

It should be added that the discrepancy was calculated using the value of μ_D/μ_P measured by Bloch, Levinthal, and Packard, who found

$$K = \mu_D/\mu_P = 0.3070126 \pm 0.0000021. \quad (5)$$

However, Bitter and Siegbahn, measuring the same ratio, have found, respectively,

$$K = 0.3070210 \pm 0.0000050 \quad (6)$$

and

$$K = 0.3070183 \pm 0.0000015. \quad (7)$$

The result (7) is larger than (5) by about two parts in one hundred thousand, and would make the dis-

crepancy (using Nafe and Nelson's determination of the h.f.s.) 1.5×10^{-4} , which would be hard to account for on the basis of this calculation alone.

In conclusion, then, we are not yet in a position to estimate structural effects. In order to do so, we need, on the one hand, a more accurate value for the deuteron-proton moment ratio, and on the other a better knowledge of the deuteron S state wave function.

ACKNOWLEDGMENT

The author wishes to thank Professor H. A. Bethe and Dr. A. Bohr, who gave generously of their time and interest, and whose help and criticism were indispensable.

Numerical Value of the Lamb Shift

H. A. BETHE AND L. M. BROWN
Laboratory of Nuclear Studies, Cornell University, Ithaca, New York

AND

J. R. STEHN
Knolls Atomic Power Laboratory, Schenectady, New York

(Received October 10, 1949)

The average excitation potential of the $2s$ state of hydrogen which occurs in the Lamb shift, is calculated numerically and found to be 16.646 ± 0.007 Ry. This gives a theoretical value of 1051.41 ± 0.15 megacycles for the Lamb shift, compared with the latest experimental value of 1062 ± 5 . It is not known whether the discrepancy of 10 Mc can be explained by relativistic effects. Simple analytical approximations are discussed which make plausible the high value of the average excitation potential and give a good approximate value for it.

IN this paper, we are reporting two independent numerical calculations of the average excitation potential of the hydrogen atom which occurs in the formula for the Lamb shift.¹ The first calculation was done in 1947 by one of us (J.R.S.) with the help of Miss Steward, the second in 1949 by L.M.B.

I

The formula for the Lamb shift of a hydrogen level n_0, l has been derived by many authors² and is for s states

$$\Delta E(n_0, 0) = \frac{8Z^4 \alpha^3}{n_0^3 3\pi} \text{Ry} \left(\ln \frac{\mu}{k_0(n_0, 0)} - \ln 2 + \frac{5}{6} - \frac{1}{5} \right) \quad (1)$$

¹ W. E. Lamb and R. C. Retherford, Phys. Rev. **72**, 241 (1947); **75**, 1325 (1949).

² N. H. Kroll and W. E. Lamb, Phys. Rev. **75**, 388 (1949); J. B. French and V. F. Weisskopf, Phys. Rev. **75**, 1240 (1949); R. P. Feynman, Phys. Rev. **74**, 1430 (1948), and correction in Phys. Rev. **76**, 769 (1949), footnote 13; J. Schwinger, Phys. Rev. **76**, 790 (1949).

and for states with $l \neq 0$

$$\Delta E(n_0, l) = \frac{8Z^4 \alpha^3}{n_0^3 3\pi} \text{Ry} \left(\ln \frac{\text{Ry}}{k_0(n_0, l)} + \frac{3}{8} \frac{c_{lj}}{2l+1} \right), \quad (2)$$

where

$$\begin{aligned} c_{lj} &= 1/(l+1) & \text{for } j = l + \frac{1}{2} \\ c_{lj} &= -1/l & \text{for } j = l - \frac{1}{2}. \end{aligned} \quad (2a)$$

In these formulas, Z is the nuclear charge, n_0 the principal and l the orbital quantum number, $\alpha = e^2/\hbar c$ the fine structure constant, Ry the Rydberg energy, $\mu = mc^2$ and k_0 the average excitation energy which we wish to calculate.

This average energy is defined by³

$$\begin{aligned} \ln \frac{k_0(n_0, l)}{\text{Ry}} &= \sum_n \frac{|(n_0 0 | p_x | n)|^2 (E_n - E_0)}{|(n_0 l | p_x | n)|^2 (E_n - E_c)} \ln \frac{E_n - E_0}{\text{Ry}}, \quad (3) \end{aligned}$$

³ H. A. Bethe, Phys. Rev. **72**, 339 (1947), quoted as A in the following. The definition is in Eq. (6).

