 4.370(4) Rydbergs, which yielded a theoretical ionization potential for this state in agreement with the best experimental values available at that time, and which remained unsurpassed until very recently.

The results presented in this letter were generated by an approach very similar to that used by Schwartz, in which the integral in Eq. (1) is split into a low $k$ region $\beta_L$ and a high $k$ region $\beta_H$. The counterterms in Eq. (1) are then brought inside the integral to cancel explicitly the divergent behavior at large $k$:

$$\beta = \beta_H + \beta_L = \int_1^\infty \frac{dk}{k} \langle \psi_0 | p \cdot (H - E_0) | \psi_H(k) \rangle$$

$$+ \int_0^1 dk \left( \langle \psi_0 | p | \psi_L(k) \rangle - \frac{\langle \psi_0 | p \cdot p | \psi_0 \rangle}{k} \right), \quad (2)$$

where $\psi_L(k)$ and $\psi_H(k)$ are solutions of the equations

$$(H - E_0 + k) \psi_L(k) = p \psi_0,$$  

$$(H - E_0 + k) \psi_H(k) = (H - E_0)p \psi_0. \quad (3)$$

Since $H$ possesses overall rotational symmetry, the solutions $\psi_L(k)$ and $\psi_H(k)$ have a total angular momentum quantum number which can differ by only $\pm 1$ from that of $\psi_0$. In this work $\psi_0$ has $S$-symmetry, so $\psi_L(k)$ and $\psi_H(k)$ have $P$-symmetry.

An elegant derivation of Eq. (3) can be found in the work of Forrey and Hill [12], which examines Schwartz’s method from a fresh perspective and provides many useful computational techniques. We evaluate the two integrals in Eq. (1) numerically, using the procedure described by Forrey and Hill, computing the matrix element of the resolvent at
each integration knot by solving variationally for \( \psi_L \) or \( \psi_H \) in Eq. (3) and Eq. (4). When \( k \) is very large, we use the asymptotic approximation:

\[
\langle \Psi_0 | p (H - E_0) | \psi_H(k) \rangle = \frac{2 Z D}{k} \left[ \sqrt{2k} - Z \ln(k) + C + \frac{D}{\sqrt{k}} + \cdots \right].
\]

(5)

The constants \( C \) and \( D \) have been computed in closed form only for the hydrogen atom; in this work they are estimated by extrapolating the values generated by the solution of Eq. (4) at successive integration knots. This equation was solved explicitly at each successive knot, running in the direction of increasing \( k \), until the relative difference between successive extrapolated estimates of \( C \) was roughly 1%. For larger \( k \) the resulting asymptotic formula was used. For the helium ground state our estimates of \( C \) and \( D \) are 4.988(1) and -18.8(3) respectively, with the errors resulting mainly from extrapolation uncertainty. These estimates can be compared with the value 5.18 computed by Schwartz [14] for \( C \) and the value -20±3 he assumed for \( D \).

The non-relativistic wavefunction \( \Psi_0 \) was computed variationally using our modification [10], [12] of the basis set first developed by Frankowski and Pekeris [4], which exploits knowledge of the analytic structure of the true wavefunction at the 2- and 3-particle coalescences to improve the convergence of the variational trial function to the exact unknown wavefunction:

\[
\Psi_0 = \sum_{\nu} c_{\nu}(\phi_{\nu}(s, t, u) \pm \phi_{\nu}(s, -t, u))
\]

\[
\phi_{\nu}(s, t, u) = s^n t^l u^m (\ln s)^\frac{\nu}{2} e^{-ax+ct}
\]

where \( s, t, \) and \( u \) are the Hylleraas coordinates defined by \( s = r_1 + r_2, t = r_2 - r_1 \) and \( u = r_{12} \) and the \( \pm \) sign is chosen so that the product of \( \Psi_0 \) and the spin function is antisymmetric under exchange of the electrons.

