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New Calculation of the Numerical Value of the Lamb Shift*

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The calculation of the second-order perturbation in hydrogen which gives the low-energy part of the Lamb Shift is attacked from a new approach, described in the preceding papers and here extended. A formula is gotten for $\ln(k_0)$ involving a double integral. The final numerical evaluation using an electronic computer to sum the series expansion of this formula yields what we believe to be the most accurate value of $\ln(k_0)$ yet given. Small discrepancies with the earlier results of Harriman are outside the realm of current physical significance, but do indicate that the reliability of the earlier results was badly overestimated. Approximate formulas for the radiative-perturbed wave functions are given; these may be quite useful for further calculations.

I. PERTURBATION CALCULATIONS IN HYDROGEN

We shall first describe a specialization of the perturbation calculation techniques of the previous papers (*1*, *2*) for the hydrogen atom. In units of $Z^2e^2/2a_0$ for energy a_0/Z for length we have

$$
\begin{aligned}
H_0 &= -\frac{d^2}{dr^2} - \frac{2}{r}\frac{d}{dr} + \frac{1}{r^2}\mathfrak{L}^2 - \frac{2}{r}, \\
E_{nlm}^{(0)} &= -\frac{1}{n^2}, \\
\psi_{nlm}^{(0)} &= Y_{lm}(\theta, \varphi)e^{-r/n}r^l P_{nl}(r),
\end{aligned} \tag{1}
$$

$$
P_{nl}(r) = \frac{1}{2}\left(\frac{2}{n}\right)^{l+2}\sqrt{\frac{(n+l)!}{(n-l-1)!}}\sum_{s=0}^{n-l-1}\binom{n-l-1}{s}\frac{\left(-2\frac{r}{n}\right)^s}{(2l+1+s)!},
$$

where $\binom{a}{b} = a!/b!(a-b)!$ and $Y_{lm}(\theta, \varphi)$ is the normalized spherical harmonic.

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We want to calculate the first-order perturbed wave function $\psi_{nlm}^{(1)}$ due to some perturbation $H_1(\mathbf{r}, \mathbf{p})$. The determining equation is [Eq. (1′) of Ref. *1*]

$$(E_n^{(0)} - H_0)\psi_{nlm}^{(1)} = (H_1 - E_{nlm}^{(1)})\psi_{nlm}^{(0)}. \tag{2}$$

Let us make the separations in angular momentum

$$(H_1 - E_{nlm}^{(1)})\psi_{nlm}^{(0)} = \sum_{l'm'} Y_{l'm'}(\theta, \varphi)e^{-r/n}r^{l'-1}h_{nl'm'}(r) \tag{3}$$

and

$$\psi_{nlm}^{(1)} = \sum_{l'm'} Y_{l'm'}(\theta, \varphi)e^{-r/n}r^{-l'-1}u_{nl'm'}(r). \tag{4}$$

For each $l'm'$ we have the equation

$$\left[r\frac{d^2}{dr^2} - 2\left(\frac{r}{n} + l'\right)\frac{d}{dr} + 2\frac{l'}{n'} + 2\right]u_{nl'm'}(r) = r^{2l'+1}h_{nl'm'}(r). \tag{5}$$

The important point is that this equation may be easily solved by a Laplace transform. Defining

$$u(p) = \int_0^\infty dre^{-pr}u(r), \qquad Q(p) = \int_0^\infty dre^{-pr}h(r)r^{2l'+1},$$

we get the *first*-order differential equation

$$\left[p\left(\frac{2}{n} - p\right)\frac{d}{dp} - 2(l' + 1)p + \frac{2}{n}(n + l' + 1)\right]u(p) = Q(p). \tag{6}$$

Since this is a first-order equation, we can always find $u(p)$ by quadrature. But if, as is usually the case, we are interested not in $\psi^{(1)}$, but in some energy shift

$$E^{(2)} = \int dv\psi^{(0)*}H_2\psi^{(1)}, \tag{7}$$

the solution may become even simpler. If H_2 consists only of powers of $\mathbf{r}$ and $\mathbf{p}$ the integrals in (7) reduce to the form

$$\int_0^\infty drr^te^{-2r/n}u(r) = \left(-\frac{d}{dp}\right)^t u(p)|_{p=2/n}.$$

From Eq. (6) we see, however, that we have

$$u\left(\frac{2}{n}\right) = \frac{n}{2(n - l' - 1)}Q\left(\frac{2}{n}\right) \tag{8}$$

as an *algebraic* solution. One can easily find derivations of $u(p)$ at $p = 2/n$ as an algebraic function of derivatives of $Q(p)$ at $p = 2/n$.