TABLE I. Oscillator strengths for hydrogen.

Transitions from to	2p		
	2s	ns	nd
n=1	—	-0.138732	—
3	0.43486	0.01359	0.69576
4	0.10276	0.00305	0.12180
5	0.04193	0.00121	0.04437
large	3.664n ⁻³	0.102n ⁻³	3.257n ⁻³

where $(n_0l|p_x|n)$ denotes the matrix element of an arbitrary momentum component p_x corresponding to the transition from the "initial" state n_0, l , of energy E_0 , to the final state n , of energy E_n . Note that on the left-hand side the matrix element from the initial state $l=0$ is involved, regardless of the value of l for which $k_0(n_0, l)$ is to be calculated: This definition is necessary because the sum on the left would vanish (see A) if we used $l \neq 0$ for the initial state. For s states, then, k_0 is actually the geometric average of the excitation energy $E_n - E_0$, with the weighting factor $p_{n_0}^2(E_n - E_0)$; for other states, k_0 is defined in as close analogy to the s states as possible. The denominator Ry in the arguments of the logarithms could be omitted for s states; for $l \neq 0$, it serves to make the argument dimensionless and appears again in Eq. (2); any other constant energy would serve as well, but Ry is most convenient.

It is convenient to introduce the oscillator strength f by putting

$$|(n_0l|p_x|n)|^2 = \frac{1}{2}m(E_n - E_0)f(n_0l, n) \quad (4)$$

and to use the energy change in Rydberg units,

$$\nu = (E_n - E_0)/\text{Ry}. \quad (5)$$

Then (3) becomes

$$\ln(k_0(n_0, l)/\text{Ry}) \sum_n f(n_0l, n) \nu^2 = \sum_n f(n_0l, n) \nu^2 \ln \nu. \quad (6)$$

The left-hand side may be evaluated by sum rules (reference 3, Eqs. (9) and (10)) and gives

$$\sum \nu^2 f(n_0, 0, n) = 16/(3n_0^3). \quad (7)$$

For our case, $n_0 = 2$, therefore

$$\ln(k_0(2, l)/\text{Ry}) = \sum_n \frac{3}{2}f(2, l, n) \nu^2 \ln \nu. \quad (8)$$

To evaluate this expression, we need the oscillator strengths for hydrogen. For transitions to the discrete spectrum, we have used the formula given by Bethe,⁴ (Eq. (41.4)) and re-evaluated his Table 16 in which some numerical mistakes were found, some of which have been previously pointed out by other authors. The corrected values are given in Table I. For large n (≥ 6), we found it sufficient to use

$$g(2s, n) \equiv \frac{3}{2}f(2s, n) \nu^2 = 0.3436n^{-3}(1 + \frac{1}{3}n^{-2}) \quad (8a)$$

$$g(2p, n) \equiv \frac{3}{2}f(2p, n) \nu^2 = 0.3149n^{-3}(1 + 4.24n^{-2}). \quad (8b)$$

⁴H. A. Bethe, *Handbuch der Physik* 24/1 (Verlag Julius Springer, Berlin, 1933), p. 273.

As is seen from Table II, the discrete final states n contribute only about 2 percent of the sum in (8) for the $2s$ state. For the $2p$ state, their absolute contribution is similar while in this case the continuum gives an almost negligible contribution. In either case, no great numerical accuracy is required for the discrete states.

For transitions to the continuum, we define the quasi-principal quantum number n by

$$E_n = +\text{Ry}/n^2. \quad (9)$$

Then the oscillator strength for transitions from the $2s$ state into an interval $d\nu$ of the continuous spectrum is

$$df(2s, n) = 4\nu^{-4}d\nu((4/3) + \nu^{-1}) \times \exp(-4n \arccot(n/2))/(1 - e^{-2\pi n}). \quad (10)$$

The summation over n in (8) should be replaced by an integration over $d\nu$. For transitions from the $2p$ state to the continuous spectrum

$$df(2p, n) = (8/9)\nu^{-5}d\nu(\frac{3}{2} + \nu^{-1}) \times \exp(-4n \arccot(n/2))/(1 - e^{-2\pi n}). \quad (11)$$

