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Another way to calculate the Lamb shift in two-electron systems

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We present a calculation of the two-electron Bethe logarithm, the main part of the theoretical expression for the Lamb shift of the atomic ground state. The basic method uses Hylleraas pseudostates to approximate the intermediate states in the slowly convergent sum defining the quantity of interest. Three tricks improve the convergence in our method. First, we choose the nonlinear parameters of the pseudostates by a variational method. Second, we extend the energy sum analytically, beyond the last pseudoenergy. Finally, we extrapolate the result using a physically reasonable parameter as the independent variable. The extrapolation proves to be remarkably linear. Results are given for helium and several two-electron ions and compared with previous calculations. The hydrogen system is also considered. [S1050-2947(98)10206-8]

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I. INTRODUCTION

One of the most difficult parts of the two-electron Lamb shift calculation is the Bethe logarithm:

$$\ln(K)=\frac{\sum_n \langle 0|V|n\rangle\langle n|V|0\rangle(E_n-E_0)^3\,\ln(E_n-E_0)}{\sum_n \langle 0|V|n\rangle\langle n|V|0\rangle(E_n-E_0)^3}\equiv\frac{N}{D},\qquad(1)$$

where $V=r_1\cos\theta_1+r_2\cos\theta_2$. The main difficulty is the slow convergence of the sums, especially the numerator, with intermediate-state basis size. In fact, the sum in the denominator would diverge if the energy difference were raised to the fourth power, rather than the third. Thus, the numerator is just on the edge of divergence due to the logarithmic factor. Several different techniques have been invented in an attempt to circumvent these problems [1–3]. For helium, the published results range from a low of 4.3313 to a high of 4.3701, and they are all surprisingly close to the value obtained [3] without interelectronic correlation, 4.3704. Some of the cited papers give estimates of the uncertainties in the calculations; these vary from 1×10^{-6} in the unpublished work of Baker *et al.* to the conservative estimate of Kabir and Salpeter of 0.2.

This paper describes a method that is quite simple in concept, although it involves several tricks and requires a significant amount of computer time. We do not claim it is necessarily the most accurate; when the calculation of Baker *et al.* is published it may turn out to be definitive. We believe the method is interesting, independent, and of accuracy comparable to most of those in the literature. So far, we have applied the method only to the ground state, but we see no reason why it could not be used for excited states equally well.

In principle, the intermediate states $|n\rangle$ should be the complete set of $L=1$ eigenstates, both bound and continuum, of the Hamiltonian describing the two-electron system. Instead, we usually use the pseudostate summation method, replacing this difficult set of functions with a large, finite set of normalizable functions. For simpler cases, like calculations of polarizabilities [4] or van der Waals coefficients [5], the method works extremely well, largely because the convergence is aided by the appearance of negative powers of the energy differences. In the present case, however, the energy differences make the convergence very slow, and the usefulness of the pseudostate summation technique is questionable.

To overcome the problem, we will use some special tricks. In Sec. II we will examine the denominator of Eq. (1) and will use it to make an optimum choice of the form of the pseudostates to be employed. In Sec. III we will improve the convergence by using a standard method to approximate the form of the terms corresponding to excitation energies above the last pseudoenergy included. In Sec. IV a physically reasonable linear extrapolation method will be introduced and used to obtain quite an accurate value for ln(*K*), and our results for various two-electron ions will be compared with previous results. An Appendix will apply the method to the case of atomic hydrogen, which should be simpler but turns out to be puzzling.

The Hamiltonian (in reduced Rydberg units) for the two-electron system with a single nucleus of charge Z is the following:

$$H=-\nabla_1^2-\nabla_2^2-K\nabla_1\cdot\nabla_2-\frac{2Z}{\rho_1}-\frac{2Z}{\rho_2}+\frac{2}{\rho_{12}},\qquad(2)$$

where $K=2/(M+1)$, M is the mass of the nucleus in units of the electron mass, $\vec{\rho}_i=[M/(M+1)](\vec{r}_i-\vec{r}_M)$, and $\vec{\rho}_{12}=\vec{\rho}_1-\vec{\rho}_2$. The two-electron ground-state function $|0\rangle$ has the form

$$\Psi_0=e^{-a(\rho_1+\rho_2)}\sum_{l,m,n=0}^{\Omega_0}C_{l,m,n}\rho_1^l\rho_2^m\rho_{12}^n+[1\leftrightarrows2].\qquad(3)$$

