see pages 272 and 299 for lowest order results

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Radiative Level Shifts, I. Formulation and Lowest Order Lamb Shift*

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In a series of papers, we shall develop and apply formal operator techniques for radiative level shift calculations. This first paper is concerned with the general formulation of the method and its application to the evaluation of the lowest order Lamb shift. An effort has been made to keep it pedagogically coherent, and a detailed review of the various theoretical contributions and comparison with experiment has been included.

I. INTRODUCTION

Since the experimental discovery of the Lamb shift in 1947 (*1*) and the very accurate measurements of the hyperfine structure in hydrogen (*2*), the theoretical calculation of radiative corrections to bound state energy levels has undergone constant refinement, both in the sophistication of the approach and the degree of accuracy attained (*3–5*). In fact, to workers on this type of problem, it is quite obvious that increased sophistication is necessary in the progress toward greater accuracy. Analytical techniques that are adequate barely to attain a given degree of approximation are generally hopelessly cumbersome at the next level of approximation.

The dimensionless parameters which one encounters in the calculation of the

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Lamb shift are the fine structure constant α, the strength of the Coulomb potential $Z\alpha$, the ratio of electron and nuclear masses m/M, and the ratio of nuclear and atomic sizes, R/a_0. In the present paper, we shall be concerned with the calculation of the one photon contributions to the Lamb shift (one power of α) as a function of $Z\alpha$, with the nucleus treated as a fixed Coulomb potential ($m/M \to 0$ and $R/a_0 \to 0$). The two photon contributions (*6–8*) and the effects of a finite nucleus (*9*, *10*) have been calculated previously to sufficient accuracy for the experiments.

In most of the early work, and in the present work as well, one is interested in the level shifts in light nuclei, and hence the Lamb shift is expanded in a series whose terms are successively smaller for small $Z\alpha$. Unlike the unshifted energy levels themselves, this is not simply a power series in $(Z\alpha)^2$, but is found to take the form

$$\Delta E_n = \frac{4}{3\pi n^3}\alpha mc^2 \{[C_{41} \ln (Z\alpha)^{-2} + C_{40}](Z\alpha)^4 + C_5(Z\alpha)^5 + [C_{62} \ln^2 (Z\alpha)^{-2} + C_{61} \ln (Z\alpha)^{-2} + C_{60}] (Z\alpha)^6 + \cdots\}. \tag{1.1}$$

The main dependence on the quantum numbers of the state is given by δ_{l0}/n^3 since, except for small "state-dependent" parts of C_{40}, C_{61}, and C_{60}, the coefficients in (1.1) are independent of the principal quantum number n and vanish for orbital angular momentum quantum number $l \neq 0$. In this and the following paper, we calculate a dominant part of C_{60} and the complete state-dependence of C_{61} and verify previous calculations of the lower order coefficients C_{41}, C_{40}, C_5, and C_{62} and of the $n = 1, 2$ parts of C_{61}. Another purpose of the present work is to give a clear exposition of the origin of the various terms and an indication of how one could, in principle, proceed systematically to higher orders.

The earliest calculations (*3*) were concerned with the lowest order terms, C_{40} and C_{41}. The logarithmic dependence on $Z\alpha$ and the major part of C_{40} can be related to the logarithmic infrared divergence which occurs in the scattering of an electron. In the bound state problem there is not an actual divergence because the emission and absorption of very soft virtual photons is suppressed by the binding effects. However, the earliest treatments of this infrared divergent behavior introduced complications. In some cases, the calculation had to be split into various parts, each of which was separately infrared divergent and had to be regulated by introducing a photon mass λ, which ultimately cancelled out. In other cases, the region of the virtual photon energy was split into a soft and a hard part which were treated by separate approximations; when added, the upper cutoff on the soft part cancelled the lower cutoff of the hard part. The actual calculation of C_{41} can be done analytically; it yields simply

$$C_{41} = \delta_{l0}. \tag{1.2}$$

A large part of the C_{40} term may also be calculated analytically, but a complete evaluation requires numerical calculation of the so-called Bethe sum (*3*, *11*).

The lowest order contributions arise entirely from nonrelativistic intermediate states, so the earliest calculations made nonrelativistic approximations at the earliest possible stage. The next task was to calculate C_5 terms. These terms have a relativistic origin; i.e., they arise from intermediate states in which the electron has relativistic momentum (of order mc) or is closer to the nucleus than an electron Compton wavelength. Their evaluation required a more careful and detailed formulation of the problem. Karplus, Klein, and Schwinger (*4*) (hereinafter referred to as KKS) calculated the energy shift by using formal operator techniques to evaluate the mass operator in the bound state. Baranger, Bethe and Feynman (*4*), in order to use techniques developed by Feynman for scattering problems, separated the energy shift into parts which were separately infrared divergent and later recombined them. Neither of these methods was particularly straightforward, and they have not been extended to higher orders. The result for C_5 is

$$C_5 = 3\pi[1 + {}^{11}\!/_{128} - {}^{1}\!/_{2}\ln 2 + {}^{5}\!/_{192}]. \tag{1.3}$$

In an attempt to find a more direct method of expanding the Lamb shift in powers of $Z\alpha$, Fried and Yennie (*12*) expanded the electron propagator part of the mass operator in powers of the potential. The method was not as convenient as had been hoped, for in each term of the expansion a spurious contribution of too low an order appeared. These could be eliminated by proper choice of the photon gauge, but the method still proved rather cumbersome. Nevertheless, it was possible to calculate the coefficient (*5*)

$$C_{62} = -{}^{3}\!/_{4}. \tag{1.4}$$

Work along a similar line was pursued by Layzer (*5*), who showed that the nonanalytic terms in $(Z\alpha)^2$ (such as $\ln(Z\alpha)^{-2}$ terms or ones which are odd powers of $Z\alpha$) could be picked out rather straightforwardly. He was able to obtain both C_{62} and

$$C_{61} = \begin{Bmatrix} 7\ln 2 - {}^{71}\!/_{80} & 1S_{1/2} \\ 4\ln 2 + {}^{63}\!/_{40} & 2S_{1/2} \\ {}^{103}\!/_{240} & 2P_{1/2} \\ {}^{29}\!/_{240} & 2P_{3/2} \end{Bmatrix}. \tag{1.5}$$

The aim of the present work is to reduce the Lamb shift operator systematically to parts each of which contributes only to a single term in (1.1). The general reduction resembles that of KKS (*4*) most closely, but the detailed techniques

are somewhat different in that KKS expressed the electron and photon propagators as integrals of exponentials and used operator tricks involving products of exponentials, while we leave the propagators as denominators and use operator tricks involving products of operators in numerators and denominators. The initial steps of our reduction are then quite in parallel to Feynman's treatment of mass renormalization (*3*). As terms of each order are extracted, the residues of course become lengthier and more complicated. However, the present method apparently is more compact than previous methods, permitting easier identification of the terms of each order.

In a calculation such as this one, there are different procedures for expanding the original Lamb shift operator so as to leave residues of higher and higher order. Basically one tries to make an expansion which is a power series in the ratio of a small operator to a large one. But since the operators we deal with are all unbounded, the meaning of the terms large and small vary with the situation, which usually emphasizes one of two different regions. The nonrelativistic region is characterized by energies of the order of the binding energy $\epsilon = (Z\alpha)^2 mc^2/2n^2$ and distances of the order of the Bohr radius $a_0 = \hbar/Z\alpha mc$, while the relativistic region is characterized by energies of the order of the rest energy mc^2 and distances of order of the electron Compton wavelength $\hbar/mc$. The effective order of magnitude of a given operator depends on which region is more important in each given situation, and in general, as the expansions are made, the contributions shift back and forth between the two regions. In trying to keep the calculation simple, one guiding principle we have followed is to avoid false expansions, i.e., expansions which leave a residue of the same order. A straightforward expansion in powers of V is such a false expansion in nonrelativistic situations since the essential expansion parameter $mV/(p^2 + 2m\epsilon)$ is then of order unity. Our guiding principle may be modified whenever it leads to a structure which is unnecessarily awkward to handle; but, in general, the requirement of simplicity seems to be satisfied by avoiding false expansions.

A careful consideration of the orders of magnitude involved in the various regions enables us to locate higher order terms in a straightforward manner. In this way, we can determine the terms contributing to C_{60}, the most important coefficient after those already listed here. Although its exact calculation would require the numerical calculation of terms like the Bethe sum in C_{40}, a good estimate is obtained from certain leading terms which are found to dominate the result. The present experimental accuracy does not seem to warrant the massive program required to complete the calculation of C_{60}.

There is a brief pedagogical point which should be mentioned. The most direct previous derivation of the lowest order terms in (1.1), that of KKS (*4*), seems to have been largely overlooked by the textbooks since it was embedded in a calculation of the higher order coefficient C_5. The present derivation is more

direct in that the exponentiation of KKS is avoided, although a λ integration is retained and a symmetric insertion notation introduced to make the higher order calculation more tractable than it would be in a derivation devoted to the minimization of the path to the lowest order results. We have, however, made every effort to arrange this paper so that it will be comprehensible to those readers interested in the Lamb shift calculation at a "textbook" level as well as to those wishing to understand the higher order corrections. To this end, we have left the higher order calculations to the second paper, and have also set off in square brackets certain passages which can be skipped without confusion.

The material to be discussed in this series of papers has been split up in the following way. The present paper (I) gives the initial considerations in the reduction of the level shift operator in Section II, the evaluation of the lowest order contributions to the Lamb shift in Section III, and a discussion of the present status of theory and experiment in Section IV. Paper II (*13*) treats the higher order corrections in detail. Section V gives a general discussion of the order of magnitude of different terms, and terms contributing to the coefficients listed in (1.1) are identified in Section VI and Section VII, and the complete higher order calculation is summarized in Section VIII. Paper III (*14*) applies the same techniques to the hyperfine structure calculation, starting with the results of Section II of the present paper.

II. PRELIMINARY DECOMPOSITION

Quantum electrodynamics leads in lowest order to two types of radiative corrections to the energy levels of an electron bound in an external electromagnetic potential. These are illustrated graphically in Fig. 1. The *vacuum polarization* contribution corresponding to Fig. 1(a) has been computed in detail (*15*) and will not be discussed here, except that the results are included in the final formulas. In the present work, we are interested in the dominant *self-energy* contribution of Fig. 1(b) along with its associated mass correction Fig. 1(c).

Our starting point is the formal expression for the energy shift in the state $|n\rangle$:

$$\Delta E_n = \frac{\alpha}{4\pi^3}\int \frac{d^4k/i}{k^2}\left\langle n\left|\gamma_\mu \frac{1}{\boldsymbol{\Pi} - \boldsymbol{k} - m}\gamma^\mu\right|n\right\rangle - \delta m\,\langle n \mid n\rangle. \qquad (2.1)$$

Aside from the factor $(\boldsymbol{\Pi} - \boldsymbol{k} - m)^{-1}$, which represents the electron propagator in the external potential in operator form, the meaning of the symbols is generally familiar; notation will be presented in greater detail below. Actually, this expression gives a complex result for ΔE_n . It is understood that the denominators in the integral each have a small positive imaginary part; the resulting imaginary part of ΔE_n represents the decay rate of the state $|n\rangle$ through photon emission. The complex energy shift then gives us the location of a pole in the

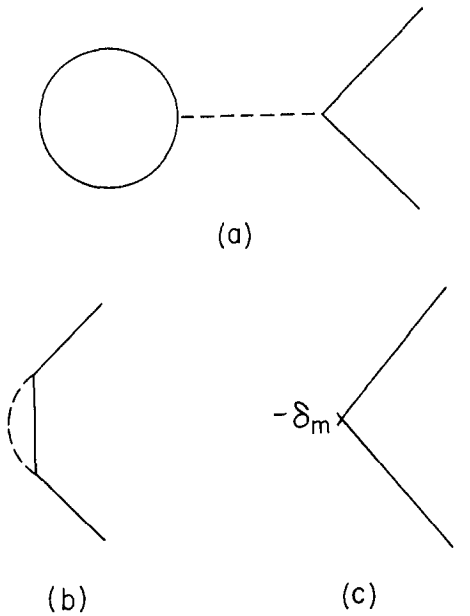

FIG. 1. Feynman graphs representing lowest order contributions to radiative level shifts.

complex energy plane corresponding to a resonance in photon scattering from the hydrogen atom. The Lamb shift refers to the real part of the shift. Further discussion of the relationship of the complex energy shift to an actual experimental measurement of the shift is contained in a paper by F. Low (*16*).

The purpose of our study is to reduce this formal expression to an expansion of the form (1.1). This will prove to be a rather involved procedure since $\mathbf{H}$ is an unbounded operator and hence cannot be assigned any definite order of magnitude. Nevertheless, our reduction procedure can frequently be guided by assigning orders of magnitude in certain situations. For example, if we know that a certain contribution is dominated by the nonrelativistic region of electron integration, we estimate its order of magnitude by making the "nominal" order of magnitude assignments

$$\begin{aligned} \mathbf{p} &= O\,(Z\alpha mc) \\ V &= O\,(Z^2\alpha^2 mc^2) \end{aligned} \qquad \text{(nonrelativistic)}. \tag{2.2}$$

where $\mathbf{p}$ and V are respectively the momentum and potential operators. On the other hand, if we know that it is the small distance or high momentum region of electron integration which is more important, we say we are in the relativistic region and make the order estimates

$$\begin{aligned} \mathbf{p} &= O\,(mc) \\ V &= O\,(Z\alpha mc^2). \end{aligned} \qquad \text{(relativistic)} \tag{2.3}$$

Although these estimates are usually reliable, it is to be emphasized that they are only a qualitative guide and their validity must always be verified by a more careful calculation.