This very powerful technique of the Laplace transform will be necessary for the more difficult problem of evaluating the Lamb shift.

II. THE LAMB SHIFT

The nonrelativistic part of the Lamb shift (*3*) of the energy of the nl-state of hydrogen is governed by the second-order perturbation problem

$$\Lambda_{nl} = P \int_0^K k\, dk \sum_{n'l'} \frac{|\langle nl \mid \mathbf{p} \mid n'l' \rangle|^2}{E_{nl}^{(0)} - E_{n'l'}^{(0)} - k}, \tag{9}$$

in which P implies the principal value of the integral to follow. There is a different first-order perturbed electronic wave function $\psi^{(1)}$ for each value of k

$$(E_n^{(0)} - H_0 - k)\psi_{nlm}^{(1)} = \mathbf{p}\psi_{nlm}^{(0)},$$

and this is what makes this problem more complicated than any we have yet discussed.[1] Proceeding as outlined in the first section, we separate $\psi^{(1)}$ into two parts as

$$Y_{l+1,m}(\theta, \varphi)e^{-r/n}r^{-l-2}u_+(r) \tag{9a}$$

and

$$Y_{l-1,m}(\theta, \varphi)e^{-r/n}r^{-l}u_-(r),$$

with appropriate numerical factors to take care of the angular integrals. We then have two equations

$$\left[r\frac{d^2}{dr^2} - 2\left(\frac{r}{n} + l \pm 1\right)\frac{d}{dr} + \frac{2}{n}(n + l \pm 1) - kr\right]u_\pm(r)$$
$$= \sum_s \binom{n-l-1}{s} \frac{\left(-\frac{2}{n}\right)^s}{(2l+s+1)!}\left(-\frac{1}{n} + \frac{s + l + \frac{1}{2} \mp l \mp \frac{1}{2}}{r}\right) r^{s+2l+2\pm1} \tag{10}$$

and the solution

$$\Lambda_{nl} = P\int_0^K k\, dk\, \frac{1}{4}\left(\frac{2}{n}\right)^{2l+4} \frac{(n+l)!}{(n-l-1)!}\int_0^\infty dr e^{-2r/n}$$
$$\times \sum_s \binom{n-l-1}{s}\frac{\left(-\frac{2}{n}\right)^s}{(2l+s+1)!}\left[\frac{l+1}{2l+1}u_+(r)\left(sr^{s-1} - \frac{r^s}{n}\right)\right. \tag{11}$$
$$\left. + \frac{l}{2l+1}u_-(r)\left((2l+s+1)r^{s+1} - \frac{r^{s+2}}{n}\right)\right].$$

[1] Brown *et al.* (*4*) suggested that one might evaluate the Lamb shift by this differential equation approach.

We now carry out the Laplace transforms.

$$\left[\left(-p^2+\frac{2}{n}p+k\right)\frac{d}{dp}-2p(l+1\pm 1)+2\frac{n+l+1\pm 1}{n}\right] \cdot u_\pm(p) = Q_\pm(p), \tag{12}$$

$$\begin{aligned} Q_+(p) &= \frac{d}{dp}\left(1-\frac{2}{np}\right)^{n-l-2}\frac{2}{np^{2l+4}}\left(np-\frac{n+l+1}{n}\right), \\ Q_-(p) &= \frac{1}{p^{2l+1}}\left(1-\frac{1}{np}\right)\left(1-\frac{2}{np}\right)^{n-l-1}, \end{aligned} \tag{13}$$

$$\begin{aligned} \Lambda_{nl} = \int_0^K kdk\,\frac{1}{4}\left(\frac{2}{n}\right)^{2l+4}\frac{(n+l)!}{(n-l-1)!}\sum_s\binom{n-l-1}{s}\frac{\left(\frac{2}{n}\right)^s}{(2l+s+1)!} \\ \times\left[\frac{l+1}{2l+1}\left\{-s\left(\frac{d}{dp}\right)^{s-1}-\frac{1}{n}\left(\frac{d}{dp}\right)^{s}\right\}u_+(p)\right. \\ \left.+\frac{l}{2l+1}\left\{-(2l+s+1)\left(\frac{d}{dp}\right)^{s+1}-\frac{1}{n}\left(\frac{d}{dp}\right)^{s+2}\right\}u_-(p)\right]_{p=2/n}. \end{aligned} \tag{14}$$

The differential Eq. (12) is solved by quadrature.