(Our best ground-state energy was obtained with the Pekeris number $\Omega_0=16$, corresponding to a total of 525 terms.) The intermediate states $|n\rangle$ also have the Hylleraas form, but with $L=1$:

$$\Psi_n = -\cos(\theta_{12}/2)(f+\tilde{f})D_1^{1+} - \sin(\theta_{12}/2)(f-\tilde{f})D_1^{1-},$$

where

$$f(\rho_1,\rho_2,\rho_{12}) = e^{-\gamma(\rho_1+\rho_2)}\rho_1 \sum_{i,j,k=0}^{\Omega_p} C_{i,j,k}\rho_1^i \rho_2^j \rho_{12}^k, \tag{4}$$

and

$$\tilde{f}(\rho_1,\rho_2,\rho_{12}) = f(\rho_2,\rho_1,\rho_{12}).$$

The rotational harmonics D used here are those defined by Bhatia and Temkin [6]. For each expansion length (Ω_p) and nonlinear parameter (γ), a set of functions (Ψ_n) and corresponding energies (E_n) are obtained variationally, to be inserted in the summations shown in Eq. (1).

II. THE DENOMINATOR

It is simple to transform the denominator D of Eq. (1) to an equivalent form—one in which the intermediate sum has been removed—which should make its evaluation both easier and more accurate. We use the commutator relation

$$\langle n|[H,V]|0\rangle = \langle n|V|0\rangle(E_n - E_0) \tag{5}$$

three times, in order to remove the factor depending on E_n:

$$D = \frac{2}{3}(2+K)^2\{\langle 0|[H,(\nabla_1+\nabla_2)]\cdot(\nabla_1+\nabla_2)|0\rangle - \langle 0|(\nabla_1+\nabla_2)\cdot[H,(\nabla_1+\nabla_2)]|0\rangle\}. \tag{6}$$

Since the only parts of H that do not commute with $\nabla_1 + \nabla_2$ are the nuclear potential terms, this expression finally can be put in the form

$$D_{\rm ex} = \frac{16\pi Z(1+K)}{3}\langle 0|\delta(\vec{\rho}_1) + \delta(\vec{\rho}_2)|0\rangle, \tag{7}$$

where closure over the set of intermediate states has been invoked, Poisson's equation has been used to introduce the convenient δ functions, and we have dropped the small term of order K^2. The only uncertainty in the value of this expression for D comes from the variational approximation used to evaluate $|0\rangle$ [Eq. (3)], and this error can be made negligibly small by using a high enough value of Ω_0. In effect, in the derivation of Eq. (7) we have inserted a complete set of exact intermediate states and assumed that the initial state is also an exact eigenstate of H.

But since it is not possible to reduce N to a similar simple form (because of the logarithm) it is important to know how well the pseudostate sum has converged. We expect that the convergence of the pseudostate expansion of D will be similar to that of N, and since we know the ‘‘exact’’ value of D we have a measure of the error in N (for each value of Ω_p) as well. But we still need some criterion for choosing the nonlinear parameter γ appearing in the trial functions of Eq. (4).

If, instead of using the commutator relation [Eq. (5)] three times we employ it four times, twice in each matrix element of Eq. (1), the following (acceleration) form is obtained:

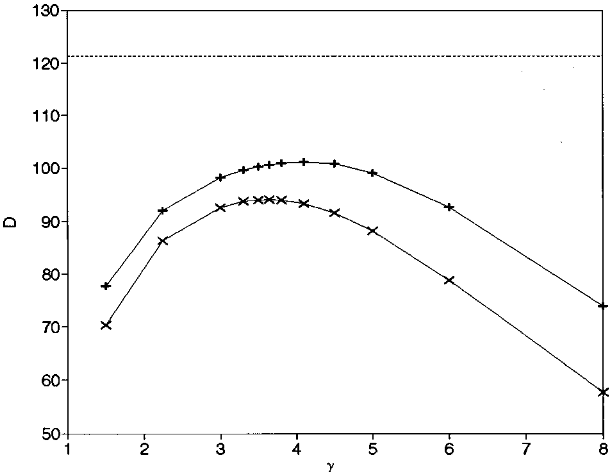

FIG. 1. Behavior of $D_{\rm acc}$ for helium as a function of the nonlinear parameter γ. The crosses are for $\Omega_p = 3$, and the plus signs are for $\Omega_p = 4$. The dotted line is the ‘‘exact’’ value, obtained from Eq. (7).