NOTATION

The bound state $|n\rangle$ satisfies the Dirac equation[1]

$$(\mathbf{\Pi} - m)|\, n\rangle = 0 \quad \text{and} \quad \langle n\,|(\mathbf{\Pi} - m) = 0 \tag{2.4}$$

where $\langle n\,|$ represents the Dirac adjoint vector (in the usual notation $\langle n\,| = \psi_n{}^{+}\beta = \bar{\psi}_n$) rather than the Hermitian conjugate vector. The "mechanical" momentum Π^μ is the gauge invariant combination

$$\Pi^\mu = (p^\mu - eA^\mu) \tag{2.5a}$$

where A^μ is the external electromagnetic potential

$$A^\mu(\mathbf{x}) \equiv (\varphi(\mathbf{x}), \mathbf{A}(\mathbf{x})) \tag{2.5b}$$

and

$$p^\mu \equiv (E_n\,, \mathbf{p}). \tag{2.5c}$$

E_n is the total energy of the state $|n\rangle$; in terms of the binding energy ϵ_n (reckoned positive), it is

$$E_n = m - \epsilon_n\,. \tag{2.5d}$$

It should be kept in mind that Π_0 depends on the state $|n\rangle$ through its energy.

The matrix element occurring in the integral of (2.1) is a shorthand for expressions that could be written out more explicitly in the coordinate or momentum representations

$$\left\langle n \left| \gamma_\mu \frac{1}{\mathbf{\Pi} - \boldsymbol{k} - m} \gamma^\mu \right| n \right\rangle \tag{2.6a}$$

$$= \int d^3x\, d^3x'\, \bar{\psi}_n(\mathbf{x})\gamma_\mu \left\langle \mathbf{x} \left| \frac{1}{\mathbf{\Pi} - \boldsymbol{k} - m} \right| \mathbf{x}' \right\rangle \gamma^\mu \psi_n(\mathbf{x}')$$

$$= \int d^3p\, d^3p'\, \bar{\psi}_n(\mathbf{p})\gamma_\mu \left\langle \mathbf{p} \left| \frac{1}{\mathbf{\Pi} - \boldsymbol{k} - m} \right| \mathbf{p}' \right\rangle \gamma^\mu\, \psi_n(\mathbf{p}') \tag{2.6b}$$

[1] The charge and mass of the electron are e and m, and natural rationalized units are used, so $\hbar = c = 1$ and $\alpha = e^2/4\pi\hbar c \approx 1/137$. The Dirac matrices are defined by $\gamma^\mu \equiv (\gamma_0\,, \boldsymbol{\gamma}) \equiv (\beta, \beta\boldsymbol{\alpha})$, so they satisfy the anticommutation relations $\{\gamma_\mu\,, \gamma_\nu\} = 2g_{\mu\nu}$, where the metric $g_{\mu\nu}$ has only diagonal elements $(+1, -1, -1, -1)$. Repeated Greek indices are summed from 0 to 3, Latin indices from 1 to 3. Scalar products are denoted by $A\cdot B \equiv g_{\mu\nu}A^\mu B^\nu = A_0B_0 - \mathbf{A}\cdot\mathbf{B}$ for two four-vectors, $A^\mu = (A_0\,, \mathbf{A})$, and by $\boldsymbol{A} \equiv \gamma\cdot A \equiv g_{\mu\nu}\gamma^\mu A^\nu = \gamma_0 A_0 - \boldsymbol{\gamma}\cdot\mathbf{A}$ for a four-vector and the Dirac matrices. We define the antisymmetric Dirac tensor $[\gamma^\mu, \gamma^\nu] \equiv 2i\sigma^{\mu\nu}$, which will be coupled to the commutator $[\Pi_\mu\,, \Pi_\nu] = -ieF_{\mu\nu}$, where $F_{\mu\nu} \equiv \partial_\mu A_\nu - \partial_\nu A_\mu$ is the electromagnetic field tensor. Since Π is not available in boldface italics, we will use the special notation $\mathbf{\Pi} = \gamma\cdot\Pi \equiv \boldsymbol{p} - e\boldsymbol{A}$ and will not use Π as a three-vector except as Π_i or $\mathbf{p} - e\mathbf{A}$.

where the wave functions in either representation are displayed explicitly. In the coordinate representation, the electron propagation from $\mathbf{x}'$ to $\mathbf{x}$ is given by

$$\left\langle \mathbf{x} \left| \frac{1}{\boldsymbol{\Pi} - \boldsymbol{k} - m} \right| \mathbf{x}' \right\rangle = e^{i\mathbf{k}\cdot\mathbf{x}} \left\langle \mathbf{x} \left| \frac{1}{\boldsymbol{\Pi} - \gamma_0 k_0 - m} \right| \mathbf{x}' \right\rangle e^{-i\mathbf{k}\cdot\mathbf{x}'} . \tag{2.6c}$$

The right side of this equation is seen to be plane wave factors representing the emission and absorption of the photon times the usual propagator of an electron of energy $E_n - k_0$ from $\mathbf{x}'$ to $\mathbf{x}$ in an external field. Corresponding remarks could be made about the propagator in the momentum representation. The propagator could be evaluated as a power series in the potential in either representation by using

$$\frac{1}{\boldsymbol{\Pi} - \boldsymbol{k} - m} = \frac{1}{\boldsymbol{p} - \boldsymbol{k} - m} + \frac{1}{\boldsymbol{p} - \boldsymbol{k} - m} e\boldsymbol{A} \frac{1}{\boldsymbol{p} - \boldsymbol{k} - m} + \cdots . \tag{2.7}$$

However, this suffers from the disadvantage of destroying gauge invariance term by term and it does not lead in a straightforward way to an expansion in powers of $Z\alpha$ (*5*, *12*). We shall avoid this expansion in our initial reduction and employ it only at the last stages of calculation where it either gives a legitimate expansion of the type (1.1) or is unavoidable.

We now proceed to the reduction of (2.1). As far as possible, we will use the same methods as would be used in the calculation of the self-energy of a free particle. Among other things, this will facilitate the identification of the part of the self-energy associated with the mass renormalization. In addition it seems to be the best way to avoid spurious expansions in the initial steps of the reduction. As a preliminary step, we regularize the photon propagator,

$$\frac{1}{k^2} = \lim_{\Lambda\to\infty} \left[\frac{1}{k^2} - \frac{1}{k^2 - \Lambda^2} \right] = \lim_{\Lambda\to\infty} \int_0^{\Lambda^2} \frac{-dL}{(k^2 - L)^2} , \tag{2.8}$$

so that later manipulations of the k integrations will be valid. Next, the bound electron propagator is formally rationalized,

$$\frac{1}{\boldsymbol{\Pi} - \boldsymbol{k} - m} = \frac{\boldsymbol{\Pi} - \boldsymbol{k} + m}{(\boldsymbol{\Pi} - \boldsymbol{k})^2 - m^2} = \frac{\boldsymbol{\Pi} - \boldsymbol{k} + m}{k^2 - 2k\cdot\Pi + \boldsymbol{\Pi}^2 - m^2} \tag{2.9}$$

and the resulting denominator is combined in the usual way with the regularized photon propagator,

$$\begin{aligned} &\frac{-1}{(k^2 - L)^2} \frac{1}{k^2 - 2k\cdot\Pi + \boldsymbol{\Pi}^2 - m^2} \\ &\qquad = \int_0^1 \frac{2(1 - z)\, dz}{[(1 - z)\, L - k^2 + z(2k\cdot\Pi - \boldsymbol{\Pi}^2 + m^2)]^3} . \end{aligned} \tag{2.10}$$

We thus have

$$\frac{1}{k^2}\frac{1}{\boldsymbol{\Pi}-\boldsymbol{k}-m}=\lim_{\Lambda\to\infty}2\int_0^1 dz\int_0^{(1-z)\Lambda^2} dK\,\frac{\boldsymbol{\Pi}-\boldsymbol{k}+m}{D^3}$$
$$=2\int_0^1 dz\int_0^{\infty} dK\,\frac{\boldsymbol{\Pi}-\boldsymbol{k}+m}{D^3} \tag{2.11a}$$

where we have transformed to a new variable of integration for regularization,

$$K=(1-z)L, \tag{2.11b}$$

whose upper limit, $(1-z)\Lambda^2\to\infty$, will be kept finite only when an explicit divergence is encountered. The denominator combination

$$D=K-k^2+2zk\cdot\Pi-z\boldsymbol{\Pi}^2+zm^2 \tag{2.12a}$$

may be rearranged and written as

$$D=z^2m^2+K-(k-z\Pi)^2+z(1-z)H-z^2M \tag{2.12b}$$

where (see footnote 1)

$$M=\boldsymbol{\Pi}^2-\Pi^2=\tfrac{1}{2}e\sigma^{\mu\nu}F_{\mu\nu}=e[\boldsymbol{\sigma}\cdot\mathfrak{IC}-i\boldsymbol{\alpha}\cdot\mathfrak{E}] \tag{2.13}$$

is the magnetic moment operator, and

$$H\equiv m^2-\boldsymbol{\Pi}^2=(m+\boldsymbol{\Pi})(m-\boldsymbol{\Pi}) \tag{2.14}$$

is the second order Dirac operator, which vanishes when acting on the given state vector, $|n\rangle$ or $\langle n|$.

For convenience, the ambiguous operator notation

$$\frac{\boldsymbol{\Pi}-\boldsymbol{k}+m}{D^3}$$

has been used, since the numerator and denominator commute and can thus be written in either order. This commutativity does not hold when the numerator terms are separated, so a definite order of the operators must then be taken. We will use the average of the two orders,

$$\frac{\boldsymbol{\Pi}-\boldsymbol{k}+m}{D^3}\equiv\frac{1}{2}\left\{(\boldsymbol{\Pi}-\boldsymbol{k}+m)\frac{1}{D^3}+\frac{1}{D^3}(\boldsymbol{\Pi}-\boldsymbol{k}+m)\right\}$$
$$\equiv\frac{1}{2}\left\{(\boldsymbol{\Pi}-\boldsymbol{k}+m),\quad\frac{1}{D^3}\right\}, \tag{2.15}$$

throughout the calculation, although for brevity usually only one order will be indicated. Thus, we may completely reverse the order of all the operators in any given term, since either order implies the average with the other order.

Before proceeding with the discussion of the reduction of our operator, it will prove convenient to introduce a shorthand for dealing with products

$$N_1 \frac{1}{D} N_2 \frac{1}{D} \cdots N_r \frac{1}{D} N_{r+1} \tag{2.16}$$

of "numerators," N_i, and "denominators," D^{-1}. A double bar notation will be used to indicate that subsequent factors are to be symmetrically inserted:

$$\begin{aligned} N_1 \frac{1}{D} N_2 \frac{1}{D} \cdots N_r \frac{1}{D} N_{r+1} \Big\| \frac{A}{D} &= N_1 \frac{1}{D} A \frac{1}{D} N_2 \frac{1}{D} \cdots N_r \frac{1}{D} N_{r+1} \\ &+ N_1 \frac{1}{D} N_2 \frac{1}{D} A \frac{1}{D} \cdots N_r \frac{1}{D} N_{r+1} + N_1 \frac{1}{D} N_2 \frac{1}{D} \cdots N_r \frac{1}{D} A \frac{1}{D} N_{r+1}; \end{aligned} \tag{2.17}$$

any of the N_i or A may be unity. In the following, N/D will denote a sum of terms of the form (2.16); $(N/D)\| AD^{-1}$ may accordingly be defined as the sum of insertions, as in (2.20a).

The *raison d'être* of the notation is the formulas for the differentiation or commutation of expressions of the form (2.16):

$$\frac{d}{d\lambda} \frac{N}{D} = \frac{dN/d\lambda}{D} - \frac{N}{D} \Big\| \frac{dD/d\lambda}{D}; \tag{2.18a}$$

$$\left[C, \frac{N}{D}\right] = \frac{[C, N]}{D} - \frac{N}{D} \Big\| \frac{[C, D]}{D}. \tag{2.18b}$$

In both (2.18a) and (2.18b), the first term in the right hand side represents the sum of terms in which each N_i separately is replaced by the indicated numerator, as should be clear from an example:

$$\begin{aligned} \frac{d}{d\lambda}\left(\frac{1}{D} M \frac{1}{D} N \frac{1}{D}\right) &= \left(\frac{1}{D} \frac{dM}{d\lambda} \frac{1}{D} N \frac{1}{D} + \frac{1}{D} M \frac{1}{D} \frac{dN}{d\lambda} \frac{1}{D}\right) \\ &- \left(\frac{1}{D} \frac{dD}{d\lambda} \frac{1}{D} M \frac{1}{D} N \frac{1}{D} + \frac{1}{D} M \frac{1}{D} \frac{dD}{d\lambda} \frac{1}{D} N \frac{1}{D} + \frac{1}{D} M \frac{1}{D} N \frac{1}{D} \frac{dD}{d\lambda} \frac{1}{D}\right) \end{aligned}$$

Since $(N/D)\| AD^{-1}$ is again a sum of terms of the form (2.16), we may insert other factors, define

$$\frac{N}{D} \Big\| \frac{A}{D} \frac{B}{D} \equiv \left(\frac{N}{D} \Big\| \frac{A}{D}\right) \Big\| \frac{B}{D} \tag{2.19}$$

and note that the usual additive, associative, and distributive laws of differentiation hold:

$$\left(\frac{N}{D} + \frac{M}{D}\right) \Big\| \frac{A}{D} = \frac{N}{D} \Big\| \frac{A}{D} + \frac{M}{D} \Big\| \frac{A}{D}; \tag{2.20a}$$

$$\frac{N}{D}\Big\|\frac{A+B}{D}=\frac{N}{D}\Big\|\left(\frac{A}{D}+\frac{B}{D}\right)=\frac{N}{D}\Big\|\frac{A}{D}+\frac{N}{D}\Big\|\frac{B}{D}; \tag{2.20b}$$

$$\left(\frac{N}{D}\frac{M}{D}\right)\Big\|\frac{A}{D}=\left(\frac{N}{D}\Big\|\frac{A}{D}\right)\frac{M}{D}+\frac{N}{D}\left(\frac{M}{D}\Big\|\frac{A}{D}\right). \tag{2.20c}$$

Repeated insertions

$$\frac{1}{D}\Big\|\frac{1}{D}\cdots(r\text{ times})\cdots\frac{1}{D}\equiv\frac{1}{D}\Big\|\frac{1}{D^r}=\frac{r!}{D^{r+1}} \tag{2.21}$$

give a factorial which appears in infinite expansions

$$\frac{N}{D-x}=\sum_{r=0}^{\infty}\frac{1}{r!}\frac{N}{D}\Big\|\left(\frac{x}{D}\right)^r \tag{2.22}$$

but cancels other factorials in integrations such as

$$\int_0^\infty dK\,\frac{N}{K+D}\Big\|\frac{1}{K+D}=\int_0^\infty dK\left(-\frac{d}{dK}\frac{N}{K+D}\right)=\frac{N}{D}. \tag{2.23}$$

Readers interested primarily in the lowest order calculation should be able to skip further details and pick up the discussion in the next subsection "Mass Renormalization".