Our bases for representing \( \psi_L(k) \) and \( \psi_H(k) \) include functions of four different types. The \( k \)-independent functions

\[
\chi_{\nu}^{(1)} = r_1 \phi_{\nu}(s, t, u) \pm r_2 \phi_{\nu}(s, -t, u)
\]

together with the single function \( \chi^{(2)} = p \Psi_0 \) provide a good solution space for small \( k \).

For large \( k \) the solution \( \psi_H(k) \) becomes concentrated in \( k \)-dependent regions of configuration space for which one electron is very close to the nucleus and the other electron is much further away, so it is essential to use explicitly \( k \)-dependent basis functions. Of primary importance is the ‘Schwartz function’ \( \chi^{(3)} \), an approximate solution of Eq. (3) that reproduces the first two terms in the asymptotic expansion in Eq. (2):

\[
\chi^{(3)} = \left( p_1 \exp \left( -\frac{\sqrt{2k} r_1}{r_1} - \frac{1}{r_1} \right) \right) \Psi_0 \pm (r_1 \leftrightarrow r_2).
\]

to help approximate that part of \( \psi_H(k) \) which is orthogonal to the ‘Schwartz function’, we also use a fourth set of functions \( \chi^{(4)}_{\nu} \), which are symmetrized sums of products of single-variable Laguerre functions \( L_i(R_j) = L_i(R_j) e^{-R_j/2} \) of the three perimetric coordinates \( R_1 = r_1 + r_2 - r_{12}, R_2 = r_1 - r_2 + r_{12}, \) and \( R_3 = -r_1 + r_2 + r_{12} \):

\[
\chi^{(4)}_{\nu} = (r_1 L_p(a R_1) L_q(b R_2) L_r(c R_3)) \pm (r_1 \leftrightarrow r_2).
\]

Combinations of the exponential parameters \( a, b, \) and \( c \) can be chosen to reflect the strong ‘in-out’ correlation in \( \psi_H(k) \) for large \( k \). For any \( k \) the overlap matrix elements for these basis functions are very small or zero far from the main diagonal, which enables us to avoid the severe problems with numerical linear dependence which prevented Schwartz from using a large basis of functions of the form of powers of \( r_1, r_2, r_{12} \) times a highly asymmetrical exponential of \( r_1 \) and \( r_2 \). We set \( a = b + c \) to eliminate from \( \chi^{(4)}_{\nu} \) any exponential \( r_{12} \)-dependence, which would complicate the evaluation of matrix elements between these functions and the other types of basis functions. Analytic considerations [12] suggest that the integrand is optimised if \( b \approx (2k)^{1/4} \) and \( c \approx Z \). We coarsely search the parameter space in the neighborhood of these values of \( b \) and \( c \) seeking to maximize the two integrands of Eq. (3) in accordance with the variational principle described in [12].

The calculation of \( \beta_L \) was fast and straightforward. In this case \( k \) was small enough that there was no need to include explicit \( k \)-dependence in the basis. \( \chi^{(3)} \) was omitted altogether, and a single average value of the parameter \( b \) was used in the \( \chi^{(4)}_{\nu} \) functions, independent of the value of \( k \) at a particular integration knot. We solved for \( \psi_L(k) \)
in a basis with 92 \( \chi_{\nu}^{(1)} \) functions, the \( \chi^{(2)} \) function, and 120 \( \chi_{\nu}^{(4)} \) functions. The parameters \( b \) and \( c \) were varied to maximize the integrand. Changes in the integrand due to small variations in \( b \) and \( c \) were used to assess convergence.