These formulas may be obtained from the expressions for the photoelectric absorption coefficient (reference 4, Eqs. (47.19), (47.20)), using the general relation between absorption coefficient and oscillator strength,

$$\tau = Nz2\pi^2e^2(\hbar/mc)(df/dE), \quad (12)$$

where N is the number of atoms per cm³, z the number of electrons in the given shell,⁵ and df/dE the oscillator strength per unit energy interval, i.e. $(1/\text{Ry})(df/d\nu)$. It should be noted that Eq. (47.20) of reference 4, like the original formula of Stobbe,⁶ is too large⁷ by a factor of 2; this mistake has been corrected in (11).

In Fig. 1 we have plotted the expression

$$g \equiv \frac{3}{2}\nu^3 df/d\nu \quad (13)$$

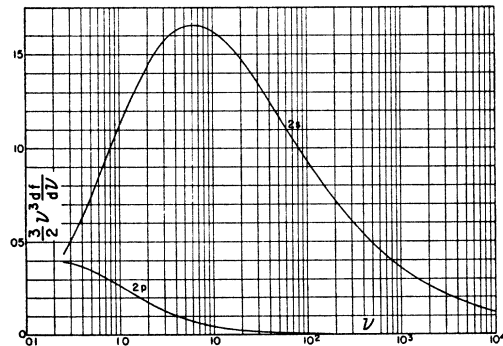


FIG. 1. The weight functions for the determination of the average excitation energy.

⁵Note that ν_2 in reference 4 is $\frac{1}{4}\text{Ry}$.

⁶M. Stobbe, *Ann. d. Physik* 7, 661 (1930).

⁷This was pointed out to one of the authors (H.A.B.) many years ago. It is most easily verified by comparing the oscillator strength $df/d\nu$ just above and just below the energy $E_n=0$. It can also be verified by checking the sum rule analogous to (7), $\sum f(2p, n) \nu^2 = 0$, see Table II.

vs. $\log \nu$, for $2s$ and $2p$. The integral under the $2s$ curve, after addition of the discrete spectrum, gives unity (Eq. (7)). The smallness of g for the $2p$ state is apparent.

For the numerical integration, we have used the integration variable n instead of ν , inserting

$$\nu = \frac{1}{4} + 1/n^2. \quad (14)$$

It is easily seen that the integrand in (7) then behaves as dn for small n , and that in (8) as $dn \log n$. Because of the singularity of $\log n$ at $n=0$, numerical integration is not feasible. However, it is easy to expand the

TABLE II. Results of numerical integration.

	2s State		2p State
	Earlier Integration	Later	Later Integration
Contribution to S :			
Discrete	0.02645	0.02645	-0.081366
Continuous	0.9736	0.97340	+0.081336
Total	1.00005	0.99985	-0.000030
Contribution to (8)			
Discrete	-0.0465	-0.04649	-0.030669
Continuous	2.8593	2.85840	+0.000685
Total	2.8128	2.81191	-0.02998
Total/ S	2.8127	2.81233	
Adopted $\ln(k_0/Ry)$	2.8121 ± 0.0004		-0.0300 ± 0.0002
k_0/Ry	16.646 ± 0.007		0.9704 ± 0.0002

integrand (apart from the log) into a power series in n , which permits analytical integration. This procedure was used for n up to 0.05, while from there to 0.1 it was used as a check on the numerical work: The results agreed within 0.00005 which is beyond the accuracy attempted (0.0001).

The numerical integration was done by Simpson's rule, using in the final calculation for the s state intervals⁸ as follows:

$$\begin{aligned} &\text{from } n=0.05 \text{ to } 0.1, && \text{interval } 0.0125 \\ &\text{from } n=0.1 \text{ to } 0.2, && \text{interval } 0.025 \\ &\text{from } n=0.2 \text{ to } 1, && \text{interval } 0.05. \end{aligned}$$

From $n=1$ to ∞ , we used $s=1/n$ as a variable, choosing intervals of 0.05 for s . The fourth differences of the integrand were of the order of 1 percent of the integrand itself (usually less) so that the error in the result may be expected to be about 1 part in 10,000. The earlier calculation was done with twice the intervals; the results of the two calculations agree within 0.0009 unit, after correction of a numerical mistake of 0.0031 unit in the earlier integration, and of 0.0007 unit in the discrete contribution, both of which were subsequently discovered. The error in Simpson's rule is roughly proportional to the fourth power of the interval used, so that the result of the second calculation should be