If different denominators occur in an expression, they may be distinguished by different subscripts such as D_0 and D_1. Then an insertion without a subscript may be used to denote the sum of the different possible insertions

$$\Big\|\frac{A}{D}\equiv\Big\|\frac{A}{D_0}+\Big\|\frac{A}{D_1} \tag{2.24}$$

and we find that the various properties of symmetric insertion hold for $\| AD_0^{-1}$, $\| AD_1^{-1}$, $\| AD^{-1}$, or any combination of them. An exception is found in the commutativity of insertions and expansions, such as

$$\frac{1}{D_1}\Big\|\frac{A}{D}=\left(\frac{1}{D_0}+\frac{1}{D_0}\times\frac{1}{D_1}\right)\Big\|\frac{A}{D}=\left(\frac{1}{D_0}+\frac{1}{D_1}\times\frac{1}{D_0}\right)\Big\|\frac{A}{D} \tag{2.25}$$

with $D_1=D_0-x$, which holds for the sum of insertions (2.24) but not for either insertion alone. A particularly neat result is the cancellation of factorials in the denominator combining formula

$$\frac{1}{D_0}\frac{1}{D_1}\Big\|\frac{1}{D_0{}^r}\frac{1}{D_1{}^s}\frac{1}{D^t}=\int_0^1\frac{du}{D_u{}^2}\Big\|\left(\frac{1-u}{D_u}\right)^r\left(\frac{u}{D_u}\right)^s\left(\frac{1}{D_u}\right)^t \tag{2.26}$$

where $D_u\equiv uD_1+(1-u)D_0$ and D_0 and D_1 are assumed to commute. Perhaps the most useful property of symmetric insertion is its commutativity

$$\frac{N}{D}\left\|\frac{A}{D}\frac{B}{D}\right. = \frac{N}{D}\left\|\frac{B}{D}\frac{A}{D}\right. \tag{2.27}$$

regardless of whether or not N, A, B, and D commute.[2] This allows us to carry out commutation, differentiation, integration, or expansion (with due regard to the limitations on (2.25)) in any convenient sequence. Thus, for example, we start with three denominators

$$\frac{2}{D^3} = \frac{1}{D}\left\|\frac{1}{D^2}\right. \tag{2.28}$$

but may validly perform initial manipulations with only one denominator, leaving the insertion of the other two until later.

Mass Renormalization

Including mass renormalization, but not vacuum polarization, the energy shift to order α is now given by

$$\Delta E_n = \frac{\alpha}{4\pi}\int_0^1 dz \int_0^\infty dK \int \frac{d^4k}{\pi^2 i}\,\langle n \mid I \mid n\rangle - \langle n \mid \delta m \mid n\rangle, \tag{2.29a}$$

where

$$I = 2\gamma_\mu \frac{\boldsymbol{\Pi} - \boldsymbol{k} + m}{D^3}\gamma^\mu \tag{2.29b}$$

is an operator which must be rearranged into calculable forms. In order to identify the mass renormalization δm, we start with a free electron, for which ΔE_n must vanish. In this case there is no external field,

$$[\Pi_\mu, \Pi_\nu] = -ieF_{\mu\nu} = 0, \tag{2.30}$$

so the only noncommuting operators are the γ matrices. However, since now $M = 0$ and $H = m^2 - \Pi^2$, there are no longer any γ matrices in D, and those in the numerator in I may be contracted, giving us

$$\begin{aligned}\gamma_\mu(\boldsymbol{\Pi} - \boldsymbol{k} + m)\gamma^\mu &= -2\boldsymbol{\Pi} + 2\boldsymbol{k} + 4m \doteq 2m + 2\boldsymbol{k} \\ &\doteq 2(1+z)m + 2(\boldsymbol{k} - z\boldsymbol{\Pi}),\end{aligned} \tag{2.31}$$

since $\boldsymbol{\Pi} \doteq m$ acting on the wave function. If the photon momentum integration is shifted[3] to new variables k_μ' given by

$$k_\mu' = (k - z\Pi)_\mu, \tag{2.32}$$

[2] Note that only the insertions commute, and that we must not forget terms like $[C, N]/D$ in Eq. (2.18b).

[3] The shift is valid here since the amount of the shift, $z\Pi$, commutes with the rest of the denominator and the integrations are convergent (by regularization).

then the integration vanishes for the term odd in $\boldsymbol{k} - z\boldsymbol{\Pi} = \boldsymbol{k}'$. For the other term, the contour for the k_0' integration may be rotated in the usual way[4] to run up the imaginary axis, so that $k_0' = ik_4'$ and we have a Euclidean four-space, with

$$d^4k'/i = d^3k'\, dk_0/i = dk_1'\, dk_2'\, dk_3'\, dk_4' = \kappa^3\, d\kappa\, d\Omega_4\,, \tag{2.33a}$$

where

$$-k'^2 = -k_0'^2 + \mathbf{k}'^2 = k_4'^2 + k_1'^2 + k_2'^2 + k_3'^2 = \kappa^2 \tag{2.33b}$$

is the squared radial variable. The four-dimensional solid angle is $2\pi^2$, so the general k integration is found to be

$$\int \frac{d^4k/\pi^2 i}{A - k^2} \left\| \frac{1}{(A - k^2)^{r+2}} = \int_0^\infty \frac{\kappa^2\, d\kappa^2}{A + \kappa^2} \right\| \frac{1}{(A + \kappa^2)^{r+2}} = \frac{1}{A} \left\| \frac{1}{A^r}\right., \tag{2.33c}$$

which in the present case is

$$2\int \frac{d^4\, k'/\pi^2\, i}{[z^2\, m^2 + K - k'^2 + z(1 - z)H]^3} = \frac{1}{z^2\, m^2 + K + z(1 - z)H} \doteq \frac{1}{z^2\, m^2 + K}\,, \tag{2.34}$$

since H vanishes when acting on the wave function. Now, for a free electron, we have

$$\Delta E_n^{\text{free}} = 0 = \lim_{\Lambda\to\infty} \frac{\alpha}{4\pi} \int_0^1 dz \int_0^{(1-z)\Lambda^2} dK \left\langle n \left| \frac{2(1 + z)m}{z^2\, m^2 + K} \right| n \right\rangle - \langle n \mid \delta m \mid n \rangle$$

so that the mass renormalization must be

$$\delta m = \lim_{\Lambda\to\infty} \frac{\alpha}{2\pi} \int_0^1 dz(1 + z)m \ln \frac{(1 - z)\Lambda^2}{z^2\, m^2} = \lim_{\Lambda\to\infty} \frac{3\alpha}{4\pi} \left(\ln \frac{\Lambda^2}{m^2} + \frac{1}{2}\right) m. \tag{2.35}$$

For a bound electron, it will prove convenient to carry out the subtraction of δm before, rather than after, integration. To do this, we simply subtract a "mass renormalization operator"

$$I_{\delta m} \equiv \frac{4(1 + z)m}{(z^2\, m^2 + K - k^2)^3} \tag{2.36a}$$

[4] The contour rotation is valid here because the singularities at

$$\pm k_0' = (z^2 m^2 + K + \mathbf{k}'^2)^{1/2} - i\epsilon$$

are not crossed and the contribution at infinity vanishes since the integration is convergent (by regularization).

from I, and calculate

$$\Delta E_n = \frac{\alpha}{4\pi}\int_0^1 dz \int_0^\infty dK \int \frac{d^4k}{\pi^2 i}\langle n \mid I - I_{\delta m} \mid n\rangle. \tag{2.36b}$$

REARRANGEMENT

The reduction of I for a bound electron will follow that for a free electron, but will yield additional terms. Thus, before contracting the numerator as in (2.31) to obtain

$$4\frac{(1+z)m}{D^3} + 4\frac{\boldsymbol{k} - z\,\boldsymbol{\Pi}}{D^3} \tag{2.37a}$$

we must bring one of the γ matrices through the denominators, obtaining terms

$$\begin{aligned}\gamma_\mu[\boldsymbol{\Pi} - \boldsymbol{k} + m][2/D^3, \gamma^\mu] = \gamma_\mu[(1-z)\boldsymbol{\Pi} + m](1/D)[\gamma^\mu, D] \\ \cdot(1/D)\|(1/D^2) - \gamma_\mu[\boldsymbol{k} - z\boldsymbol{\Pi}](1/D)[\gamma^\mu, D](1/D)\|(1/D^2)\end{aligned} \tag{2.37b}$$

which vanish for a free electron because they contain a factor of the field,

$$[\gamma^\mu, D] = [\gamma^\mu, -z\boldsymbol{\Pi}^2] = -2z[\Pi^\mu, \boldsymbol{\Pi}]. \tag{2.37c}$$

Since the nonrelativistic order of magnitude of the field

$$[\Pi_i, \Pi_0] = [p^i, V]$$

is $(Z\alpha)^3 m^2 c^3$, we would expect terms containing more powers of the field to be of higher order. This is found to be true, and an expansion of I in powers of the field will be seen in the following paper to yield an expansion of the form (1.1) for ΔE. Our general aim now, therefore, is to write such an expansion for I. In particular, the leading term has been seen to be $I_{\delta m}$, and the terms linear in the $F_{\mu\nu}$ will give the lowest order terms, of order $(Z\alpha)^4$, in the exapnsion (1.1). Terms containing more than one factor of the field contribute to the higher order calculations in the following paper and their discussion will be set off in square brackets ([ ]) in this paper.

The only term here which is nonvanishing for a free electron is the first term in (2.37a),

$$I_1(D) \equiv \frac{4(1+z)m}{D^3}. \tag{2.38}$$

This is the leading term in I, yielding a contribution of zeroth order in $Z\alpha$, which is cancelled by $I_{\delta m}$. It is easy to see that in the nonrelativistic region the complete denominator,

$$D = z^2m^2 + K - (k - z\Pi)^2 + z(1-z)H - z^2M,$$

(2.12b), differs from the free electron denominator

$$z^2m^2 + K - k^2 \equiv D_{00}$$

in $I_{\delta m}$ by terms of relative order $(Z\alpha)^2$. This would indicate that the leading order of the Lamb shift is proportional to $(Z\alpha)^2$. In fact these leading terms precisely cancel and the correct leading order is proportional to $(Z\alpha)^4$. One may get a rough idea of the reasons for this cancellation and the nature of the actual leading terms by observing the structure of D. It is noted that: (a) The $-z^2M$ term is of relative order $(Z\alpha)^4$ and hence causes no trouble. (b) The k integration could be shifted as in (2.32) if the amount of the shift, $z\Pi_\mu$, was still an operator which commuted with I. The correction thus involves the commutator $[\Pi_\mu, \Pi_\nu]$, which by itself contains a factor of $F_{\mu\nu}$, of order $(Z\alpha)^3$. We will label these terms "L," in contrast to the "M" term in (a). (c) Finally, if we can drop $-z^2M$ and let $(k - z\Pi)^2$ become k^2 to order $(Z\alpha)^2$, the operator H can act on the state $|n\rangle$ and vanish. At this stage, I_1 would be exactly cancelled out by $I_{\delta m}$. It is clear from the preceding discussion that the reduction must be handled very carefully in order not to introduce terms which are separately of too low an order. Such a poor reduction would be obtained, for example, by expanding D^{-1} in powers of A_μ, which would split H into two parts and lead to terms of order $(Z\alpha)^2$ whose sum would be zero (*12*).

The first step in the reduction of I_1 is clearly to expand in powers of the magnetic term $-z^2M$ in the denominator

$$D = D_1 - z^2M, \tag{2.39a}$$

where

$$D_1 \equiv z^2m^2 + K - (k - z\Pi)^2 + z(1 - z)H. \tag{2.39b}$$

Then, using (2.22) and (2.25) we find the remainder

$$I_1(D) - I_1(D_1) \equiv I_{M1} \equiv \sum_{r=1}^{\infty} \frac{4(1+z)m}{r!} \frac{1}{D_1^3} \Big\| \left(\frac{z^2M}{D_1}\right)^r \tag{2.40a}$$

$$= 2(1+z)m \frac{1}{D_1} z^2M \frac{1}{D_1} \Big\| \frac{1}{D_1^2} + 2(1+z)m \frac{1}{D_1} z^2M \frac{1}{D_1} z^2M \frac{1}{D_1} \Big\| \frac{1}{D_1^2} + \cdots, \tag{2.40b}$$

which is an explicit expansion in powers of the field.

