Bethe logarithm for the $1\,^1S$ and $2\,^1S$ states of helium

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We present variational calculations of the Bethe logarithm for the $1\,^1S$ and $2\,^1S$ states of helium. The approach is based on the explicit second-order perturbation formula and closely follows the method of Schwartz. The final values are $\ln[K_0(1\,^1S)/(1\ \mathrm{Ry})]=4.370\,157\,9(5)$ and $\ln[K_0(2\,^1S)/(1\ \mathrm{Ry})]=4.366\,409\,1(7)$. The latter result reduces the difference between theoretical and experimental values for the ionization potential of the $2\,^1S$ state to 0.15 MHz. [S1050-2947(99)03305-3]

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It is known that the most difficult part in the numerical calculation of the $O(\alpha^3)$ contribution to the Lamb shift in helium is the Bethe logarithm:

$$\ln\frac{k_0}{(1\ \mathrm{Ry})}=\frac{\sum_n |\langle 0|\mathbf{p}|n\rangle|^2(E_n-E_0)\ln\{|E_n-E_0|/(1\ \mathrm{Ry})\}}{\sum_n |\langle 0|\mathbf{p}|n\rangle|^2(E_n-E_0)}. \tag{1}$$

It is extremely surprising that the early calculation of Schwartz [1] was the most accurate for over 30 years. The present work has appeared as a byproduct of our study of antiprotonic helium atoms [2]. So, not all the stages of the present work are the most optimal for the calculation. However, the final result is the most accurate to date, and that encourages us to present our calculations to the audience.

According to [3], the two-electron self-energy can be expressed in a form

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

where $\psi_0^2(0)=\langle\delta(\mathbf{r}_1)+\delta(\mathbf{r}_2)\rangle$ is the expectation value (in atomic units) of the operator $[\delta(\mathbf{r}_1)+\delta(\mathbf{r}_2)]$.

To calculate the Bethe logarithm we use an approach similar to the method of Schwartz [1]. So, we start from the direct perturbation formula (derived from the Bethe-Salpeter textbook (19.7) [4])

$$\begin{aligned}\Delta E_{LS}&=-\frac{2}{3\pi}\frac{\alpha^3}{m^2}\int_0^K dk\ \sum_n\frac{\langle 0|\boldsymbol{\nabla}|n\rangle(E_0-E_n)\langle n|\boldsymbol{\nabla}|0\rangle}{k(E_0-E_n-k)}\\&=-\frac{2}{3\pi}\frac{\alpha^3}{m^2}\int_0^K dk\ \langle 0|\boldsymbol{\nabla}(E_0-H)\\&\quad\times(E_0-H-k)^{-1}\boldsymbol{\nabla}|0\rangle\\&=-\frac{2}{3\pi}\frac{\alpha^3}{m^2}\int_0^K dk\ \langle 0|[H,\boldsymbol{\nabla}](E_0-H-k)^{-1}\boldsymbol{\nabla}|0\rangle.\end{aligned}$$

Here $\boldsymbol{\nabla}=\boldsymbol{\nabla}_1+\boldsymbol{\nabla}_2$ is the sum of gradient operators of two electrons and $[a,b]\equiv ab-ba$.

Let us denote the integrand by

$$I(k)=-\langle 0|[H,\boldsymbol{\nabla}](E_0-H-k)^{-1}\boldsymbol{\nabla}|0\rangle,$$

then noting that the solution of an equation $(E_0-H-k)\psi_1=\boldsymbol{\nabla}\psi_0$ can be presented in a form (asymptotic for $k\to\infty$)

$$\psi_1=-(1/k)\boldsymbol{\nabla}\psi_0+U,$$

one gets after substituting ψ_1 into $I(k)$ that

$$I(k)=\frac{2\pi Z}{k}\psi_0^2(0)-\frac{1}{k}\tilde{w}(k),$$

where

$$\tilde{w}(k)=\langle 0|[H,\boldsymbol{\nabla}](E_0-H-k)^{-1}[H,\boldsymbol{\nabla}]|0\rangle.$$

The asymptotic behavior of $\tilde{w}(k)$ for $k\to\infty$ is (see [1])

$$\tilde{w}(k)\sim\frac{4\pi Z_1^2}{k}\left[(2k)^{1/2}-Z_1\ln k+\sum_{m=0}^{\infty}C_m k^{-m/2}\right]\psi_0^2(0). \tag{3}$$