⁸ The integrand was calculated at the intervals h stated. The integral from x to $x+2h$ is then $\frac{1}{3}h[f(x)+4f(x+h)+f(x+2h)]$.

high by 0.00006, an error considerably smaller than the rough estimate of 1 part in 10,000 from the fourth differences. As a check, the sum in (8) *without* the logarithmic factor was also calculated (denoted by S); according to (7), this should give unity for $2s$ and zero for $2p$. The deviation of 1.5 parts in 10,000 (Table II) for the s state indicates the accuracy attained; for the p state, the error is one-fifth of this. One can be doubtful whether it is more accurate to use the result (8) as it stands, or to divide it by the numerically calculated S ; both results are given in Table II, and their mean is used as the final result. The probable error is taken as the whole difference between the two results; the main source of error is presumably in evaluation of the integrand (or of the discrete contribution) since the error from Simpson's rule should be less than 0.0001. The probable error for the $2p$ state was estimated from the difference of the earlier and the later calculation which was 0.0002.

II

These results can now be inserted into the Lamb effect formulas (1), (2). In the numerical factor in front, we should insert the Rydberg constant for hydrogen, rather than for infinite mass. This can be seen from the derivation,³ the velocity matrix elements in A Eq. (6) are the same whether the reduced mass or the full mass is used for the electron whereas the energy differences $E_n - E_m$ are proportional to the electron mass and thus to Ry_H . This can also be traced through A Eqs. (8) to (11). There is some doubt whether to use the reduced mass of the electron also in $\mu = mc^2$ in (1); we shall do so which may cause an error of $1/1840 = 0.0005$ in the value of the parenthesis in (1). A larger uncertainty exists because of the neglect of relativistic corrections in (1) (see below).

For α we take the value deduced from hyperfine structure⁹

$$1/\alpha = 137.041 \pm 0.005. \quad (15)$$

Then the constant factor in (1), the "Lamb constant," is, when expressed in frequency units:

$$(\alpha^3/3\pi)Ry = 135.549 \pm 0.015 \text{ megacycles}. \quad (16)$$

The uncertainty arises entirely from that of α . The first term in the parenthesis in (1) is

$$\ln(\mu/k_0(2s)) = 10.5336 - 2.8121 = 7.7215 \pm 0.0006. \quad (17)$$

The error includes 0.0004 from Table II, and 0.0005 from the questionable use of the reduced mass in μ . The value quoted by French and Weisskopf, 7.6906, referred to the *difference*

$$\ln(\mu/k_0(2s)) - \ln(Ry/k_0(2p)) = 7.7215 - 0.0295 = 7.6920,$$

according to our present calculation, the small difference between this and 7.6906 being due to numerical mis-

⁹ H. A. Bethe and C. Longmire, Phys. Rev. **75**, 306 (1949).

takes in our earlier calculation. The results are given in Table III. The error of the shift of $2s$ includes 0.11 Mc from the uncertainty of the Lamb constant (16), i.e. mostly of α , and 0.08 Mc from that of $\ln(\mu/k_0(2s))$, of which only 0.05₅ arises from the numerical calculation. For the p levels, the uncertainty is all due to the calculation of $k_0(2p)$.

The measured Lamb shift is the difference between the shifts of $2s$ and $2p_{1/2}$ state, viz.

$$L(2s) - L(2p_{1/2}) = 1051.41 \pm 0.15 \text{ megacycles} \quad (18)$$

in agreement with the calculated values previously given by French and Weisskopf, and Lamb and Kroll.² The latest published experimental value¹⁰ is

$$L(\text{experimental}) = 1062 \pm 5 \text{ Mc.} \quad (19)$$

The discrepancy between (18) and (19) is twice the experimental error, which probably has been generously estimated. It is possible that this discrepancy is due to the neglect of relativistic corrections in the derivation of formula (1). These may not be negligible because the wave function of the hydrogen ground state has large Fourier components of high wave number. A rough estimate shows that these corrections are of relative order α , but without the logarithmic factor which gives the main contribution to (1). Thus the rough estimate would give a correction of order 1 Mc, too small to explain the discrepancy. Moreover, superficial reasoning would lead one to expect a decrease of the theoretical value. However, an explicit calculation of the relativistic corrections is now very urgent and may give a different result.