The next step is to formally shift the k integration by letting the denominator become

$$D_0 = z^2m^2 + K - k^2 + z(1 - z)H. \tag{2.41}$$

As in (c) above, the resulting $I_1(D_0)$ then exactly cancels $I_{\delta m}$. The correction

for the formal shift from D_1 to D_0 could be handled by a straightforward expansion such as

$$\frac{1}{D_1} - \frac{1}{D_0} = \frac{1}{D_1}\left(-2zk\cdot\Pi + z^2\,\Pi^2\right)\frac{1}{D_0} \tag{2.42}$$

but this pedestrian approach seems to conceal the essential nature of the correction and to complicate the higher order terms since factors of $F_{\mu\nu}$ do not readily appear. It is preferable to consider D_1 and D_0 as a single denominator

$$D_\lambda \equiv z^2m^2 + K - (k - \lambda z\Pi)^2 + z(1-z)H \tag{2.43}$$

evaluated at $\lambda = 1$ and $\lambda = 0$, so that the shift correction may be expressed as the integral of a derivative,

$$\begin{aligned} I_1(D_1) - I_1(D_0) &= \int_0^1 d\lambda\,\frac{\partial}{\partial\lambda} I_1(D_\lambda) \\ &= -4(1+z)m\int_0^1 d\lambda\left\{\frac{1}{D_\lambda}\frac{\partial D_\lambda}{\partial\lambda}\frac{1}{D_\lambda^3} + \frac{1}{D_\lambda^2}\frac{\partial D_\lambda}{\partial\lambda}\frac{1}{D_\lambda^2} + \frac{1}{D_\lambda^3}\frac{\partial D_\lambda}{\partial\lambda}\frac{1}{D_\lambda}\right\} \\ &= -2(1+z)m\int_0^1 d\lambda\,\frac{1}{D_\lambda}\left(2zk\cdot\Pi - 2\lambda z^2\,\Pi^2\right)\frac{1}{D_\lambda}\left\|\frac{1}{D_\lambda^2}\right., \end{aligned} \tag{2.44}$$

a technique previously used by KKS (*4*). In any event, we find that I_1 has the most complicated higher order parts since it is the term which contains the very lowest order part, $I_{\delta m}$.

In (2.44), (2.37), and in later steps we encounter terms containing a factor of $k - z\Pi$ or $k - \lambda z\Pi$. These terms contain an implicit factor of the field since they vanish if the field vanishes, as may be seen by the following argument: the vanishing of these terms by symmetry in a shifted k_ν integration is prevented only by the noncommutativity of the shift; any commutator of the shift vanishes if the basic commutator $[\Pi_\nu, \Pi_\mu] = ieF_{\mu\nu}$ vanishes. In order to exhibit an explicit factor of the field, we may integrate by parts, using a formula analogous to but more general than Eq. (2.14) and (2.15) of KKS (*4*). We note that a perfect derivative such as

$$\frac{\partial}{\partial k^\nu}\frac{N}{D} = \frac{N}{D}\left\|\frac{2k_\nu - 2z\,\Pi_\nu}{D}\right. \tag{2.45}$$

will vanish when integrated over all k_ν; it is assumed here that N is independent of k and that the integration of N/D is convergent (by regularization). Thus, for a term in I with N independent of k, we always have an equivalence

$$\frac{N}{D}\left\|\frac{k_\nu}{D}\right. \doteq \frac{N}{D}\left\|\frac{z\,\Pi_\nu}{D}\right. \qquad \text{or} \qquad \frac{N}{D_\lambda}\left\|\frac{k_\nu}{D_\lambda}\right. \doteq \frac{N}{D_\lambda}\left\|\frac{\lambda z\,\Pi_\nu}{D_\lambda}\right.. \tag{2.46a, b}$$

We thus see that factors of $(k - z\Pi)_\nu$ may be reduced to commutators of $z\Pi_\nu$

(and then to fields) since the k_ν will cancel the $z\Pi_\nu$ in an integration by parts when the $z\Pi_\nu$ are commuted to symmetrically inserted positions.

Using this in the shift correction (2.44), we can write the derivative as a double commutator,

$$\begin{aligned}\frac{1}{D_\lambda}\frac{\partial D_\lambda}{\partial\lambda}\frac{1}{D_\lambda}\Big\|\frac{1}{D_\lambda^2} &= \frac{1}{D_\lambda}(2zk\cdot\Pi - 2\lambda z^2\,\Pi^2)\frac{1}{D_\lambda}\Big\|\frac{1}{D_\lambda^2}\\ &\doteq \frac{1}{D_\lambda}2z\,\Pi^\nu\frac{1}{D_\lambda}\Big\|\frac{\lambda z\,\Pi_\nu}{D_\lambda^2} - \frac{1}{D_\lambda}2\lambda z^2\,\Pi^2\frac{1}{D_\lambda}\Big\|\frac{1}{D_\lambda^2}\\ &= 2\lambda\frac{1}{D_\lambda}\left[z\,\Pi_\nu, \left[\frac{1}{D_\lambda}, z\,\Pi^\nu\right]\right]\frac{1}{D_\lambda}\Big\|\frac{1}{D_\lambda}\\ &= 2\lambda\frac{1}{D_\lambda}\left[z\,\Pi_\nu, \frac{1}{D_\lambda}\left[z\,\Pi^\nu, D_\lambda\right]\frac{1}{D_\lambda}\right]\frac{1}{D_\lambda}\Big\|\frac{1}{D_\lambda},\end{aligned} \tag{2.47a}$$

which shows explicitly that the validity of the shift depends on the commutativity of the amount shifted. Let us use the form

$$\int_0^1 d\lambda\,\frac{\partial}{\partial\lambda}I_1(D_\lambda) \doteq -4(1+z)z^2\,m\int_0^1 d\lambda^2\,\frac{1}{D_\lambda}\Pi_\nu\frac{1}{D_\lambda}[\Pi^\nu, D_\lambda]\frac{1}{D_\lambda^2}\Big\|\frac{1}{D_\lambda} \tag{2.47b}$$

which must be averaged with the reversed order to regain the double commutator. There are two parts to the commutator

$$\begin{aligned}-[\Pi^\nu, D_\lambda] &= -[\Pi^\nu, z(1-z)H] + [\Pi^\nu, (k-\lambda z\Pi)^2]\\ &= z(1-z)\{\mathbf{\Pi}, [\Pi^\nu, \mathbf{\Pi}]\} - \lambda z\{(k-\lambda z\Pi)_\mu, [\Pi^\nu, \Pi^\mu]\},\end{aligned} \tag{2.48}$$

the first due to the shift not commuting with H, and the second due to the shift not commuting with itself. In the first part the second order nature of H may be removed by bringing the anticommuted $\mathbf{\Pi}$ to the outside, where it becomes m, yielding a lowest order term of type "L,"

$$I_{L1} \equiv 8(1-z^2)\,z^3\,m^2\int_0^1 d\lambda^2\,\frac{1}{D_\lambda}\Pi_\nu\frac{1}{D_\lambda}[\Pi^\nu, \mathbf{\Pi}]\frac{1}{D_\lambda^2}\Big\|\frac{1}{D_\lambda}. \tag{2.49}$$

[The higher order corrections in the first part of (2.48) are for commuting the $\mathbf{\Pi}$ through Π_ν,

$$I_{a1} \equiv 4(1-z^2)\,z^3\,m\int_0^1 d\lambda^2\,\frac{1}{D_\lambda}[\Pi_\nu, \mathbf{\Pi}]\frac{1}{D_\lambda}[\Pi^\nu, \mathbf{\Pi}]\frac{1}{D_\lambda^2}\Big\|\frac{1}{D_\lambda}, \tag{2.50}$$

and through the four denominators,

$$\begin{aligned}I_b \equiv 4(1-z^2)z^3\,m\int_0^1 d\lambda^2\Big\{&\frac{1}{D_\lambda}\Pi_\nu\left[\frac{1}{D_\lambda}, \mathbf{\Pi}\right]\left[\Pi^\nu, \mathbf{\Pi}\right]\frac{1}{D_\lambda^2}\\ &+\left[\frac{1}{D_\lambda}, \mathbf{\Pi}\right]\Pi_\nu\frac{1}{D_\lambda}[\Pi^\nu, \mathbf{\Pi}]\frac{1}{D_\lambda^2} + \frac{1}{D_\lambda}\Pi_\nu\frac{1}{D_\lambda}[\Pi^\nu, \mathbf{\Pi}]\left[\mathbf{\Pi}, \frac{1}{D_\lambda^2}\right]\Big\}\Big\|\frac{1}{D_\lambda}.\end{aligned} \tag{2.51}$$

In the second part of (2.48), the contribution of the k_μ part may be rewritten as

$$-8(1+z)\,z^3\,m\int_0^1 d\lambda^2\,\lambda\,\frac{1}{D_\lambda}\,\Pi_\nu\,\frac{1}{D_\lambda}\,[\Pi^\nu,\,\Pi^\mu]\,\frac{1}{D_\lambda^2}\,\Big\|\,\frac{\lambda z\,\Pi_\mu}{D_\lambda}$$
$$=\,-4(1+z)\,z^4\,m\int_0^1 d\lambda^2\,\lambda^2\,\frac{1}{D_\lambda}\,\Pi_\nu\,\frac{1}{D_\lambda}\,[\Pi^\nu,\,\Pi^\mu]\,\frac{1}{D_\lambda}\,\Pi_\mu\,\frac{1}{D_\lambda}\,\Big|\,\frac{1}{D_\lambda} \tag{2.52}$$

by using (2.46) and then averaging with μ and ν interchanged and with the operator order reversed. Except for commuting Π_μ through a denominator, the contribution of one of the $\lambda z\Pi_\mu$ parts of (2.48) exactly cancels (2.52) and the contribution of the other part becomes

$$I_c \equiv 2(1+z)\,z^4\,m\int_0^1 d\lambda^2\,\lambda^2\,\frac{1}{D_\lambda}\,[\Pi_\nu\,,\,\Pi_\mu]\,\frac{1}{D_\lambda}\,[\Pi^\nu,\,\Pi^\mu]\,\frac{1}{D_\lambda^2}\,\Big\|\,\frac{1}{D_\lambda} \tag{2.53}$$

when averaged with μ and ν interchanged. The higher order corrections for commuting the Π_μ's through a denominator are

$$I_d \equiv 4(1+z)\,z^4\,m\int_0^1 d\lambda^2\,\lambda^2\Big\{\frac{1}{D_\lambda}\,\Pi_\nu\Big[\frac{1}{D_\lambda}\,,\,\Pi_\mu\Big]\,[\Pi^\nu,\,\Pi^\mu]\,\frac{1}{D_\lambda^2}$$
$$+\,\frac{1}{D_\lambda}\,\Pi_\nu\,\frac{1}{D_\lambda}\,[\Pi^\nu,\,\Pi^\mu]\Big[\Pi_\mu\,,\,\frac{1}{D_\lambda}\Big]\,\frac{1}{D_\lambda}\Big\}\,\Big\|\,\frac{1}{D_\lambda}\,.] \tag{2.54}$$

We have thus reduced $I_1 - I_{\delta m}$ to I_{M1}, I_{L1}, I_{a1}, I_b, I_c, and I_d.

In the first term of (2.37b), we anticommute the $\mathbf{\Pi}$ outside of γ_μ, so it acts on the wave function and becomes m. By then bringing γ_μ next to the commutator,

$$\gamma_\mu[\gamma^\mu,\,D] \,=\, -4zM, \tag{2.55}$$

we obtain another magnetic moment term,

$$I_{M2} \equiv\, -4m\,\frac{1}{D}\,z^2\,M\,\frac{1}{D}\,\Big\|\,\frac{1}{D^2}\,, \tag{2.56}$$

whose expansion in powers of the magnetic moment operator z^2M,

$$I_{M2} = \sum_{r=1}^{\infty}\frac{-8m}{(r-1)!}\,\frac{1}{D_1^3}\,\Big\|\,\Big(\frac{z^2\,M}{D_1}\Big)^r \tag{2.57a}$$
$$=\,-4m\,\frac{1}{D_1}\,z^2\,M\,\frac{1}{D_1}\,\Big\|\,\frac{1}{D_1^2} - 8m\,\frac{1}{D_1}\,z^2\,M\,\frac{1}{D_1}\,z^2\,M\,\frac{1}{D_1}\Big\|\,\frac{1}{D_1^2} + \cdots \tag{2.57b}$$

may be combined term by term with the expansion of I_{M1}, (2.40b). In anticommuting the $\mathbf{\Pi}$ through γ_μ,

$$\{\gamma_\mu\,,\,\mathbf{\Pi}\} \,=\, 2\Pi_\mu\,, \tag{2.58}$$

we obtain another term of type "L,"

$$I_{L2} \equiv -4z(1-z)\,\Pi_\mu \frac{1}{D}[\Pi^\mu, \mathbf{\Pi}]\frac{1}{D}\Big\|\frac{1}{D^2}. \tag{2.59}$$

[The higher order correction for commuting γ_μ through D^{-1},

$$I_{a2} \equiv zm\left[\gamma_\mu, \frac{1}{D}\right][\gamma^\mu, D]\frac{1}{D}\Big\|\frac{1}{D^2} = -4z^3 m \frac{1}{D}[\Pi_\mu, \mathbf{\Pi}]\frac{1}{D}[\Pi^\mu, \mathbf{\Pi}]\frac{1}{D}\Big\|\frac{1}{D^2}, \tag{2.60}$$

is very similar to I_{a1}, (2.50).]