The \( \beta_H \) integral was computationally expensive, primarily because including the ‘Schwartz function’ \( \chi_{\nu}^{(3)} \) requires evaluating algorithmically complicated matrix elements. Since \( \chi_{\nu}^{(3)} \) is intended primarily to accelerate the convergence for very large \( k \), and since over half of the knots in our integration scheme correspond to \( k < 40 \), we chose to omit \( \chi_{\nu}^{(3)} \) from the basis for knots below \( k \approx 40 \). At each node we solved for \( \psi_{\Omega} \) in a basis consisting of 92 \( \chi_{\nu}^{(1)} \) functions, the \( \chi^{(2)} \) function, the \( \chi_{\nu}^{(3)} \) function (for high \( k \)), and 220 \( \chi_{\nu}^{(4)} \) functions. We then recomputed the solution of Eq. (4) after first reducing the number \( N \) of \( \chi_{\nu}^{(4)} \) functions in the existing matrices to study convergence of the integrand. A simple polynomial fit in the variable \( 1/N \) was applied to the sequence of results with \( N = 220, 165, 120, \) and 84 to generate the values of the Bethe logarithms in this letter. The error associated with the finiteness of the basis for \( \psi_{\Omega} \) was taken as the entire difference between the extrapolated value and the value corresponding to \( N = 220 \).

Other sources of numerical error arise from the numerical integration itself (for which there are good analytic error bounds (3), and the finiteness of the basis used to approximate \( \Psi_0 \). The latter error is assumed to be comparable to the relative error in \( D \) in all cases. For neutral helium, independent runs with less accurate representations of \( \Psi_0 \) indicate that this estimate of this error is somewhat conservative. The numerical integration was parametrized to keep the absolute error in \( \beta_H \) and \( \beta_{\Omega} \) below \( 10^{-8} \). The results of independent calculations carried out for neutral helium with a coarser mesh were consistent with the analytic error bound.

The uncertainties assigned to the Bethe logarithms in this letter are the sums of the uncertainty due to extrapolation of \( \psi_{\Omega} \) and the uncertainty due to approximation of \( \Psi_0 \) in a finite basis. The uncertainty in \( \psi_{\Omega} \) and the numerical integration error bounds are negligible by comparison.

Our Bethe logarithms for the 1\( ^1 \)S, 2\( ^2 \)S, and 2\( ^2 \)\( ^2 \)S states are listed in Tables I, II, and III, respectively. The values of \( k_0 \) have been divided by \( Z^2 \) to illustrate their approach to the hydrogenic limit as \( Z \) becomes large. Scaled values of the nonrelativistic binding energy \( E_{\text{NR}}/Z^2 \) and \( D/Z^2 \) are also listed to provide some measure of the accuracy of \( \Psi_0 \). Uncertainties in \( D \) were computed by comparison with highly accurate results for \( <\delta(r_1) \rangle \) provided by Drake (4).

The exact hydrogenic limits of \( \ln(k_0/\text{Ry}) \) (13), (17) and of \( E_{\text{NR}} \) and \( D \) are displayed in the bottom row of each table, labeled by \( 1/\infty \) (exact). Immediately above the bottom row, in the row labeled \( 1/\infty \), we list the hydrogenic values and the corresponding uncertainties computed using the method described in this letter with \( 1/Z = 0 \) so that the \( 1/r_{12} \) term is removed from the Hamiltonian.

For \( Z = 1 \) the Hamiltonian \( H \) has a single bound state of 1\( ^1 \)S symmetry. As \( Z \to 1 \) from above all the singly excited bound states of a two-electron ion disappear into the continuum as the ‘outer’ electron moves infinitely far away. Hence as \( Z \to 1 \) from above, the energies and all other finite-range properties of the states should tend toward those for a single hydrogen atom in its ground state with \( Z = 1 \). The approach of the Bethe logarithms and other properties toward their hydrogenic values as \( Z \to 1 \) from above is visible in Tables II and III for the 2\( ^2 \)S and 2\( ^2 \)\( ^2 \)S states, respectively.

We have fit our ionic results to the \( 1/Z \) expansion developed by Goldman and Drake (18)

\[
\ln(k_0/\text{Ry}) = C_0 + C_1/Z + C_2/Z^2 + \cdots
\]

where \( \ln(k_H/\text{Ry}) \) is the weighted sum of the two hydrogenic Bethe logarithms corresponding to the state. Table IV displays the results of a three parameter polynomial fit for \( C_1, C_2, \) and \( C_3 \) using data for \( Z = 4, 8, \) and 16. The listed uncertainties come from the formal propagation of error through the regression formula and do not include truncation errors from higher-order terms in the expansion.