It has often been pointed out that a higher theoretical result would be obtained if the vacuum polarization effect were left out of (1), and that this effect can be separated from the main part of the Lamb effect in a relativistically invariant way. The vacuum polarization is represented by the term $-\frac{1}{5}$ in (1) and therefore contributes an amount

$$-27.110 \text{ Mc} \quad (20)$$

to the Lamb effect. If it were excluded, the result would be 16 Mc higher than the experimental value so that the agreement is not improved.

III

In this section, we shall try to give a qualitative understanding of the very large result, 16.646 Ry, which we found for the average excitation potential of the $2s$ state. As was pointed out, $\ln k_0$ is the average of $\ln(E_n - E_0)$ with the weight factor $\nu^2 f$. If we take the average of $E_n - E_0$ itself, rather than of its logarithm, with the same weight factor $\nu^2 f$, we get infinity. This

¹⁰ R. C. Retherford and W. E. Lamb, Phys. Rev. **75**, 1325 (1949).

TABLE III. Lamb shifts.

	$2s$	$2p_{1/2}$	$2p_{3/2}$
First term in parenthesis	7.7215 ± 0.0006	$+0.0300 \pm 0.0002$	$+0.0300 \pm 0.0002$
Total parenthesis	7.6707 ± 0.0006	-0.0950 ± 0.0002	$+0.0925 \pm 0.0002$
Level shift in megacycles	1038.53 ± 0.14	-12.88 ± 0.03	$+12.54 \pm 0.03$

is because we have (neglecting constant factors)

$$\begin{aligned} \sum (E_n - E_0) \nu^2 f &\sim \sum (E_n - E_0)^2 |p_{0n}^x|^2 \sim \sum |(\partial V / \partial x)_{0n}|^2 \\ &= \langle (\partial V / \partial x)^2 \rangle_{00} = \frac{1}{3} \langle (\nabla V)^2 \rangle_{00} = \frac{1}{3} \int \frac{e^4}{r^4} \psi_0^2 4\pi r^2 dr. \quad (21) \end{aligned}$$

This integral diverges at $r=0$ as dr/r^2 if ψ_0 refers to an s state. If the angular momentum of the state ψ_0 is not zero, the integral is finite. Now since the average of $E_n - E_0$ is infinite (for an s state), it is understandable that the average of $\ln(E_n - E_0)$ is large.

Further information can be obtained from the asymptotic behavior of the oscillator strength f , given by Eq. (10), for large frequencies; this is, considering (14):

$$\nu^2 df = (8/3\pi) \nu^{-3/2} d\nu = (16/3\pi) dn. \quad (22)$$

This shows that already the average of $\nu^{3/2} \sim (E_n - E_0)^{3/2}$, with the weight factor $\nu^2 df$, is infinite. The small contribution of the discrete transitions (Table II) is further evidence.

The most concrete picture is obtained from Fig. 1 in which $\frac{3}{2} \nu^2 df / d\nu$ is plotted against $\log \nu$. The maximum of the curve is seen to come at $\nu=7$ which is reasonably high, and the curve falls off much more slowly towards higher than towards lower ν . The required average $\log k_0$ is simply the center of gravity of the curve of Fig. 1, and a value of 16.6 for k_0 looks entirely reasonable.

It is easy to obtain simple analytic estimates of $\ln k_0$. This can be done by approximating the exact oscillator strength (10) by a simpler expression which can be easily integrated. Since we know already that the high frequencies are the most important, the simpler expression must be a close approximation to f at the high frequency end but need not be so for low frequencies. The simplest approximation is to set

$$dG \equiv \frac{3}{2} \nu^2 df = (8/\pi) dn e^{-an}, \quad (23)$$

which agrees with (22) for small n , and to choose a in such a way that the integral of (23) over all n is unity as it must be according to (7). This gives