Another term which has yet to be expressed in powers of the field is the second term of (2.37a); using again the equivalence (2.46) we find

$$\begin{aligned} 2\frac{1}{D}(\boldsymbol{k} - z\,\mathbf{\Pi})\Big\|\frac{1}{D^2} &\doteq 2\frac{1}{D}z\,\Pi_\nu\frac{1}{D}\gamma^\nu\Big\|\frac{1}{D} - 2\frac{1}{D^2}z\,\mathbf{\Pi}\Big\|\frac{1}{D} \\ &= 2z\frac{1}{D}\Pi_\nu\frac{1}{D}[\gamma^\nu, D]\frac{1}{D}\Big\|\frac{1}{D} - 2z\frac{1}{D^2}[\mathbf{\Pi}, D]\frac{1}{D}\Big\|\frac{1}{D}. \end{aligned} \tag{2.61}$$

By using the identity

$$[\mathbf{\Pi}, D] = [\mathbf{\Pi}, 2zk\cdot\Pi] = -2z[\Pi^\nu, \mathbf{\Pi}]k_\nu \tag{2.62}$$

and the equivalence (2.46) again, we may further rearrange the second term of (2.61),

$$\begin{aligned} 4z^2\frac{1}{D^2}[\Pi^\nu, \mathbf{\Pi}]\frac{1}{D}\Big\|\frac{k_\nu}{D} &\doteq 4z^2\frac{1}{D^2}[\Pi^\nu, \mathbf{\Pi}]\frac{1}{D}\Big\|\frac{z\,\Pi_\nu}{D} \\ &= 4z^2\left(\frac{1}{D}z\,\Pi_\nu\frac{1}{D}\Big\|\frac{1}{D}\right)[\Pi^\nu, \mathbf{\Pi}]\frac{1}{D} \\ &\qquad + 4z^2\frac{1}{D^2}[\Pi^\nu, \mathbf{\Pi}]\frac{1}{D}z\,\Pi_\nu\frac{1}{D} \\ &= 4z^3\frac{1}{D}\Pi_\nu\frac{1}{D}[\Pi^\nu, \mathbf{\Pi}]\frac{1}{D}\Big\|\frac{1}{D} \\ &\qquad - 4z^3\frac{1}{D}\left[\Pi_\nu, \frac{1}{D}[\Pi^\nu, \mathbf{\Pi}]\frac{1}{D}\right]\frac{1}{D}. \end{aligned} \tag{2.63}$$

By the use of the identity (2.37c), the first terms of (2.61) and (2.63) may now be combined,

$$I_{L3} \equiv -4z^2(1-z)\frac{1}{D}\Pi_\nu\frac{1}{D}[\Pi^\nu, \mathbf{\Pi}]\frac{1}{D}\Big\|\frac{1}{D}. \tag{2.64}$$

The second term of (2.63) will be written as

$$I_{L4} \equiv -8z^3 \frac{1}{D} \Pi_\nu \frac{1}{D} [\Pi^\nu, \mathbf{\Pi}] \frac{1}{D^2}, \tag{2.65}$$

which must be averaged with its reversed order to regain the double commutator structure.

[Let us now show that the $\nu = 0$ parts of I_L are all quadratic in the field. When averaged with its reversed order, I_{L2} becomes

$$\begin{aligned} I_{L2}(\nu = 0) &= -2z(1 - z) \left[\Pi_0 , \frac{1}{D} [\Pi^0, \mathbf{\Pi}] \frac{1}{D} \right] \Big\| \frac{1}{D^2} \\ &= 2z(1 - z) \frac{1}{D} [\Pi^0, \mathbf{\Pi}] \frac{1}{D} \Big\| \frac{[\Pi_0 , D]}{D^3} \end{aligned} \tag{2.66}$$

for $\nu = 0$ since the commutator of Π_0 with the field $[\Pi^0, \mathbf{\Pi}]$ vanishes because only functions of position are involved. We get similar expressions for $I_{L1}(\nu = 0)$ and $I_{L4}(\nu = 0)$ since they were originally expressed in terms of a commutator of Π_ν with D^{-1} and the field. However, when $I_{L3}(\nu = 0)$ and its reversed order are averaged,

$$I_{L3}(\nu = 0) = -2z^2(1 - z) \frac{1}{D} \left\{ \Pi_0 \frac{1}{D} [\Pi^0, \mathbf{\Pi}] - [\Pi^0, \mathbf{\Pi}] \frac{1}{D} \Pi_0 \right\} \frac{1}{D} \Big\| \frac{1}{D}, \tag{2.67}$$

we obtain not only a commutator of Π_0 with D^{-1} and the field,

$$\begin{aligned} &-2z^2(1 - z) \frac{1}{D} \left[\Pi_0 , \frac{1}{D} [\Pi^0, \mathbf{\Pi}] \right] \frac{1}{D} \Big\| \frac{1}{D} \\ &\qquad = 2z^2(1 - z) \frac{1}{D^2} [\Pi_0 , D] \frac{1}{D} [\Pi^0, \mathbf{\Pi}] \frac{1}{D} \Big\| \frac{1}{D}, \end{aligned} \tag{2.68}$$

but also a term

$$\begin{aligned} &-2z^2(1 - z) \frac{1}{D} \left[\frac{1}{D} , [\Pi^0, \mathbf{\Pi}] \right] \Pi_0 \frac{1}{D} \Big\| \frac{1}{D} \\ &\qquad = -2z^2(1 - z) \frac{1}{D^2} [[\Pi^0, D], \mathbf{\Pi}] \frac{1}{D} \Pi_0 \frac{1}{D} \Big\| \frac{1}{D} \end{aligned} \tag{2.69a}$$

involving a commutator of the field,

$$[[\Pi^0, \mathbf{\Pi}], D] = [[\Pi^0, D], \mathbf{\Pi}] + [\Pi^0, [\mathbf{\Pi}, D]], \tag{2.69b}$$

in which the term

$$[\Pi^0, [\mathbf{\Pi}, D]] = 2zk_\nu [\Pi^0, [\mathbf{\Pi}, \Pi^\nu]] = 0 \tag{2.69c}$$

may be reduced to a vanishing commutator of Π^0 with the field by means of the identity (2.62). As in the first part of (2.48), the $\mathbf{\Pi}$ in (2.69a) is brought to the

outside to become m, but this contribution vanishes now because we have a commutator rather than an anticommutator. The higher order correction for commuting $\mathbf{\Pi}$ through Π_0 is identical to (2.68) and that for commuting $\mathbf{\Pi}$ through the denominators is given by

$$2z^2(1-z)\,\frac{1}{D^2}\,[\Pi^0, D]\,\frac{1}{D}\,\Pi_0\,\frac{1}{D}\,\Big\|\,\frac{[\mathbf{\Pi}, D]}{D^2}$$

$$= 2z^2(1-z)\,\frac{1}{D}\left[\frac{1}{D}, \Pi^0\right]\Pi_0\,\frac{1}{D}\,\Big\|\,\frac{[\mathbf{\Pi}, 2zk\cdot\Pi]}{D^2} \tag{2.70a}$$

$$\doteq 4z^4(1-z)\,\frac{1}{D}\left[\frac{1}{D}, \Pi^0\right]\Pi_0\,\frac{1}{D}\,\Big\|\,\frac{[\mathbf{\Pi}, \Pi^\nu]}{D}\,\frac{\Pi_\nu}{D}$$

$$= 4z^4(1-z)\left\{\frac{1}{D^2}\,[\Pi_\nu, \Pi^0]\,\frac{1}{D}\,\Pi_0\,\frac{1}{D}\right.$$

$$\left. + \frac{1}{D^2}\,[\Pi^0, D]\,\frac{1}{D}\,\Pi_0\,\frac{1}{D}\,\Big\|\,\frac{\Pi_\nu}{D}\right\}\Big\|\,\frac{[\mathbf{\Pi}, \Pi^\nu]}{D}\,, \tag{2.70b}$$

where we have again used the identity (2.62) and the equivalence (2.46).]

[Finally, the last term of (2.37b)

$$2z\gamma_\nu(\boldsymbol{k} - z\mathbf{\Pi})\,\frac{1}{D}\,[\Pi^\mu, \mathbf{\Pi}]\,\frac{1}{D}\,\Big\|\,\frac{1}{D^2} \tag{2.71}$$

is a higher order term since it vanishes for a free electron not only because it has a factor of the field, like the first term of (2.37b), but also because it has a factor of $(k - z\Pi)^\lambda$, like the second term of (2.37a). It should be noted that these two factors are independent here only because the amount of the required shift, $z\Pi^\lambda$, commutes with the field in lowest order. That is, when the γ matrices in the numerator of (2.71) are brought together, their product with the commutator

$$[z\Pi^\lambda, F^{\mu\nu}] \tag{2.72}$$

vanishes,[5]

$$\begin{aligned}\gamma_\mu\gamma_\lambda\gamma_\nu[\Pi^\lambda, [\Pi^\mu, \Pi^\nu]] &= \gamma_\mu\gamma^i\gamma_\nu[p_i, [\Pi^\mu, \Pi^\nu]]\\ &= \gamma_\mu\gamma^i\gamma_\nu\{[\Pi^\mu, [p_i, \Pi^\nu]] - [\Pi^\nu, [p_i, \Pi^\mu]]\}\\ &= (\gamma_\mu\gamma^i\gamma_\nu - \gamma_\nu\gamma^i\gamma_\mu)[\Pi^\mu, [p_i, \Pi^\nu]]\\ &= (\gamma^j\gamma^i\gamma_\nu - \gamma_\nu\gamma^i\gamma^j)[p_j, [p_i, \Pi^\nu]] = 0.\end{aligned} \tag{2.73}$$

[5] In (2.73), note that $[\Pi^\lambda, F^{\mu\nu}(\mathbf{x})] = g^{i\lambda}[p_i, F^{\mu\nu}(\mathbf{x})]$, that $(\gamma^j\gamma^i\gamma_\nu - \gamma_\nu\gamma^i\gamma^j)$ is antisymmetric in i and j, and that $[p_j, [p_i, \Pi^\nu]] = [p_i, [p_j, \Pi^\nu]]$.

One higher order correction, for commuting γ_ν through the denominator, is

$$I_e \equiv 2z\gamma_\mu(\not{k} - z\not{\Pi}) \frac{1}{D} [\gamma_\nu, D] \frac{1}{D} [\Pi^\mu, \Pi^\nu] \frac{1}{D} \Big\| \frac{1}{D^2}$$
$$= -4z^2\gamma_\mu(\not{k} - z\not{\Pi}) \frac{1}{D} [\Pi_\nu, \not{\Pi}] \frac{1}{D} [\Pi^\mu, \Pi^\nu] \frac{1}{D} \Big\| \frac{1}{D^2} \tag{2.74}$$

and the other higher order correction, for the shift not commuting with the denominator, is

$$\begin{aligned} I_f &\equiv 2z\gamma_\mu \gamma_\lambda \gamma_\nu (k - z\Pi)^\lambda \frac{1}{D} [\Pi^\mu, \Pi^\nu] \frac{1}{D} \Big\| \frac{1}{D^2} \\ &\doteq 2z\gamma_\mu \gamma_\lambda \gamma_\nu \left\{ \frac{1}{D} [\Pi^\mu, \Pi^\nu] \frac{1}{D} \Big\| \frac{z\Pi^\lambda}{D^2} - z\Pi^\lambda \frac{1}{D} [\Pi^\mu, \Pi^\nu] \frac{1}{D} \Big\| \frac{1}{D^2} \right\} \\ &= 2z^2\gamma_\mu \gamma_\lambda \gamma_\nu \left\{ \frac{1}{D} [\Pi^\lambda, D] \frac{1}{D^2} [\Pi^\mu, \Pi^\nu] \frac{1}{D} \right. \\ &\qquad \left. + \frac{1}{D} [\Pi^\mu, \Pi^\nu] \frac{1}{D} [\Pi^\lambda, D] \frac{1}{D^2} + \frac{1}{D} [\Pi^\lambda, D] \frac{1}{D} [\Pi^\mu, \Pi^\nu] \frac{1}{D^2} \right\} \Big\| \frac{1}{D} . \end{aligned} \tag{2.75}$$

At this stage all the integrals over k converge because the only divergence, in I_1, has been cancelled in (2.44) by the divergence in $I_{\delta m}$. Thus, the upper limit of the K integration, $(1 - z)\Lambda^2$, will now be taken to be infinite since it is no longer needed to regularize the divergence in δm, (2.35). The K integration could now be easily carried out as in (2.23) for all terms except I_{L4} and (2.70). In those terms, the K integration avoided the introduction of a computational device analogous to the z integration used by KKS (4) in their Eqs. (2.15), (2.25), and (2.26). That is, our discussion of (2.46) assumed that a symmetrically inserted factor of $1/D$ would always be available to be associated with the numerator factor of k_ν, which would not be true in (2.63) or (2.70), if the K integration had already been carried out. We might note that, if further symmetrically inserted denominators were needed, they could be provided by integrating by parts:

$$\begin{aligned} \int_0^\infty dK \frac{N}{K + A} &= \frac{K}{1!} \frac{N}{K + A} \Big|_0^\infty - \int_0^\infty dK \frac{K}{1!} \frac{d}{dK} \frac{N}{K + A} \\ &= \int_0^\infty dK \frac{K}{1!} \frac{N}{K + A} \Big\| \frac{1}{K + A} \\ &= \cdots = \frac{1}{r!} \int_0^\infty dK \frac{N}{K + A} \Big\| \left(\frac{K}{K + A} \right)^r . \end{aligned} \tag{2.76}$$

We have thus rearranged the operator $I - I_{\delta m}$ as the sum of the magnetic

moment terms,

$$I_M \equiv I_{M1} + I_{M2}, \tag{2.77}$$

and the other lowest order terms,

$$I_L \equiv I_{L1} + I_{L2} + I_{L3} + I_{L4}, \tag{2.78}$$

plus the higher order terms,

$$I_a \equiv I_{a1} + I_{a2}, \tag{2.79}$$

I_b, I_c, I_d, I_e, and I_f. In the next section, the contributions to order $\alpha(Z\alpha)^4 m$ of I_M and I_L are calculated. Their higher order contributions, and the contributions of the higher order terms, are calculated in the following paper to order $\alpha(Z\alpha)^6 m$.