Our results for the 1\( ^1 \)S state and the 2\( ^2 \)S states of neutral helium are in complete agreement with the recent calculations of Korobov and Korobov (19). The most accurate previous value of the Bethe logarithm of the 2\( ^2 \)S state came from Goldman and Drake’s 1st-order \( 1/Z \) expansion (17), (18). A numerical comparison of results for neutral helium appears in Table V.

Preliminary values of our Bethe logarithms for the 1\( ^1 \)S, 2\( ^2 \)S (20) and 2\( ^2 \)\( ^2 \)S states of helium were used in a recent comparison of theory and experiment by Drake and Martin (21). The values in this letter make slight corrections to the theoretical ionization energies of the 2\( ^2 \)S and the 2\( ^2 \)\( ^2 \)S levels in that work, while the 1\( ^1 \)S state is unaffected. Modifying “Bethe log cor.” contribution in Drake and Martin’s Table II to include the values in this letter yields the theoretical results in Table VI, which are compared with results from several recent experiments (22), (23), (24), (25).

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[1] E.A. Hylleraas, Z. Phys. 54, 347 (1929).
[2] T. Kinoshita, Phys. Rev. 105, 1490 (1957); *ibid.* 115, 366 (1959).
[3] C.L. Pekeris, Phys. Rev. 112, 1649 (1958); *ibid.* 115, 1216 (1959); *ibid.* 127, 509 (1962).
[4] K. Frankowski and C.L. Pekeris, Phys. Rev. 146, 46 (1966); K. Frankowski, Phys. Rev. 160, 1 (1967).
[5] Y. Accad, C.L. Pekeris, B. Schiff Phys. Rev. A 4, 516 (1971).
[6] E. Giacobino and F. Biraben, J. Phys. B: At. Mol. Phys. 15, L385 (1982); L. Hlousek, S. A. Lee, and W. M. Fairbank, Jr., Phys. Rev. Lett. 50, 328 (1983); P. Juncar, H. G. Berry, R. Damschini, and H. T. Duong, J. Phys. B: At. Mol. Phys. 16, 381 (1983); C. J. Sansonetti and W. C. Martin, Phys. Rev. A 29, 159 (1984); C. J. Sansonetti, J. D. Gillaspy, and C. L. Cromer, Phys. Rev. Lett. 65, 2539 (1990).
[7] P.K. Kabir and E.E. Salpeter, Phys. Rev. 108, 1256 (1957).
[8] H.A. Bethe, Phys. Rev. 72, 399 (1947).
[9] S.P. Goldman, Phys. Rev. A 30, 1219 (1984).
[10] J.D. Baker, R.N. Hill, and J.D. Morgan III, “High Precision Calculation of Helium Atom Energy Levels”, in *AIP Conference Proceedings* 189, *Relativistic, Quantum Electrodynaminc, and Weak Interaction Effects in Atoms* (AIP, New York, 1989), 123.
[11] G.W.F. Drake and R.A. Swainson, Phys. Rev. A 41, 1243 (1990).
[12] R. C. Forrey and R. N. Hill, Ann. Phys. 226, 88 (1993).
[13] R. Bukowski, B. Jeziorski, R. Moszyński, and W. Kolos, Int. J. Quantum Chem. 42, 287 (1992).
[14] C. Schwartz, Phys. Rev. 123, 1700 (1961).
[15] D.E. Freund, B.D. Huxtalbe and J.D. Morgan III, Phys. Rev. A 29, 980 (1984); J.D. Baker, D.E. Freund, R.N. Hill, and J.D. Morgan III, Phys. Rev. A 41, 1247-1273 (1990).
[16] G.W.F. Drake, private communication.
[17] G.W.F. Drake, “High Precision Calculations for Rydberg States of Helium”, in *Long Range Casimir Forces: Theory and Recent Experiment on Atomic Systems* (Plenum Press, New York, 1993), 163.
[18] S. P. Goldman and G.W.F. Drake, J. Phys. B 16, L183 (1983); 17, L197 (1984).
[19] V.I. Korobov and S.V. Korobov, Phys. Rev. A 59, 3394 (1999).
[20] J.D. Baker, R.C. Forrey, J.D. Morgan III, R.N. Hill, M. Jeziorska, J. Shertzer, Bull. Am. Phys. Soc., 38, 1127 (1993).
[21] G.W.F. Drake and W.C. Martin, Can. J. Phys. 76, 597 (1998).
[22] K.S.E. Eikema, W. Ubachs, W. Vassen, and W. Hogervorst, Phys. Rev. Lett. 76, 1216 (1996); K.S.E. Eikema, W. Ubachs, W. Vassen, and W. Hogervorst, Phys. Rev. A 55, 1866 (1997).