$$\begin{aligned} u_\pm\left(\frac{2}{n}\right) = u_\pm^0\left(\frac{2}{n}\right)\left[\int_{(1/n)+\lambda-\epsilon}^{2/n} dp\,\frac{Q_\pm(p)}{\left(-p^2+\frac{2}{n}p+k\right)u_\pm^0(p)}\right. \\ \left.-Q_\pm\left(\frac{1}{n}+\lambda\right)(2\lambda)^{1/\lambda+l\pm1}\int^{\epsilon} dx\,x^{l\pm1-1/\lambda}\right]_{\epsilon\to 0}, \end{aligned} \tag{15}$$

where

$$u_\pm^0(p) = \left(\frac{\lambda+\frac{1}{n}-p}{\lambda-\frac{1}{n}+p}\right)^{1/\lambda}\left(-p^2+\frac{2}{n}p+k\right)^{-l-1\mp1}.$$

and

$$\lambda = \sqrt{k+\frac{1}{n^2}}.$$

The necessary derivatives of $u_\pm$ are gotten from the differential equation (12). The answer is to be compared with the logarithm of the mean excitation energy defined by Bethe (*3*).

$$\ln[k_0(nl)] = \lim_{K\to\infty}\left[-\frac{n^3}{4}\Lambda_{nl}-\frac{n}{4}K+\ln K\delta_{l0}\right]$$

The desired result appears now as a double integral. We shall carry through the evaluation for the $2s$ and $2p$ states.

III. THE $2s$-STATE

Starting with $l = 0$, $\psi^{(1)}$ contains only p-states, so only u_+ enters. Introducing the new variables of integration

$$e^q = \frac{\lambda - \frac{1}{2} + p}{\lambda + \frac{1}{2} - p} \quad \text{and} \quad y = \frac{1}{2\lambda} \tag{16}$$

we have

$$\ln[k_0(2s)] = \lim_{K\to\infty}\left[\ln K - \frac{1}{2}K + \int_{(4K+1)^{-1/2}}^{1} dy I(y)\right], \tag{17}$$

where

$$I(y) = \frac{y^2-1}{8y^5}u_+(1) = \frac{192}{(y-1)(1+y)^5}\left(\frac{1-y}{1+y}\right)^{2y} \times \int_{\infty}^{\ln 1+y/1-y} dq \frac{\left[e^{-q(3-2y)} - \left(\frac{1-y}{1+y}\right)e^{-q(2-2y)}\right]}{\left[1-\left(\frac{1-y}{1+y}\right)e^{-q}\right]^5},$$

and we shall evaluate the q integral by a power series expansion in $(1-y)/(1+y)e^{-q} < 1$.

$$I(y) = \frac{-3}{4y^3} + \frac{192(1-y)}{(1+y)^7}\sum_{m=0}^{\infty}\binom{m+3}{3}\left(\frac{1-y}{1+y}\right)^{2m}\frac{1}{m+2-2y}. \tag{18}$$

We shall take care of the singularities at $K \to \infty$ $(y \to 0)$ by extracting

$$J(y) = \frac{-3}{4y^3} + \frac{192(1-y)}{(1+y)^7}\sum_{m=0}^{\infty}\binom{m+3}{3}\left(\frac{1-y}{1+y}\right)^{2m} \times \left[\frac{1}{m+2} + \frac{2y}{(m+2)(m+3)}\right] = \frac{1}{4y^3} - \frac{2(3y+1)}{y(1+y)^3}.$$

We have

$$\int_{(4K+1)^{-1/2}}^{1} dy\, J(y) = \frac{k}{2} - \ln K - \frac{1}{2},$$

whence

$$\ln[k_0(2s)] = -\frac{1}{2} + \int_0^1 dy\, \frac{192(1-y)}{(1+y)^7} \sum_{m=0}^{\infty} \left(\frac{1-y}{1+y}\right)^{2m} \times \frac{(m+1)y(2y+1)}{m+2-2y} \tag{20}$$

$$= \frac{187}{60} + 64 \int_0^1 dy\, \frac{y(1-y)(2y+1)(2y-1)}{(1+y)^7} \sum_{m=1}^{\infty} \left(\frac{1-y}{1+y}\right)^{2m} \frac{1}{m+2-2y}.$$