III. LOWEST ORDER LAMB SHIFT

Order Estimates for the Coulomb Potential

The preliminary decomposition in Section II, is gauge-invariant and holds for any potential $A^\mu(\mathbf{x})$. From this point on, we shall usually restrict ourselves to the Coulomb gauge and the scalar Coulomb potential,

$$A_0 = \phi(\mathbf{x}) = -Ze/4\pi r \qquad (\mathbf{A} = 0), \tag{3.1}$$

so that

$$\Pi^\mu = (E_n - V, \mathbf{p}), \tag{3.2}$$

where the potential energy V is a multiplicative operator in configuration space,

$$V = e\phi = -Z\alpha/r, \tag{3.3}$$

and an integral operator in momentum space, defined by

$$Vf(\mathbf{p}) \equiv -\frac{Z\alpha}{2\pi^2}\int \frac{d^3\mathbf{p}'}{(\mathbf{p}-\mathbf{p}')^2} f(\mathbf{p}'). \tag{3.4}$$

There is only an electric field, so the magnetic moment operator becomes

$$M = -ie\boldsymbol{\alpha}\cdot\boldsymbol{\mathcal{E}} = ie\boldsymbol{\alpha}\cdot\nabla\phi = i\boldsymbol{\alpha}\cdot\nabla V = -\boldsymbol{\alpha}\cdot[\mathbf{p}, V]. \tag{3.5}$$

Let us next review some pertinent features of the operators and wave functions for the Coulomb potential. For preliminary estimates of orders of magnitude, let us consider the nonrelativistic region; this requires small $Z\alpha$ since

$$\left\langle \left(\frac{v}{c}\right)^2 \right\rangle^{\mathrm{NR}} = \left\langle \frac{\mathbf{p}^2}{m^2} \right\rangle^{\mathrm{NR}} = \left(\frac{Z\alpha}{n}\right)^2 \ll 1.$$

The nonrelativistic Schrödinger equation for the electron is

$$\left(\frac{\mathbf{p}^2}{2m} + V\right)\phi_n^{\mathrm{NR}} = -\epsilon_n^{\mathrm{NR}}\phi_n^{\mathrm{NR}}, \tag{3.6}$$

the binding energies are given by the Bohr formula,

$$2m\epsilon_n^{\mathrm{NR}} = \left(\frac{Z\alpha m}{n}\right)^2 \equiv \beta^2 = \left(\frac{Z}{na_0}\right)^2, \tag{3.7}$$

and we have the nonrelativistic orders of magnitude indicated in (2.2):

$$\begin{aligned} \frac{1}{r} &\sim |\,\mathbf{p}\,| \sim \beta \sim Z\alpha m, \\ V &\sim Z\alpha\,|\,\mathbf{p}\,| \sim (Z\alpha)^2 m. \end{aligned} \tag{3.8}$$

These may be combined to assign "nominal" orders of magnitude to various operators. For example, the second order Dirac operator may be written as

$$\begin{aligned} \frac{H}{2m} &= \frac{m^2 - (m - \epsilon_n - V)^2 + \mathbf{p}^2 - M}{2m} \\ &= \left[\frac{\mathbf{p}^2}{2m} + V + \epsilon_n^{\mathrm{NR}}\right] + \left[\epsilon_n - \epsilon_n^{\mathrm{NR}} - \frac{(\epsilon_n + V)^2}{2m} - \frac{M}{2m}\right] \end{aligned} \tag{3.9}$$

in which the first bracket is the nonrelativistic operator, of order $(Z\alpha)^2 m$, and the second bracket contains the relativistic corrections, including the magnetic moment or spin-orbit term, of order $(Z\alpha)^4 m$.

For small $Z\alpha$, the large components of the Dirac wave function[6] become the nonrelativistic wave function, ϕ_n^{NR}, and the small components become

$$\chi_n^{\mathrm{NR}} = \frac{\boldsymbol{\sigma}\cdot\mathbf{p}}{2m}\phi_n^{\mathrm{NR}}. \tag{3.10}$$

For operators coupling large components together, the small components may be dropped as higher order in $Z\alpha$. An important example of such an operator is

$$[p_i\,,\,[V,\,p_i]] = \nabla^2 V = 4\pi Z\alpha\delta(\mathbf{x}), \tag{3.11}$$

for which we find

$$\begin{aligned} \langle n\,|\,\nabla^2 V\,|\,n\rangle^{\mathrm{NR}} &= 4\pi Z\alpha \int d^3\mathbf{x}\phi_n^{*\mathrm{NR}}(\mathbf{x})\delta(\mathbf{x})\phi_n^{\mathrm{NR}}(\mathbf{x}) \\ &= 4\pi Z\alpha\,|\,\phi_n^{\mathrm{NR}}(\mathbf{x} = 0)\,|^2 = 4Z\alpha\beta^3\delta_{l0}\,. \end{aligned} \tag{3.12}$$

However, for operators only coupling large to small components, we must use (3.10). For the example of the operator in (3.9)

$$-\frac{M}{2m} = \frac{ie}{2m}\,\boldsymbol{\alpha}\cdot\boldsymbol{\mathcal{E}}, \tag{3.13}$$

[6] We use the usual representation, in which

$$\psi_n = \begin{pmatrix}\phi_n \\ \chi_n\end{pmatrix}, \qquad \beta = \begin{pmatrix}I & 0 \\ 0 & -I\end{pmatrix}, \qquad \boldsymbol{\alpha} = \begin{pmatrix}0 & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & 0\end{pmatrix}.$$

we find

$$\begin{aligned}\left\langle n \left| \frac{-M}{2m} \right| n \right\rangle^{\mathrm{NR}} &= \frac{ie}{2m} \left\langle \left[\boldsymbol{\sigma}\cdot\mathbf{E}, \frac{\boldsymbol{\sigma}\cdot\mathbf{p}}{2m} \right] \right\rangle^{\mathrm{NR}} \\ &= \frac{-e}{4m^2} \langle div\mathbf{E} + 2\boldsymbol{\sigma}\cdot\mathbf{E}\times\mathbf{p} \rangle^{\mathrm{NR}} \\ &= \frac{1}{4m^2} \left\langle \nabla^2 V + \frac{2}{r}\frac{dV}{dr}\,\boldsymbol{\sigma}\cdot\mathbf{L} \right\rangle^{\mathrm{NR}} \\ &= \frac{(Z\alpha)^4 m}{n^3} \frac{C_{lj}}{2l+1}\,,\end{aligned} \tag{3.14a}$$

where

$$C_{lj} \equiv \begin{cases} 1/(l+1) & \text{for } j = l + \tfrac{1}{2} \\ -1/l & \text{for } j = l - \tfrac{1}{2}. \end{cases} \tag{3.14b}$$

The *nominal* order of magnitude, $(Z\alpha)^{\mathrm{N}}$, is obtained for any term in I by combining the above nonrelativistic order estimates for the numerator, omitting dimensional factors of m and state-dependent factors of n for brevity. Thus, the nonvanishing components of the field tensor,

$$[\Pi^i, \Pi^0] = [p_i\,, V] \sim Z\alpha m (Z\alpha)^2 m, \tag{3.15}$$

are of nominal order $(Z\alpha)^3$, and the higher order terms in I are all at least of nominal order $(Z\alpha)^6$, as most of them are quadratic in the fields. However, it should be noted that the actual order is less than the nominal order if the neglect of operators in the denominators would cause a divergence. For example, the S-state expectation value of the square of the field,

$$\begin{aligned}\langle n \mid [p_i\,, V][V, p_i] \mid n \rangle^{\mathrm{NR}} = \left\langle \frac{(Z\alpha)^2}{r^4} \right\rangle^{\mathrm{NR}} &= (Z\alpha)^2 \int \frac{d^3\mathbf{x}}{r^4} \mid \phi_n^{\mathrm{NR}}(\mathbf{x}) \mid^2 \\ &\to (Z\alpha)^2 \mid \phi_n^{\mathrm{NR}}(\mathbf{x}=0) \mid^2 \int \frac{d^3\mathbf{x}}{r^4} \sim (Z\alpha)^5 m^3 \int_0 \frac{dr}{r^2}\end{aligned} \tag{3.16a}$$

(or, in the momentum representation,

$$\begin{aligned}&= \left(\frac{-Z\alpha}{2\pi^2}\right)^2 \int d^3\mathbf{p}\phi_n^{*\mathrm{NR}}(\mathbf{p}) \int \frac{d^3\mathbf{p}'}{(\mathbf{p}-\mathbf{p}')^2} \\ &\quad \cdot \int \frac{d^3\mathbf{p}''}{(\mathbf{p}'-\mathbf{p}'')^2} \phi_n^{\mathrm{NR}}(\mathbf{p}'')(\mathbf{p}-\mathbf{p}')\cdot(\mathbf{p}''-\mathbf{p}') \\ &\quad \to \left| \frac{Z\alpha}{2\pi^2} \int d^3\mathbf{p}\phi_n^{\mathrm{NR}}(\mathbf{p}) \right|^2 \int \frac{d^3\mathbf{p}'}{\mathbf{p}'^2} \sim (Z\alpha)^5 m^3 \int^\infty d\mathbf{p}'\Big),\end{aligned} \tag{3.16b}$$

diverges linearly at small distances (or large momenta). The omitted denominators D effectively cut off the divergence at the Compton wavelength of the electron, $r \sim 1/m$ (corresponding to the relativistic momentum, $p \sim m$, at which $z(1-z)H \sim z(1-z)\mathbf{p}^2$ becomes comparable to z^2m^2 in D), so the actual order is $(Z\alpha)^5$, which is the nominal order, $(Z\alpha)^6$, reduced by the degree of divergence. The effects of electron divergences such as (3.16) and similar apparent infrared photon divergences on order estimates are discussed in detail later, but we can state here that none of the higher order terms is of lower order than $(Z\alpha)^5$.

Evaluation of Lowest Order Contributions

For the lowest order evaluation of a term in I, say $I_x(D)$, we will try to use the same steps which were used to reduce I to $I_{\delta m}$, again leaving correction terms which are of higher order than the given term. The first step is to drop any terms in I_x which are of higher order because of their numerator structure. The second step is to drop the magnetic moment operator z^2M from the denominators:

$$I_x(D) \to I_x(D_1). \tag{3.17}$$

A third step is to formally shift the k integration:

$$I_x(D_1) \to I_x(D_0). \tag{3.18}$$

The next step is to let the operator H vanish:

$$I_x(D_0) \to I_x(D_{00}), \quad \text{where} \quad D_{00} \equiv z^2m^2 + K - k^2; \tag{3.19a), (3.19b}$$

this leaves no corrections for denominators acting on the wave function. Finally, nonrelativistic wave functions are used to evaluate the remaining operator. Actually, these steps will be modified from term to term in such a way that the corrections will always be of higher order whenever possible. This will be discussed in more detail in the next paper.

For the magnetic moment term I_M, dropping z^2M is the same as omitting the terms after $r = 1$ in (2.40) and (2.57), so that we have

$$I_M(D_1) = [2(1+z) - 4]m \frac{1}{D_1} z^2M \frac{1}{D_1} \Big\| \frac{1}{D_1^2}. \tag{3.20}$$

After the shift ($D_1 \to D_0$) is carried out, the denominators automatically become the c-numbers D_{00} (since they all act on wave functions), whose k and K integrations are straightforward

$$\int_0^\infty dK \int \frac{d^4k/\pi^2 i}{D_{00}^2} \Big\| \frac{1}{D_{00}^2} = \int_0^\infty \frac{dK}{[z^2m^2 + K]^2} = \frac{1}{z^2m^2}, \tag{3.21}$$

as in (2.33c) and (2.23). Finally, the z integration yields

$$\Delta E_n(M) = \frac{\alpha}{4\pi}\int_0^1 dz[2z-2]m\left\langle n\left|\frac{M}{m^2}\right|n\right\rangle = \frac{\alpha}{2\pi}\left\langle n\left|\frac{-M}{2m}\right|n\right\rangle, \quad (3.22)$$

which is obviously the lowest order contribution of the anomalous moment of the electron, $(\alpha/2\pi) + 0(\alpha^2)$ times the Dirac moment in (3.13).

For the other lowest order terms, I_L, we first drop the numerator terms with $\nu = 0$ since we have found them to be quadratic in the field, like (2.66) and (2.70); the remaining numerators are like

$$\Pi_i[\Pi^i, \mathbf{\Pi}] = p_i[p_i, V]\gamma_0 \sim \mathbf{p}\cdot\boldsymbol{\mathcal{E}}. \quad (3.23)$$

Then, as in I_M, we drop z^2M and shift the k integration, so the H's vanish in the denominators which act directly on a wave function. The denominators "inside" p_i and $[p_i, V]$ do not act on any wave function and remain as D_0, but may be combined with the "outside" c-number denominators, D_{00}, by a u integration,

$$\frac{1}{D_0}\frac{1}{D_{00}} = \int_0^1 \frac{du}{D_{0u}^2} \quad (3.24a)$$

where

$$D_{0u} \equiv uD_0 + (1-u)D_{00} = z^2m^2 + K - k^2 + uz(1-z)H. \quad (3.24b)$$

The denominator combining rules (2.26) then give us

$$I_L = I_{L1} + I_{L2} + I_{L3} + I_{L4} = p_i\int_0^1 \frac{du}{D_{0u}^2}\Big\|\left\{4(1-z^2)z^3m^2\frac{(1-u)^2}{D_{0u}^3} - 4z(1-z)\frac{1}{D_{0u}^2} - 4z^2(1-z)\frac{1-u}{D_{0u}^2} - 4z^3\frac{(1-u)^2}{D_{0u}^2}\right\}[p_i, V]\gamma_0. \quad (3.25)$$

The k and K integrations are as for I_M in (3.21), with

$$z^2m^2 \to z^2m^2 + uz(1-z)H, \quad (3.26a)$$

except that the extra inserted factor z^2m^2/D_{0u} in I_{L1} in (3.25) becomes an extra factor of

$$\frac{z^2m^2}{z^2m^2 + uz(1-z)H} \quad (3.26b)$$

which may then be replaced by $2u/(1-u)$ by an integration by parts,

$$\int_0^1 \frac{(1-u)^2z^2m^2\,du}{[z^2m^2 + uz(1-z)H]^2} = \int_0^1 \frac{2(1-u)u\,du}{z^2m^2 + uz(1-z)H}. \quad (3.26c)$$