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1Certain commercial equipment, instruments, or materials are identified in this paper to foster understanding. Such identification does not imply recommendation or endorsement by the National Institute of Standards and Technology, nor does it imply that the materials or equipment identified are necessarily the best available for the purpose.
[23] S.D. Bergeson, A. Balakrishnan, K.G.H. Baldwin, T.B. Lucatorto, J.P. Marangos, T.J. McIlrath, T.R. O’Brian, S.L. Rolston, C.J. Sansonetti, J. Wen, and N. Westbrook, Phys. Rev. Lett. 80, 3475 (1998).
[24] W. Lichten, D. Shiner, and Z.-X. Zhou, Phys. Rev. A 43, 1663 (1991); *ibid.* 45, 8295 (1992).
[25] C.J. Sansonetti and J.D. Gillaspy, Phys. Rev. A 45, R1 (1992), and unpublished data (1996).
[26] C. Dorrer, F. Nez, B. de Beauvoir, L. Julien and F. Biraben, Phys. Rev. Lett. 78, 3658 (1997).
[27] G.W.F. Drake, Can. J. Phys. 66, 586 (1988).
TABLE I. $\ln\left(\frac{k_0}{Z^2\text{Ry}}\right)$, $E_{nr}/Z^2$ and $D/Z^4$ for the $1^1S$ state.

| $1/Z$ | $\ln\left(\frac{k_0}{Z^2\text{Ry}}\right)$ | $E_{nr}/Z^2$ (a.u.) | $D/Z^4$ (a.u.) |
|-------|---------------------------------|------------------|---------------|
| 1/1   | 2.99297(5)                      | -0.527 751 015 308 | 2.067 80(4)    |
| 1/2   | 2.983 864(2)                    | -0.725 931 094 259 | 2.843 815 67(5) |
| 1/3   | 2.982 624(2)                    | -0.808 879 268 074 | 3.189 069 9(1)  |
| 1/4   | 2.982 503(1)                    | -0.853 472 889 901 | 3.376 853 2(1)  |
| 1/8   | 2.982 948(2)                    | -0.924 321 798 793 | 3.677 270 3(1)  |
| 1/16  | 2.983 448(1)                    | -0.961 551 275 290 | 3.835 853 3(2)  |
| 1/$\infty$ | 2.984 128 6(7)               | -1.0              | 4.0            |
| 1/$\infty$ (exact) | 2.984 128 556               | -1.0              | 4.0            |

TABLE II. $\ln\left(\frac{k_0}{Z^2\text{Ry}}\right)$, $E_{nr}/Z^2$ and $D/Z^4$ for the $2^1S$ state.