Now setting $(1-y)/(1+y) = x$ and using

$$W_m(N) = \int_0^1 \frac{x^N dx}{m + x(m+4)} = \frac{1}{(m+4)}\left[\left(\frac{-m}{m+4}\right)^N \ln\left(2+\frac{4}{m}\right) + \sum_{l=0}^{N-1} \frac{1}{N-l}\left(\frac{-m}{m+4}\right)^l\right],$$

we come to

$$\ln[k_0(2s)] = \frac{187}{60} - 1024 \sum_{m=1}^{\infty} \frac{m(m+1)(m+2)(m+3)}{(m+4)^6} W_m(2m) + X, \tag{21}$$

where

$$X = 2\sum_{m=1}^{\infty} \frac{1}{m+4} \sum_{s=1}^{6} c_s \sum_{t=1}^{s} \frac{1}{2m+t}\left(\frac{-m}{m+4}\right)^{s-t},$$

$$c_s = (3, -7, -10, 10, 7, -3).$$

After much algebra X is evaluated:

$$X = \frac{1}{12} + \frac{4582}{5625} + \frac{5120}{117649} - 4\ln 2\left[\frac{266}{625} - \frac{2}{3} - \frac{30720}{117649}\right] - 8\left[\frac{3840}{16807} + \frac{234}{1000}\right]\zeta_5(2) - 32\left[\frac{480}{2401} - \frac{1}{100}\right]\zeta_5(3) + 128\left[\frac{21}{10} - \frac{60}{343}\right]\zeta_5(4) - 256\left(\frac{211}{49}\right)\zeta_5(5) + \frac{6144}{7}\zeta_5(6), \tag{22}$$

where

$$\zeta_n(s) = \sum_{m=n}^{\infty} \frac{1}{m^s} \tag{23}$$

and values of $\zeta_5(s)$ are given in Table I.

TABLE I

VALUES OF THE TRUNCATED ZETA FUNCTION $\zeta_5(s)$, EQ. (23)

s	$\zeta_5(s)$		
2	0.22132	29557	37116
3	0.02439	48661	22557
4	0.00357	13046	98793
5	0.00058	59663	05921
6	0.00010	21792	46966
7	0.00001	84948	54845
8	0.00000	34316	18605

We are now left with

$$\ln[k_0(2s)] = 3.1779148969 - 1024 \sum_{m=1}^{\infty} F_m,$$

$$F_m = \frac{(m+3)!}{(m-1)!(m+4)^7} \left[\sum_{l=0}^{2m-1} \frac{1}{2m-l} \left(\frac{-m}{m+4} \right)^l + \left(\frac{m}{m+4} \right)^{2m} \cdot \ln\left(2 + \frac{4}{m}\right) \right]. \quad (24)$$

For more rapid convergence we calculate the sum of

$$F_m' = F_m - \frac{1}{4} \frac{(m+3)!}{m!(m+4)^7},$$

with

$$-\frac{1024}{4} \sum_{m=1}^{\infty} \frac{(m+3)!}{m!(m+4)^7} = -256[\zeta_5(4) - 6\zeta_5(5) + 11\zeta_5(6) - 6\zeta_5(7)]$$

$$= -0.273538422.$$

The first 100 terms of $\sum F_m'$ were computed using the Stanford University IBM 650 (15 minutes computing time).

$$1024 \sum_{m=1}^{100} F_m' = 0.092605684,$$

with estimated probable roundoff error ± 28 in the last two places. In order to get the remainder of the sum we write

$$F_m' = \frac{(m+3)!}{(m-1)!(m+4)^7} \left[-\frac{1}{4m} + \int_0^1 dx \frac{x^{2m}}{x + \frac{m}{m+4}} \right],$$

and by performing partial integrations we get an asymptotic series in inverse powers of m.

$$F_{m-4}' \sim \frac{7}{16m^5} - \frac{15}{8m^6} + \frac{193}{128m^7} + \cdots . \tag{25}$$

This, together with the formula

$$\sum_{m=M+1}^{\infty} \frac{1}{m^s} = \frac{1}{(s-1)M^{s-1}} - \frac{1}{2M^s} + \frac{s}{12M^{s+1}} - \cdots$$

gives the remainder

$$1024 \sum_{m=101}^{\infty} F_m' = 0.000000908.$$

Finally our result:[2]

$$\ln[k_0(2s)] = \underset{\pm 28}{2.811769883}. \tag{26}$$

Harriman's (*6*) result is $\underset{\pm 9}{2.811798}$. The difference is three times Harriman's stated error but amounts to an insignificant 0.004-megacycle increase in the level shift. Bethe *et al.* (*5*) got the value $\underset{\pm 4}{2.8121}$ which just overlaps ours.