Using the nonrelativistic approximations for H and the wave functions, we then

find

$$\Delta E_n(L) = \frac{\alpha}{\pi}\int_0^1 du \int_0^1 dz P(z,u) \left\langle n \left| p_i \frac{1}{\Delta}[V, p_i] \right| n \right\rangle^{\mathrm{NR}} \tag{3.27a}$$

in which the polynomial is

$$P(z,u) = -2(1-z^2)u(1-u) + (1-z) + z(1-z)(1-u) + z^2(1-u)^2 \tag{3.27b}$$

and the reduced denominator is

$$\Delta \equiv zm^2 + u(1-z)H^{\mathrm{NR}}, \tag{3.28a}$$

where

$$H^{\mathrm{NR}} \equiv \mathbf{p}^2 + \beta^2 + 2mV = 2m\left[\frac{\mathbf{p}^2}{2m} + V + \epsilon_n^{\mathrm{NR}}\right]. \tag{3.28b}$$

Even though the H_{NR} in the Δ in (3.27) is of order $(Z\alpha)^2m^2$, we cannot drop it, since the z integration would then diverge logarithmically at $z = 0$. Instead, we will use the identity

$$\int_0^1 \frac{dzP(z,u)}{\Delta} = \frac{P(0,u)}{m^2}\ln\frac{m^2}{uH^{\mathrm{NR}}} + \int_0^1 dz \frac{P(z,u) - P(0,u)}{zm^2} + \frac{uH^{\mathrm{NR}}}{m^2}\int_0^1 \frac{dz}{\Delta}\left[\frac{P(0,u) - (1-z)P(z,u)}{z}\right] \tag{3.29}$$

and drop the contribution of the last term, of nominal relative order $(Z\alpha)^2$. If we replace H^{NR} by its order of magnitude, the wave function integration reduces to (3.12),

$$\frac{1}{m^2}\langle p_i[V, p_i]\rangle^{\mathrm{NR}} = \frac{1}{2m^2}\langle [p_i, [V, p_i]]\rangle^{\mathrm{NR}} = \frac{1}{2m^2}\langle \nabla^2 V\rangle^{\mathrm{NR}} = 2\frac{(Z\alpha)^4 m}{n^3}\delta_{l0}, \tag{3.30}$$

and the integrals over z and u are straightforward,

$$2\int_0^1 du\left[P(0,u)\ln\frac{1}{u(Z\alpha)^2} + \int_0^1 dz\frac{P(z,u) - P(0,u)}{z}\right] = \frac{4}{3}\left[\ln\frac{1}{(Z\alpha)^2} + \frac{13}{12} - \frac{5}{8}\right] \tag{3.31}$$

To treat the operator H^{NR} exactly, we may insert a sum over a complete set of nonrelativistic states in (3.27a), so we have

$$H^{\mathrm{NR}}|n'\rangle^{\mathrm{NR}} = 2m(\epsilon_n^{\mathrm{NR}} - \epsilon_{n'}^{\mathrm{NR}})|n'\rangle^{\mathrm{NR}} \tag{3.32a}$$

The Lamb shift itself is given by

From Wikipedia

$$\Delta E_{\text{Lamb}} = \alpha^5 m_e c^2 \frac{k(n,0)}{4n^3} \text{ for } \ell = 0$$

with $k(n, 0)$ around 13 varying slightly with n, and

$$\Delta E_{\text{Lamb}} = \alpha^5 m_e c^2 \frac{1}{4n^3}\left[k(n,\ell) \pm \frac{1}{\pi(j+\frac{1}{2})(\ell+\frac{1}{2})}\right] \text{ for } \ell \neq 0 \text{ and } j = \ell \pm \frac{1}{2},$$

with $k(n,\ell)$ a small number (< 0.05).

For a derivation of ΔE_{Lamb} see for example:[6]

$$\begin{aligned}\langle n' \mid [V, p_i] \mid n\rangle^{\text{NR}} &= \left\langle n' \left| \left[\frac{H^{\text{NR}}}{2m}, p_i\right] \right| n \right\rangle^{\text{NR}} \\ &= (\epsilon_n^{\text{NR}} - \epsilon_{n'}^{\text{NR}})\langle n' \mid p_i \mid n\rangle^{\text{NR}},\end{aligned} \tag{3.32b}$$

where, as in (3.6), $-\epsilon_{n'}^{\text{NR}}$ is the nonrelativistic energy of the state n'. We thus arrive at Bethe's original definition of an average excitation energy $\Delta\epsilon_n$ in terms of a sum over states,

$$\begin{aligned}&\frac{1}{m^2}\left\langle n \left| p_i \ln\left[\frac{(Z\alpha)^2 m^2}{H^{\text{NR}}}\right][V, p_i] \right| n \right\rangle^{\text{NR}} \\ &\quad = \sum_{n'} \left| \left\langle n \left| \frac{p_i}{m} \right| n' \right\rangle^{\text{NR}} \right|^2 (\epsilon_n^{\text{NR}} - \epsilon_{n'}^{\text{NR}}) \ln\left[\frac{(Z\alpha)^2 m}{2\,|\,\epsilon_n^{\text{NR}} - \epsilon_{n'}^{\text{NR}}\,|}\right] \\ &\quad \equiv 2\frac{(Z\alpha)^4 m}{n^3} \ln\frac{(Z\alpha)^2 m}{2\Delta\epsilon_n}\end{aligned} \tag{3.33}$$

in which the final coefficient of the logarithm is the S-state expectation value of the original operator without the logarithm, (3.30).

The Lamb shift to order $(Z\alpha)^4$ is thus given by

$$\begin{aligned}\Delta E_n^{(4)} = \frac{4\alpha(Z\alpha)^4 m}{3\pi n^3}\Bigg\{&\left[\ln\frac{1}{(Z\alpha)^2} + \frac{11}{24} - \frac{1}{5}\right]\delta_{l0} \\ &+ \ln\frac{(Z\alpha)^2 m}{2\Delta\epsilon_n} + \frac{3}{8}\frac{C_{lj}}{2l+1}\Bigg\},\end{aligned} \tag{3.34}$$

$$C_{lj} \equiv \begin{cases} 1/(l+1) & \text{for } j = l + \frac{1}{2} \\ -1/l & \text{for } j = l - \frac{1}{2}. \end{cases} \tag{3.14b}$$

order of magnitude which we obtain for the vacuum polarization contribution, corresponding to Fig. 1(a). Equation (3.34) contributes about 1052 Mc/sec to the difference between the $2S_{1/2}$ and $2P_{1/2}$ levels in hydrogen. The relative orders of magnitude of the separate parts of (3.34) may be compared by noting that

$$\ln\frac{1}{\alpha^2} \approx 10 \quad \text{and} \quad \ln\frac{(Z\alpha)^2 m}{2\Delta\epsilon_n} \approx -3\delta_{l0}\,. \tag{3.35}$$

Apparent Infrared Divergences and the Bethe Log

In the rest of this section we will discuss singular behavior at $z = 0$, such as that which yields the logarithm in (3.29). We first note that the divergence that would occur if we dropped the H in the denominator is an infrared divergence, which is usually regulated by keeping the photon mass, λ_{min}, finite. Then the lower limit of the K integration would be $(1 - z)\lambda_{\text{min}}^2$, so the denominator in (3.26) would become

$$z^2 m^2 + (1 - z)\lambda_{\text{min}}^2 + uz(1 - z)H.$$

From this we see that, if H vanishes, as for a freely propagating electron, a divergence at $z = 0$ would be cut off at

$$z \sim \lambda_{\min}/m \tag{3.36}$$

and would therefore be an infrared divergence. For our bound electron, however, such an infrared divergence is instead cut off at

$$z \sim \frac{uH}{m^2} \sim \frac{\Delta\epsilon_n}{m} \sim (Z\alpha)^2. \tag{3.37}$$

Thus, the logarithmic infrared divergence in (3.27) yields the $\ln(Z\alpha)^{-2}$ in (3.34), and a linear infrared divergence would yield a term of order $1/(Z\alpha)^2$ relative to the nominal order.

From the foregoing, it is apparent that we must again modify our order estimates, so that the actual order is the nominal order reduced by twice the degree of the apparent infrared divergence.

The principal corollary of this is that no part of H of order $(Z\alpha)^2m^2$ may be dropped as being small compared to zm^2 in the denominator of such an infrared divergent term. In particular, an expansion in powers of the potential V will not be an expansion in powers of $Z\alpha$ for infrared divergent terms. Even for a term which is not infrared divergent, an expansion of our denominators in powers of the potential,

$$\frac{1}{\Delta} = \frac{1}{\Delta_0} - 2u(1-z)m\frac{1}{\Delta_0}V\frac{1}{\Delta_0} + [2u(1-z)m]^2\frac{1}{\Delta_0}V\frac{1}{\Delta_0}V\frac{1}{\Delta_0} - \cdots, \tag{3.38a}$$

where

$$\Delta = zm^2 + u(1-z)(\mathbf{p}^2 + \beta^2 + 2mV) \tag{3.38b}$$

and

$$\Delta_0 \equiv zm^2 + u(1-z)(\mathbf{p}^2 + \beta^2), \tag{3.38c}$$

may be an expansion in powers of $(Z\alpha)^2$ for the first few terms, but the increasing powers of $1/\Delta_0 \sim 1/zm^2$ will eventually cause an infrared divergence for some term, and all succeeding terms will be of the same order since the increasing degrees of apparent infrared divergence will cancel the increasing powers of $(Z\alpha)^2$. For an example, let us consider the expansion of the operator which becomes the Bethe log in (3.33).

An alternate formulation of the Bethe log may be obtained by expanding the formal logarithmic operator in (3.29) in powers of the potential like (3.38), before the z integration is performed,

$$\ln\frac{m^2}{uH^{\mathrm{NR}}} = \int_0^1 \frac{dz(m^2 - uH^{\mathrm{NR}})}{zm^2 + u(1-z)H^{\mathrm{NR}}} = \int_0^1 \frac{dz}{1-z}\left[\frac{m^2}{\Delta} - 1\right]$$
$$= \int_0^1 \frac{dz}{1-z}\left[\left(\frac{m^2}{\Delta_0} - 1\right) - 2u(1-z)m^3\frac{1}{\Delta_0}V\frac{1}{\Delta_0} + \cdots\right] \tag{3.39}$$
$$= \ln\left[\frac{m}{u(\mathbf{p}^2+\beta^2)}\right] - \frac{2mV}{\mathbf{p}^2 - \mathbf{p}'^2}\ln\left[\frac{\mathbf{p}^2+\beta^2}{\mathbf{p}'^2+\beta^2}\right] + \cdots,$$

where $\mathbf{p}$ and $\mathbf{p}'$ are the momenta on the opposite sides of the integral operator V, (3.4), in the momentum representation. By substituting the expansion (3.39) into (3.33), we may express the Bethe log as an infinite series,

$$2Z\alpha\beta^3 \ln\frac{(Z\alpha)^2 m}{2\Delta\epsilon_n} \equiv 2Z\alpha\beta^3\{L_n^{(0)} + L_n^{(1)} + \cdots\}$$
$$\equiv \left\langle n \left| p_i \left\{ \ln\left(\frac{(Z\alpha)^2 m^2}{\mathbf{p}^2+\beta^2}\right) \right.\right.\right. \tag{3.40}$$
$$\left.\left.\left. - \frac{2mV}{\mathbf{p}^2 - \mathbf{p}'^2}\ln\left(\frac{\mathbf{p}^2+\beta^2}{\mathbf{p}'^2+\beta^2}\right) + \cdots\right\} [V, p_i] \right| n \right\rangle^{\mathrm{NR}},$$

whose leading term for S-states is found in the Appendix to be

$$L_{nS}^{(0)} \equiv \frac{1}{2Z\alpha\beta^3}\left\langle nS \left| p_i \ln\frac{(Z\alpha)^2 m^2}{\mathbf{p}^2+\beta^2}[V, p_i] \right| nS \right\rangle^{\mathrm{NR}}$$
$$= 2\ln\frac{n}{2} + 2 - 4\left(1 + \frac{1}{3} + \frac{1}{5} + \cdots + \frac{1}{2n-1}\right). \tag{3.41}$$

In Table I, (3.41) is seen to be a good approximation of the exact results, calculated by the sum over states in (3.33). Note that the n dependence is very small. Note also that the Bethe log does not depend on $Z\alpha$, as can be seen by use of the dimensionless momentum variable

$$\mathbf{t} = \mathbf{p}/\beta \tag{3.42}$$

in (3.40), so that the contribution of the Bethe log to the Lamb shift in (3.34) is entirely of order $(Z\alpha)^4$.

TABLE I

BETHE LOGARITHMS FOR S-STATES

n =	1	2	3	4	∞
(3.41)	−3.386	−3.333	−3.322	−3.318	−3.313
Exact[a]	−2.984	−2.812	−2.768	−2.750	−2.721

[a] Reference *11*.

IV. RESULTS

The calculations (*17*, *18*) accompanying the final experimental results have been amended many times, so that by now most of the "constants" used have been changed. Instead of adding more corrections to the latest calculation[7] and thereby repropagating previous errors, we will list in detail all the terms that enter and will tabulate a new set of values. The discussion given by Bethe and Salpeter (*19*) is quite accurate and complete, so we will not give detailed references for terms they discuss in their sections 20 and 21 (including the associated Addenda and Errata at the end of the book) unless the exact formula is not given there.