Following Schwartz, we want to introduce as well a function

$$J(k)=\langle 0|\boldsymbol{\nabla}(E_0-H-k)^{-1}\boldsymbol{\nabla}|0\rangle,$$

which relates to $I(k)$ and $\tilde{w}(k)$ as

$$\begin{aligned}J(k)&=-\frac{1}{k}\langle\boldsymbol{\nabla}^2\rangle-\frac{1}{k}I(k)\\&=-\frac{1}{k}\langle\boldsymbol{\nabla}^2\rangle-\frac{2\pi Z}{k^2}\psi_0^2(0)+\frac{1}{k^2}\tilde{w}(k).\end{aligned} \tag{4}$$

The first term in the final expression corresponds to the mass renormalization, the second brings the logarithmic term $\alpha^3\ln\alpha$ in Eq. (2), and $\tilde{w}(k)$ contributes to the Bethe logarithm: $\ln[K_0(n,l)/(1\ \mathrm{Ry})]$.

TABLE I. The binding energies and expectation values of the $\langle \nabla^2 \rangle$ and $4\pi[\delta(\mathbf{r}_1)+\delta(\mathbf{r}_2)]$ operators for the $1\,^1S$ and $2\,^1S$ states of helium.

	$1\,^1S$	$2\,^1S$
No. of terms in ψ_0	600	600
Binding energy	2.903 724 377 034	2.145 974 046 052
$\langle \nabla^2 \rangle$	−6.125 587 704 24	−4.310 955 820 922
$4\pi\psi_0^2(0)$	45.501 047 1	32.910 336 8

Variational wave functions describing the $1\,^1S$ and $2\,^1S$ states of a two-electron system are given in a form

$$\psi_0=\sum_{i=1}^{\infty}\{U_i\,\mathrm{Re}[\exp(-\alpha_i r_1-\beta_i r_2-\gamma_i r_{12})] + W_i\,\mathrm{Im}[\exp(-\alpha_i r_1-\beta_i r_2-\gamma_i r_{12})]\}+(\mathbf{r}_1\leftrightarrow\mathbf{r}_2).$$

Here α_i, β_i, and γ_i are complex parameters generated in a quasirandom manner [5,6]:

$$\alpha_i=\left\lfloor\frac{1}{2}i(i+1)\sqrt{p_\alpha}\right\rfloor[(A_2-A_1)+A_1] + i\left\{\left\lfloor\frac{1}{2}i(i+1)\sqrt{q_\alpha}\right\rfloor[(A_2'-A_1')+A_1']\right\},$$

where $\lfloor x\rfloor$ designates the fractional part of x, p_α and q_α are some prime numbers, and $[A_1,A_2]$ and $[A_1',A_2']$ are real variational intervals. Parameters β_i and γ_i are obtained in a similar way. The numerical values of energies and other constants necessary for the Bethe logarithm calculation are shown in Table I.

The perturbed functions ψ_1 are expanded in the same way [7]:

$$\psi_1=\sum_{i=1}^{\infty}\mathbf{r}_1\{\hat{U}_i\,\mathrm{Re}[\exp(-\alpha_i r_1-\beta_i r_2-\gamma_i r_{12})] + \hat{W}_i\,\mathrm{Im}[\exp(-\alpha_i r_1-\beta_i r_2-\gamma_i r_{12})]\}+(\mathbf{r}_1\leftrightarrow\mathbf{r}_2).$$

As k goes to infinity, the upper limit of the interval for the parameter β increases proportionally to $k^{1/2}$. There is no need to set the upper limit exactly to this value since the convergence is satisfactory, as can be seen from Tables II and III.

The following numerical scheme was adopted in [1]. The whole integration over k was split onto three intervals. The first interval was for low energies from $k=0$ to $k=50$ and

TABLE II. Convergence of $J(k)$ with the number of basis functions and comparison with the calculations of Schwartz.

No. of terms in ψ_1	$J(0)$	$J(15)$	$J(50)$
300	3.000 000 000	0.325 713 805 6	0.112 051 494 7
500	3.000 000 000	0.325 713 805 8	0.112 051 494 8
[1]	3.000 51	0.325 73	0.112 04

TABLE III. Convergence of $\tilde{w}(k)$ with the number of basis functions and comparison with the calculations of Schwartz.