| $1/Z$ | $\ln\left(\frac{k_0}{Z^2\text{Ry}}\right)$ | $E_{nr}/Z^2$ (a.u.) | $D/Z^4$ (a.u.) |
|-------|---------------------------------|------------------|---------------|
| 1/1 (exact limit) | 2.984 128 556               | -0.5              | 2.0            |
| 1/2   | 2.980 115(1)                    | -0.536 493 511 514 | 2.056 896 21(2) |
| 1/3   | 2.976 362(2)                    | -0.560 416 177    | 2.103 636 0(3)  |
| 1/4   | 2.973 976(1)                    | -0.574 618 459    | 2.132 593 0(7)  |
| 1/8   | 2.969 797(4)                    | -0.597 028 931    | 2.185 583 1(1)  |
| 1/16  | 2.967 459(3)                    | -0.610 515 708    | 2.216 320 3(6)  |
| 1/$\infty$ | 2.964 977 7(4)               | -0.625             | 2.25           |
| 1/$\infty$ (exact) | 2.964 977 593              | -0.625             | 2.25           |

TABLE III. $\ln\left(\frac{k_0}{Z^2\text{Ry}}\right)$, $E_{nr}/Z^2$ and $D/Z^4$ for the $2^3S$ state.

| $1/Z$ | $\ln\left(\frac{k_0}{Z^2\text{Ry}}\right)$ | $E_{nr}/Z^2$ (a.u.) | $D/Z^4$ (a.u.) |
|-------|---------------------------------|------------------|---------------|
| 1/1 (exact limit) | 2.984 128 556               | -0.5              | 2.0            |
| 1/2   | 2.977 742(1)                    | -0.543 807 344 559 | 2.074 008 93(2) |
| 1/3   | 2.973 852(1)                    | -0.567 858 969 952 | 2.124 087 18(4) |
| 1/4   | 2.971 735(1)                    | -0.581 072 911 861 | 2.152 566 56(2) |
| 1/8   | 2.968 414(2)                    | -0.602 260 114 376 | 2.199 147 9(4)  |
| 1/16  | 2.966 705(1)                    | -0.613 440 895 056 | 2.224 062 6(2)  |
| 1/$\infty$ | 2.964 977 6(2)               | -0.625             | 2.25           |
| 1/$\infty$ (exact) | 2.964 977 593              | -0.625             | 2.25           |

TABLE IV. Coefficients of the 1/Z expansion using a 3 parameter fit. The exact values of $C_1$ are due to Drake [17].

| 1/Z coeff | $1^1S$ | $2^1S$ | $2^3S$ |
|-----------|--------|--------|--------|
| $C_1$ (exact) | -0.0123 03(1) | 0.040 771(1) | 0.027 760(1) |
| $C_1$ | -0.0123 2(5) | 0.040 78(10) | 0.027 73(5) |
| $C_2$ | 0.0228(8) | -0.016(2) | -0.001 0(6) |
| $C_3$ | 0.002(2) | -0.011(6) | -0.007 2(2) |

TABLE V. Comparison of $\ln\left(\frac{k_0}{\text{Ry}}\right)$ for neutral helium. The uncertainty in the 1st-order 1/Z expansion due to uncalculated higher-order terms could not be readily estimated until more exact calculations were done.

| State | 1st-order 1/Z expansion | Schwartz | Korobov | This work |
|-------|-------------------------|----------|---------|-----------|
| $1^1S$ | 4.364(?)                | 4.370(4) | 4.370 157 9(5) | 4.370 159(2) |
| $2^1S$ | 4.372(?)                | -       | 4.366 409 1(5) | 4.366 409(1) |
| $2^3S$ | 4.365(?)                | -       | -       | 4.364 036(1) |
TABLE VI. Ionization potentials, in MHz, as described in [21], but with theoretical values corrected slightly by the results in this letter. a: from [22], b: from [23], c: an average of values from [24] and [25], d: from [26].

| State | This work | Experiment | Difference |
|-------|-----------|------------|------------|
| 1S    | 5 945 204 226(91) | 5 945 204 238(45)\(^a\) | 12(102) |
|       |           | 5 945 204 356(48)\(^b\) | 130(103) |
| 2S    | 960 332 040.9(25.0) | 960 332 041.01(15)\(^c\) | 0.1(25.0) |
| 2P    | 1 152 842 738.2(25.2) | 1 152 842 742.87(6)\(^d\) | 4.7(25.2) |