$$D_{\rm acc} = -8Z^2(1+K)\sum_n \frac{\langle 0|U|n\rangle\langle n|U|0\rangle}{E_0 - E_n},$$

where

$$U = \frac{\cos\,\theta_1}{\rho_1^2} + \frac{\cos\,\theta_2}{\rho_2^2}. \tag{8}$$

This expression for D looks like the second-order energy shift induced by the potential U, and it is a variational bound in the following sense. Let us apply the Rayleigh-Ritz variational method to the following trial function:

$$|\Psi_T\rangle = |0\rangle + \sum_n C_n|n\rangle \tag{9}$$

assuming that $H' = H + U$ is the Hamiltonian and that U is so small that only the leading order in U must be kept. Then the sum in Eq. (8) gives the variationally correct value for the total energy, and we choose γ to maximize $D_{\rm acc}$ as calculated from Eq. (8). In Fig. 1 we show the behavior of $D_{\rm acc}$ as γ is varied, for several different values of Ω_p; the ‘‘exact’’ value is also shown.

Now that we have set up a good way to specify the form of the intermediate states, using the ‘‘acceleration’’ form of the matrix elements shown in Eq. (8), we must calculate the corresponding value of $N_{\rm acc}$, as a function of Ω_p. This simply involves repeating the computation that led to the variational value of $D_{\rm acc}$ but with the logarithm included. Then ln(K) can be evaluated at each stage of the expansion. In Table I we display the results for $\Omega_0 = 16$ (525 terms) with $\Omega_p \leqslant 13$ (560 terms). The slow convergence can be seen.

III. EXTENDING THE UPPER LIMIT

In using this kind of pseudostate expansion, it is usually assumed that the contribution of each term is almost exact, and that the remaining error in the total is due to the fact that the sum does not extend to high enough energies. In this section we use a method due to Dalgarno and Stewart [2] to

TABLE I. Uncorrected values of numerator, denominator, and Bethe logarithm of helium as Ω_p increases. The value of the nonlinear parameter γ [Eq. (4)] that maximizes D_{acc} is also shown. (The last value of γ was obtained by extrapolation from those above, since computer time at these large expansions is quite long.) The exact value $D_{\mathrm{ex}}=121.335\,143$ is obtained from Eq. (7).

Ω_p	γ	D_{acc}	N_{acc}	ln(K)
3	3.644 529	94.114 569	301.053 261	3.198 796
4	4.080 394	101.216 416	346.195 202	3.420 346
5	4.425 096	104.957 668	373.513 205	3.558 703
6	4.849 542	108.413 460	399.676 322	3.686 593
7	5.179 484	110.403 345	416.057 508	3.768 523
8	5.588 226	112.320 411	432.319 315	3.848 983
9	5.888 226	113.508 976	442.840 189	3.901 367
10	6.305 080	114.676 534	453.744 402	3.956 373
11	6.623 156	115.446 146	461.125 678	3.994 293
12	7.004 813	116.207 693	468.586 094	4.032 316
13	7.3	116.735 692	473.876 067	4.059 393

account for the remainder of the sums beyond the highest pseudoenergy. They used experimental values of oscillator strength up to some maximum energy and used an asymptotic formula from there onward. For high energies they used the following simplified form:

$$\Psi_{n,\vec{k}}(\vec{r}_1,\vec{r}_2)=\frac{1}{2\pi}\left(\frac{k}{2}\right)^{1/2}[u_n(\vec{r}_1)e^{i\vec{k}\cdot\vec{r}_2}+u_n(\vec{r}_2)e^{i\vec{k}\cdot\vec{r}_1}] \tag{10}$$

to represent singly ionized states in the expression that replaces the discrete one used in Eq. (8):

$$\begin{aligned} F_n(\epsilon)&\equiv(I_n+\epsilon)^2\,\frac{df_n}{d\epsilon} \\ &=\frac{16Z^2(1+K)}{3(I_n+\epsilon)}\left|\langle\Psi_0|\left[\frac{\vec{r}_1}{r_1^3}+\frac{\vec{r}_2}{r_2^3}\right]|\Psi_{n,\vec{k}}\rangle\right|^2. \end{aligned} \tag{11}$$

Here $\epsilon=k^2$, I_n is the ionization-excitation potential of the two-electron system, and u_n is the wave function of the one-electron system left after single ionization. Integrating Eq. (11) over $d\epsilon$ from some lower limit ϵ_0 to ∞ gives the desired high-energy correction. For convenience, and without loss of accuracy, we fitted $F_n(\epsilon)$ to the form $[A_n+(B_n/k)\tan^{-1}(C_n/k)]\epsilon^{-3/2}$ and included s states up to $n=4$. Higher s states were included approximately by an expression falling like $1/n^4$.