IV. THE $2p$-STATE

The s- and d-wave parts of $\psi^{(1)}$ are separated and the two calculations proceed similarly to that just detailed for the $2s$-state. The principal value of the integral must be taken on account of the possible real transition $2p - 1s$. The $\ln K$-divergence exactly cancels between s- and d-wave parts as it should. The resulting formula is

$$\begin{aligned} \ln [k_0(2p)] = & -\frac{256}{3} \sum_{m=1}^{\infty} \frac{(m+2)^3(11m^2+44m+32)}{(m+4)^8} \\ & \times \left[\sum_{l=0}^{2m-1} \frac{1}{2m-l} \left(\frac{-m}{m+4} \right)^l + \left(\frac{m}{m+4} \right)^{2m} \ln\left(2 + \frac{4}{m}\right) \right] \\ & -\frac{59}{360} + \frac{256 \ln 2 + 33/5 - 270}{3^7} + \frac{421}{(72)(35)} + Y, \end{aligned} \tag{27}$$

$$Y = -\frac{2}{3} \sum_{m=1}^{\infty} \frac{1}{m+4} \sum_{s=1}^{8} d_s \sum_{t=1}^{s} \frac{1}{2m+t} \left(\frac{-m}{m+4} \right)^{s-t},$$

$$d_s = (2, -9, 5, 16, -16, -5, 9, -2);$$

[2] The stated error is our estimate of the roundoff error in the numerical computation. The electronically computed part of the work has been redone with extra precision and agrees with the above, within these stated errors.

and finally we get

$$\ln[k_0(2p)] = \underset{\pm 12}{-0.030016697}, \tag{28}$$

while Harriman (*6*) had $\underset{\pm 1}{-0.03001637}$ and Bethe *et al.* (*5*) got $\underset{\pm 2}{-0.0300}$. The discrepancy here is 33 times the stated uncertainty, but is much too small to be physically significant.

V. APPROXIMATE CALCULATIONS

The actual functional form of the electron wave function $\psi^{(1)}$ perturbed by the emission of a photon of energy k may be useful in other calculations. The solution contained in (9a), (15) is however quite complex, and we seek a simple approximation here. For the 1s- and 2s-states we have found that the function

$$\chi = \frac{\exp(-r)\left[\sqrt{\frac{1}{n^2} + k} - \frac{1}{n}\right] - 1}{k} \, \mathbf{p}\psi^{(0)} \tag{29}$$

has the same form as the exact $\psi^{(1)}$ for small r, small k, and large k. Setting $\psi^{(1)} = C\chi$ we construct a variational expression for Λ Eq. (9) [see Eqs. (9) and (10) of Ref. *1*].

$$\begin{aligned} \Lambda &\approx 2CI_1 - C^2 I_2 , \\ I_1 &= \int_0^K k\,dk \int dv \psi^{(0)*}\mathbf{p}\cdot\chi, \\ I_2 &= \int_0^K k\,dk \int dv \chi^* \cdot (E^{(0)} - H_0 - k)\chi. \end{aligned} \tag{30}$$

Then varying with respect to C

$$C = I_1/I_2 ,$$

$$\Lambda \cong I_1^2/I_2 .$$

For the 1s state we find

$$I_1 = 6 - K,$$

$$I_2 = -K - 4 \ln K + 20 + 4 \ln 2;$$

dropping terms of order $1/K$. Finally

$$\begin{aligned} \Lambda_{1s} &\approx -K + 4 \ln K - 8 - 4 \ln 2 \\ &\to -K + 4 \ln K - 4 \ln[k_0(1s)], \end{aligned}$$

so $\ln[k_0(1s)] \approx 2 + \ln 2 = 2.69$, instead of 2.98. For the 2s state we have

$$I_1 = -\tfrac{1}{4}K + \tfrac{13}{16}$$

$$I_2 = -\tfrac{1}{4}K - \tfrac{1}{2}\ln K + \tfrac{37}{6} - \tfrac{19}{4}\ln 2,$$

$$\Lambda_{2s} \approx -\tfrac{1}{4}K + \tfrac{1}{2}\ln K + \tfrac{19}{4}\ln 2 - \tfrac{109}{24}$$

$$\rightarrow -\tfrac{1}{4}K + \tfrac{1}{2}\ln K - \tfrac{1}{2}\ln[k_0(2s)]$$

so $\ln[k_0(2s)] \approx \tfrac{109}{12} - \tfrac{19}{2}\ln 2 = 2.50$ instead of 2.81.

It seems remarkable that so simple a form as (29) could give exactly the two leading terms for large K and still give values of $\ln k_0$ which are accurate to within 10 percent.

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