$$(8/\pi) \int_0^\infty dn e^{-an} = (8/\pi a) = 1. \quad (24)$$

Then the average of $\ln \nu$ becomes

$$\begin{aligned} \ln(k_0/\text{Ry}) &= \langle \ln \nu \rangle = -2 \langle \ln n \rangle = -2a \int dn e^{-an} \ln n \\ &\equiv 2(\ln a + C) = 2(\ln(8/\pi) + C), \quad (25) \end{aligned}$$

where C is Euler's constant. Inserting numerical values, we get

$$\ln(k_0/\text{Ry}) = 3.026, \quad k_0 = 20.6 \text{ Ry}, \quad (26)$$

which is slightly larger than the correct values

$$\ln(k_0/\text{Ry}) = 2.812, \quad k_0 = 16.65 \text{ Ry}. \quad (27)$$

This simple calculation therefore gives the correct order of magnitude for k_0 .

To get a closer approximation, we consider the asymptotic behavior of f in more detail. Expanding (10) in a power series in n , but keeping the power series in the denominator, one gets

$$\begin{aligned} dG \equiv \frac{3}{2} \nu^2 df &= \frac{(8/\pi)dn}{1 + \pi n + (\frac{2}{3}\pi^2 - 2\frac{1}{4})n^2 + \dots} \\ &= \frac{(8/\pi)dn}{1 + 3.14n + 4.33n^2 + \dots}. \end{aligned} \quad (28)$$

The exponential in (23) gives instead

$$\begin{aligned} dG \equiv \frac{3}{2} \nu^2 df &= \frac{(8/\pi)dn}{1 + (8/\pi)n + 32\pi^{-2}n^2 + \dots} \\ &= \frac{(8/\pi)dn}{1 + 2.55n + 3.24n^2 + \dots}. \end{aligned} \quad (29)$$

Obviously, this expression falls off too slowly with increasing n . This error is compensated by a too-rapid decrease for very large n : Actually, g should behave as $d\nu \sim n^{-3}dn$ for $n \rightarrow \infty$, whereas (23) gives an exponential decrease. It is therefore understandable that (23) gives too high a value for the average $\ln k_0$.

To improve on the behavior for small n , we choose

$$dG = \frac{(8/\pi)dn}{(1+an)^{k+1}} \quad (30)$$

and determine the two constants a and k so that the linear term in n in the denominator of (28) is correctly given, as well as the integral. The latter condition requires

$$ka = 8/\pi. \quad (31)$$

The former condition gives

$$(k+1)a = \pi. \quad (32)$$

The solution is

$$k = 8/(\pi^2 - 8) = 4.279, \quad a = (\pi^2 - 8)/\pi = 0.5951. \quad (33)$$

The average of $-\ln n$ is then

$$\begin{aligned} -\langle \ln n \rangle &= \ln a + \int \frac{kadn}{(1+an)^{k+1}} \ln an \\ &= \ln a + \Psi(k-1) - \Psi(0) \end{aligned} \quad (34)$$

where $\Psi(n)$ is the logarithmic derivative of the factorial function, i.e. of $\Gamma(n+1)$ (Jahnke-Emde's definition). With our numerical values

$$\begin{aligned} \ln(k_0/\text{Ry}) = \langle \ln \nu \rangle &= -2\langle \ln n \rangle = 2.7818 \\ k_0 &= 16.148. \end{aligned} \quad (35)$$

This is very close to the correct values (27), and somewhat smaller. Expansion of (30) for small n gives

$$\begin{aligned} g &= \frac{(8/\pi)dn}{1 + (k+1)an + \frac{1}{2}(k+1)ka^2n^2 + \dots} \\ &= \frac{(8/\pi)dn}{1 + \pi n + 4n^2 + \dots}, \end{aligned} \quad (36)$$

which is rather close to the correct expression (28), even in the quadratic term. (36) is still above (28) for small n , so that we might still have expected a too large result for $\ln k_0$; it seems that the curve of (30) crosses the correct curve (10) three times.

These calculations make the large value of the average excitation potential appear plausible. Moreover, they make it likely that k_0 is nearly independent of the principal quantum number: The asymptotic expression for the oscillator strength for small n , including terms of relative order n , is independent of n_0 , except for a factor n_0^{-3} which also occurs in the sum rule (7). Therefore, all the information we used in determining the constants a and k in (30) is independent of n_0 , and the estimate (36) applies to all values of n_0 .