In Ref. [2] the lower limit ϵ_0 is just the last experimental value of the oscillator strength available, but in our method it is not clear that the last pseudoenergy plays that role. Instead, we adjust ϵ_0 so that

$$D_{\mathrm{ex}}=D_{\mathrm{acc}}+\int_{\epsilon_0}^{\infty}d\epsilon\sum_n F_n(\epsilon). \tag{12}$$

The critical step is now to correct N using the same value of ϵ_0 as for the denominator, modifying the integral by the inclusion of the appropriate logarithmic factor. In Table II we show this improved value of ln(K); the convergence with increasing Ω_p is significantly improved.

TABLE II. Corrected values of numerator and Bethe logarithm of helium as Ω_p increases. The exact value of the denominator is used in each case. The lower limit ϵ_0 of the correction integral is also shown.

Ω_p	ϵ_0	N_{corr}	ln(K)
3	361.0613	520.267 518	4.287 855
4	724.0096	521.248 382	4.295 939
5	1143.441	523.110 217	4.311 284
6	1912.977	524.085 779	4.319 324
7	2734.433	525.086 045	4.327 568
8	4108.808	525.799 439	4.333 447
9	5524.324	526.334 777	4.337 859
10	7729.503	526.911 785	4.342 614
11	9964.945	527.307 234	4.345 874
12	13 253.52	527.650 177	4.348 700
13	16 564.86	527.870 611	4.350 517

IV. EXTRAPOLATION AND RESULTS

Although inclusion of the integral accounting for most of the asymptotic contribution to the numerator has improved the convergence of ln(K), an accurate result is still not at hand, and it will be necessary to use some method of extrapolation. To do this we need to find some reasonable independent parameter, not necessarily Ω_p itself, on which to base the procedure. That parameter should measure how close to convergence we have come at each stage.

An obvious choice is the deviation ΔD of the denominator from its exact value:

$$\Delta D\equiv D_{\mathrm{ex}}-D_{\mathrm{acc}}. \tag{13}$$

This quantity approaches zero as Ω_p increases and it should represent, at least approximately, the degree of completeness

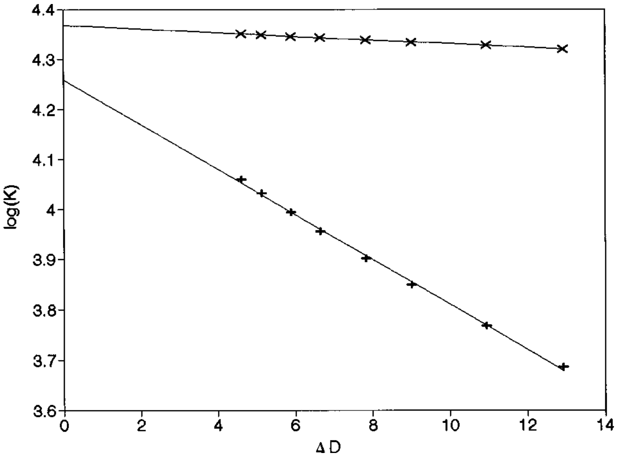

FIG. 2. ln(K) for helium as a function of ΔD. The plus signs show the uncorrected values, using the data from Table I, and the crosses are the corrected values from Table II. Linear fits have been made in both cases, and the improved convergence of the corrected values is clear.

TABLE III. Results for a series of two-electron systems.

System	Z	ln(K)	ln(K)^a
He	2	4.367 578	4.364 263
Li$^+$	3	5.177 763	5.177 249
Be^{+2}	4	5.753 615	5.753 640
Ne^{+8}	10	7.586 072	7.588 068

^{a}From Eq. (14) (Ref. [3]).

of the set of intermediate pseudostates. In Fig. 2 we have plotted the values of ln(K) from the tables with ΔD as the abscissa and have fitted straight lines to the calculated points both corrected and uncorrected. The slope of the line fitted to the corrected points is 12 times smaller than the uncorrected slope, indicating the improved convergence we expected. The extrapolated result for helium is ln(K)=4.367 58(46), where the uncertainty in parentheses is due to the linear regression analysis.