No. of terms in ψ_1	$\tilde{w}(50)/4$	$\tilde{w}(300)/4$	$\tilde{w}(3000)/4$
500	4.8375997	2.6048513	1.002786
700	4.8375997	2.6048520	1.002800
900			1.002802
[1]	4.8370	2.6045	0.94

results of a calculation for $J(k)$ were integrated numerically. Then, at intermediate energies from $k=50$ to $k=1000$, the calculated values for $\tilde{w}(k)$ were used. And finally, an integration over the high-energy region was carried out with the help of the asymptotic expansion (3).

However, the calculation of $\tilde{w}(k)$ requires solving of the equation

$$(E_0-H-k)U=-\frac{1}{k}[H,\nabla]\psi_0,$$

which defines the function U singular at $r_i\to 0$. That is slowing down the convergence of the computed value for $\tilde{w}(k)$ with respect to the number of terms in the variational expansion of U. On the contrary, even for high k the calculated value for $J(k)$ is stable and very accurate, and, in spite of strong cancellations during evaluation of $\tilde{w}(k)$ via Eq. (4), the value of $\tilde{w}(3\,000)$ obtained through $J(k)$ is several digits more accurate than that obtained through direct calculation of $\tilde{w}(k)$ (see Table III). For the asymptotic region, the fitting of five to seven unknown parameters C_n in expansion (3) is applied to get more accurate integration over the infinite interval of $k\to\infty$.

In Table IV different calculations of the Bethe logarithm for the ground state are listed. As can be seen from the table, the present result improves substantially the theoretical value of $\ln[K_0(1\,^1S)/(1\ \mathrm{Ry})]$.

The computed value for the $2\,^1S$ state is

$$\ln[K_0(2\,^1S)/(1\ \mathrm{Ry})]=4.366\,409\,1(7).$$

It can be used to get an improved theoretical value for the ionization energy of the $2\,^1S$ state of helium. In the previous calculation [11] of this state the Bethe logarithm value of 4.366 329(8) a.u. [10] has been used. Comparing these two values we see that a correction to the ionization energy due

TABLE IV. Comparison of theoretical calculations of $\ln[K_0(1\,^1S)/(1\ \mathrm{Ry})]$ for the ground state of helium.

Schwartz [1] (1961)	4.370(4)
Goldman and Drake[a] [8] (1983)	4.364
Baker *et al.* [10] (1993)	4.37012
Bhatia and Drachman [9] (1998)	4.367
Present work	4.370 157 9(5)

[a]Approximate analytical expression: $\ln K_0/(1\ \mathrm{Ry}) = \ln[19.769\,267(Z-0.006\,15)^2]$, based on an expansion over Z^{-1}.

to the Bethe logarithm improvement is -1.43 MHz. Adding this correction to the theoretical value of [11] we finally get

$$-960\,332\,040.86(2)\pm(mc^2\alpha^6 \text{ and higher-order terms that are not calculated}) \text{ MHz}, \quad (5)$$

which is to be compared with the experimental value [12]

$$-960\,332\,041.01(5)\ \text{MHz}.$$

This shift reduces the difference between theory and experiment to the bounds of experimental uncertainty: 0.15 ± 0.15 MHz. However, it is worthwhile to mention here that an estimate of contribution that comes from not yet calculated terms in Eq. (5) varies from 1 MHz [11] to 25 MHz [12] (see the paper of Drake and Martin [12]). But discussion of higher-order terms is beyond the scope of our work. The main goal was to reduce the error bars in $O(mc^2\alpha^5)$ terms at least to the level of the experimental uncertainties and it was achieved. The numerical error in the value of the Bethe logarithm for the $2\,^1S$ state corresponds to the level of 0.02 MHz.

TABLE V. Comparison with recent calculations by Baker *et al.* [13].

	$1\,^1S$ state	$2\,^1S$ state
Our work	4.3701579(5)	4.3664091(7)
Baker *et al.* [13]	4.370159(2)	4.366409(1)

Recently, we become aware of new calculations by Baker *et al.* [13] that are in excellent agreement with our results (see Table V).

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