In Table III we show the values of ln(K), obtained by this method, for a range of atomic numbers Z. Goldman and Drake [3] have used an expansion in 1/Z to derive an approximate expression for the Bethe logarithm:

$$\ln(K)=\ln[19.769\,266\,9(Z-0.006\,15)^2], \tag{14}$$

which is exact in the limit of large Z. We have included the results of Eq. (14) in Table III for comparison. (But notice that the mass polarization term was not included in [3]; this should make a difference in the fourth decimal place.) We have also fitted our four values to obtain the following formula:

$$\ln(K)=\ln[19.705\,61Z^2-0.000\,42Z+0.002\,10]. \tag{15}$$

This is not in the same factored form as Eq. (14), but a good fit is also obtained in that form:

$$\ln(K)=\ln[19.705\,541(Z+1.35\times10^{-5})^2]. \tag{16}$$

Since neither of these expressions goes exactly to the known (hydrogenic) high-Z limit, neither one can be completely satisfactory for all Z, but the present results may represent the two-electron ground-state Bethe logarithm well over the range $2\leqslant Z\leqslant 10$.

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APPENDIX

Although the main point of this paper is to calculate the ground-state Lamb shift for two-electron systems, it is an obviously interesting question to see how well the method works for the simpler and better known one-electron (atomic hydrogen) case. We replace the Hylleraas function of Eq. (3) by the exact hydrogen ground-state eigenfunction and Eq. (4) by a simple one-electron form:

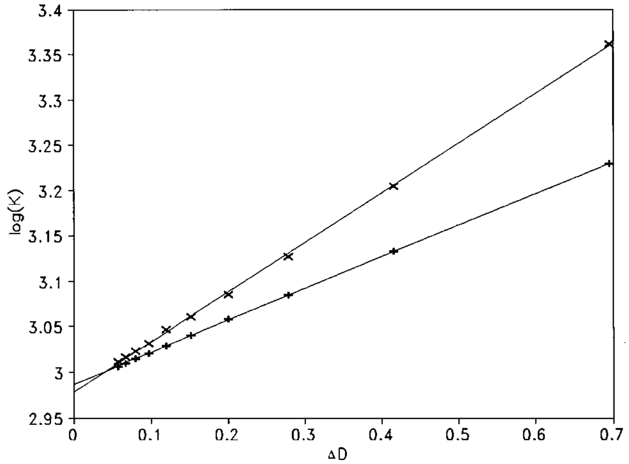

FIG. 3. ln(K) for hydrogen as a function of ΔD. The alternating convergence pattern discussed in the text leads to two distinct lines: crosses are for even values and plus signs are for odd values of Ω_p.

$$\Psi_0=\frac{e^{-r}}{\pi^{1/2}},\quad \Psi_n=e^{-\gamma r}P_1(\theta)\sum_{j=1}^{\Omega_p}C_jr^n. \tag{A1}$$

Again, the denominator can be transformed into a form like that of Eq. (7) and can be evaluated exactly: $D=16/3$. All the other steps described above are carried out, simplified to apply to the one electron system.

In Fig. 3 we show the unexpected results. In place of the linear relation found in the two-electron cases treated above and illustrated in Fig. 2, we obtain an alternating convergence pattern. As Ω_p increases from an odd value to the next even value the numerator increases significantly while the denominator remains unchanged to 7 or 8 significant figures. With the next increase in Ω_p the increase in D resumes. This effect produces the two distinct lines seen on the graph. We were able to carry the calculation up to $\Omega_p=22$, at which point D is about 1% from the exact value ($\Delta D=0.057$). It seems reasonable to extrapolate each of the two curves independently to $\Delta D=0$ and obtain the two estimates ln(K) =2.987 125 (from odd values of Ω_p) and ln(K)=2.978 329 (from even values). Combining these two values we can report a ‘‘best’’ value of ln(K)=2.9827±0.0044, where the indicated error measures the discrepancy between the two extrapolations. This should be compared with the accurate value [7] ln(K)=2.984 129; our generous error does include this value.

We have not been able to understand this irregular convergence, but we suspect that it involves some symmetry obeyed by hydrogen and not by the more complicated two-electron systems. This remains an interesting unanswered question.

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