When the reduced mass

$$\mu \equiv \frac{mM}{m+M},$$

where M is the nuclear mass, is used in the atomic wave functions in calculating

$$\langle \nabla^2 V \rangle = 4\pi Z\alpha \mid \phi_n^{\mathrm{NR}}(0) \mid^2 = 4Z\alpha \left(\frac{Z\alpha\mu}{n}\right)^3 \delta_{l0}$$

and

$$\Delta\epsilon_n \propto \mu,$$

we have

$$\Delta E_n^{(4)}(L, V.P.) = \frac{4\alpha(Z\alpha)^4 m}{3\pi n^3}\left(1 - 3\frac{m}{M}\right)\left\{\left[\ln\frac{1}{(Z\alpha)^2} + \ln\left(1+\frac{m}{M}\right) + \frac{11}{24} - \frac{1}{5}\right]\delta_{l0} + \ln\frac{(Z\alpha)^2\mu}{2\Delta\epsilon_n}\right\} \tag{4.1a}$$

for the lowest order contribution of I_L and the vacuum polarization diagram (Fig. 1a), where the reduced mass correction

$$\left(\frac{\mu}{m}\right)^3 = \left(\frac{M}{m+M}\right)^3 \simeq 1 - 3\frac{m}{M} \tag{4.1b}$$

is only taken to lowest order in m/M. For the magnetic moment terms, the reduced mass factors are given by

$$\Delta E_n^{(4)}(M) = \frac{\alpha}{2\pi}\frac{(Z\alpha)^4 m}{n^3}\begin{cases}\left(1 - 3\dfrac{m}{M}\right)(+1) & l = 0\\ \left(1 - 2\dfrac{m}{M}\right)\begin{matrix}(-\frac{1}{3} & j = \frac{1}{2})\\ (+\frac{1}{6} & j = \frac{3}{2})\end{matrix} & l = 1\end{cases}. \tag{4.2}$$

[7] Layzer's results in ref. *5*, which were added to a summary by A. PETERMANN, *Fortschr. Physik* **6**, 505 (1958).

The higher order contributions are given by (*4*, *5*, *13*)

$$\Delta E_n^{(5)} = \frac{4\alpha(Z\alpha)^5 m}{n^3}\left[1 + \frac{11}{128} - \frac{1}{2}\ln 2 + \frac{5}{192}\right]\delta_{l0} \tag{4.3}$$

and

$$\Delta E_n^{(6)} = \frac{4\alpha(Z\alpha)^6 m}{3\pi n^3}\left\{\left[-\frac{3}{4}\ln^2\frac{1}{(Z\alpha)^2} + \left(4\ln 2 - \frac{1}{10}\right)\ln\frac{1}{(Z\alpha)^2} - \left(\frac{4}{3}\pi^2 + 4 + 4\ln^2 2\right)\right]\delta_{l0} + a_n \ln\frac{1}{(Z\alpha)^2} + b_n\right\}, \tag{4.4a}$$

where

$$a_n = \left[3\left(\ln\frac{2}{n} + 1 + \frac{1}{2} + \cdots + \frac{1}{n}\right) - \frac{601}{240} - \frac{77}{60n^2}\right]\delta_{l0} + \left(1 - \frac{1}{n^2}\right)\left(\frac{1}{10} + \frac{1}{4}\delta_{j1/2}\right)\delta_{l1} + \frac{6 - 2l(l+1)/n^2}{(2l+3)l(l+1)(4l^2-1)}(1 - \delta_{l0}) \tag{4.4b}$$

and

$$|\, b_n \,|_{\text{estimated}} < 5. \tag{4.4c}$$

The fourth order radiative corrections corresponding to I_L contribute (*7*)

$$2(0.52 \pm 0.21)\frac{\alpha^2(Z\alpha)^4 m}{\pi^2 n^3}\delta_{l0}, \tag{4.5}$$

the magnetic moment term $-0.328\,\alpha^2/\pi^2$ contributes (*8*)

$$\left(-0.328\frac{C_{lj}}{2l+1}\right)\frac{\alpha^2}{\pi^2}\frac{(Z\alpha)^4 m}{n^3} \tag{4.6a}$$

where

$$-0.328 \equiv \frac{197}{144} + \frac{\pi^2}{12} + \frac{3}{4}\zeta(3) - \frac{\pi^2}{2}\ln 2 = -0.328\,479\,0, \tag{4.6b}$$

and the vacuum polarization contribution is (*6*)

$$-\left(1 + \frac{1}{81}\right)\frac{\alpha^2(Z\alpha)^4 m}{\pi^2 n^3}\delta_{l0}. \tag{4.7}$$

The nuclear motion, besides giving reduced mass factors, shifts *all* fine structure levels by

$$-\frac{(Z\alpha)^4 m}{8n^4}\frac{m}{M}. \tag{4.8}$$

This does not contribute to the Lamb shift or fine structure splittings, but is included for completeness since it shifts levels differently for different n.

The lowest order effects of the relativistic bound state equation were calculated by Salpeter (*9*) and checked by Fulton and Martin (*9*)[8] and are given by

$$\frac{4(Z\alpha)^5 m}{3\pi n^3}\frac{m}{M}\left\{2\left[\left(\ln\frac{1}{(Z\alpha)^2}+\frac{11}{24}\right)\delta_{l0}+\ln\frac{(Z\alpha)^2 m}{2\Delta\epsilon_n}\right]-\delta_{l0}-\frac{7}{4}\left[\delta_{l0}\ln\frac{1}{(Z\alpha)^2}+\tilde{a}_n\right]\right\} \tag{4.9a}$$

where the first line is $2Zm/M$ times the lowest order term $\Delta E_n^{(4)}(L)$, and $\tilde{a}_n$ is probably like

$$\tilde{a}_n \stackrel{?}{=} -2\left(\ln\frac{2}{n}+1+\frac{1}{2}+\cdots+\frac{1}{n-1}+1+\frac{1}{2n}\right)\delta_{l0}+\frac{1-\delta_{l0}}{l(l+1)(2l+1)} \tag{4.9b}$$

but has only been calculated for $n = 2$; although (4.9b) for $n \neq 2$ is only an educated guess based on calculations in the following paper, we shall use it for the $1S$ state since it probably does not depend strongly on n in any case.

The additional potential energy

$$\Delta V(r) = \int_{r_N>r} d^3 r_N\, \rho(r_N)\left(\frac{Z\alpha}{r}-\frac{Z\alpha}{r_N}\right) \tag{4.10a}$$

due to the nucleus having a charge distribution, $-Ze\rho(r_N)$, of finite extent contributes an amount

$$\langle\Delta V\rangle = \int d^3 r \int_{r<r_N} d^3 r_N \mid \phi_n(r)\mid^2 \rho(r_N)\left(\frac{Z\alpha}{r}-\frac{Z\alpha}{r_N}\right) \approx \frac{2\pi}{3} Z\alpha \mid \phi_n^{NR}(0)\mid^2 \int d^3 r_N\, \rho(r_N)\, r_N{}^2 \equiv \frac{2(Z\alpha)^4 m}{3n^3}\left(\frac{R_N}{1/m}\right)^2 \delta_{l0}\,, \tag{4.10b}$$

where only the nonrelativistic atomic wave function at the nucleus is important since R_N, the root-mean-square radius of the nuclear charge distribution, is much smaller than either $1/m$, the Compton wavelength of the electron, or $n/Z\alpha m$, the Bohr radius of the atom. We will use the values

$$R_N = \begin{cases} 0.805 \pm 0.011 \text{ F} & \text{Proton } (20) \\ 1.96 \pm 0.07 \text{ F} & \text{Deuteron}^9 \\ 1.68 \pm 0.04 \text{ F} & \text{Alpha particle } (22) \end{cases} \tag{4.10c}$$

obtained from electron scattering experiments.

[8] Besides correcting a small term Salpeter called ΔE_{cc}, Fulton and Martin find an exact result $\frac{4}{3}(1 - \ln 2)$ for an integral previously evaluated numerically as 0.411.

[9] We use the values of $G_{Ed}(0.3\ F^{-2})$ and $G_{Ed}(0.6\ F^{-2})$ given by Drickey and Hand (*21*) to solve $G_{Ed}(q^2) = 1 - R_d^2(q^2/6) + Cq^4$ for C and $R_d^2 = 3.84 \pm 0.25\ F^2$.

We shall use the new values for the physical constants as recommended by the NAS-NRC (*23*),

$$\alpha^{-1} = 137.0388 + \epsilon_\alpha \times 10^{-4}$$

$$\cdot(\ln \alpha^{-2} = 9.840\ 528\ 195 + 1.46\epsilon_\alpha \times 10^{-6})$$

$$R_\infty = 109{,}737.31 + \epsilon_R \times 10^{-2}\ \text{cm}^{-1} \tag{4.11a}$$

$$c = (2.997\ 925 + \epsilon_c \times 10^{-6}) \times 10^{10}\ \text{cm sec}^{-1},$$

to calculate the "Lamb constant,"

$$\left.\frac{4\alpha(Z\alpha)^4 m}{3\pi n^3}\right|_{Z=1;n=2} \equiv L$$

$$= \frac{\alpha^3}{3\pi} R_\infty c = 135.635\ 479 + (-2.97\,\epsilon_\alpha + 0.12\epsilon_R + 0.45\,\epsilon_c) \times 10^{-4}\ \text{Mc/sec}, \tag{4.11b}$$

where three standard deviations are

$$\epsilon_\alpha = \pm 19, \qquad \epsilon_R = \pm 3, \qquad \epsilon_c = \pm 3 \tag{4.11c}$$

in the last digits. For the Bethe log, we will use the very accurate calculations of Schwartz and Tiemann (*11*) for the $2S$ and $2P$ states and those of Harriman (*11*) for the others:

$$\ln \frac{(Z\alpha)^2 m}{2\Delta\epsilon_n} = \begin{Bmatrix} -2.984\ 149 \pm 3 \times 10^{-6} & 1S \\ -2.811\ 769\ 883 \pm 28 \times 10^{-9} & 2S \\ +0.030\ 016\ 697 \pm 12 \times 10^{-9} & 2P \end{Bmatrix}. \tag{4.12}$$

The mass values need not be so accurate; we shall use (*23*, *24*)

$$\frac{M_p}{m_e} = 1836.096; \qquad \frac{M_d}{M_p} = 1.999\ 007\ 5; \qquad \frac{M_\alpha}{M_p} = 3.972\ 605. \tag{4.13}$$

The results are listed in Table II for the $1S_{1/2}$, $2S_{1/2}$, $2P_{1/2}$, and $2P_{3/2}$ states of hydrogen, deuterium, and singly ionized helium. The totals may be corrected for changes in α or the other physical constants (4.11a) by multiplying by the factor

$$1 + (-2.0\epsilon_\alpha + 0.1\epsilon_R + 0.3\epsilon_c) \times 10^{-6}. \tag{4.14}$$

Let us now list the terms that are not included here. The largest nonnuclear term is (4.4c), which is estimated to be no larger than

$$\pm 5\,\frac{4\alpha(Z\alpha)^6 m}{3\pi n^3} = \pm 0.036; \qquad \pm 2.31\ \text{Mc/sec}\ (Z = 1; 2) \tag{4.15}$$

TABLE II[a]

ENERGY SHIFTS $(n/2)^3 \Delta E_n$ (Mc/sec)

Order and term		Eq.	State	Massive point nucleus		Nuclear corrections		
				$Z = 1$	$Z = 2$	H	D	He^+
$\alpha(Z\alpha)^4$	$\ln Z\alpha$	(4.1)	S	1334.725	18347.10	−2.107	−1.054	−7.25
			$1S$	−342.590	−5481.44	0.560	0.280	2.25
	L	(4.1)	$2S$	−319.209	−5107.35	0.522	0.261	2.10
			$2P$	4.071	65.14	−0.007	−0.003	−0.03
			S	50.863	813.81	−0.083	−0.042	−0.33
	M	(4.2)	$P_{1/2}$	−16.954	−271.27	0.018	0.009	0.07
			$P_{3/2}$	8.477	135.64	−0.009	−0.005	−0.04
	VP	(4.1)	S	−27.127	−434.03	0.044	0.022	0.18
$\alpha(Z\alpha)^5$		(4.3)	S	7.140	228.48			
$\alpha(Z\alpha)^6$	$\ln^2 Z\alpha$	(4.4)	S	−0.525	−24.78			
	$\ln Z\alpha$	(4.4)	$1S$	0.282	15.49			
			$2S$	0.309	16.99			
			$2P_{1/2}$	0.030	1.68			
			$2P_{3/2}$	0.017	0.94			
	est. const.	(4.4)	S	−0.138	−8.82			
$\alpha^2(Z\alpha)^4$	L	(4.5)	S	0.245	3.93			
			S	−0.078	−1.24			
	M	(4.6)	$P_{1/2}$	0.026	0.41			
			$P_{3/2}$	−0.013	−0.21			
	VP	(4.7)	S	−0.239	−3.83			
$(m/M)(Z\alpha)^4$			$n = 1$			−2.982	−1.492	−12.01
		(4.8)	$n = 2$			−1.491	−0.746	−6.00
$(m/M)(Z\alpha)^5$	$\ln Z\alpha$		$1S$			0.302	0.151	2.22
		(4.9)	$2S$			0.342	0.171	2.55
			$2P$			−0.017	−0.009	−0.14
$(R_N m)^2(Z\alpha)^4$		(4.10)	S			0.127	0.752	8.84
Totals			$1S_{1/2}$	1022.558	13454.67	−4.139	−1.382	−6.09
			$2S_{1/2}$	1045.966	13830.26	−2.646	−0.635	0.08
			$2P_{1/2}$	−12.827	−204.04	−1.496	−0.748	−6.09
			$2P_{3/2}$	12.553	201.51	−1.524	−0.762	−6.21
			$2S_{1/2}$–$2P_{1/2}$	1058.793	14034.30	−1.150	0.113	6.18
			$2P_{3/2}$–$2P_{1/2}$	25.380	405.55	−0.028	−0.014	−0.11

[a] To avoid cumulative round-off errors in the totals, all entries were calculated to more figures than given here, except the contributions of Eq. (4.5), for which only the three figures given here were used.

for $n = 2$. The next higher order term in that series is estimated to be

$$+\pi^3 \frac{4\alpha(Z\alpha)^7 m}{3\pi n^3} = +0.002; \qquad +0.21 \text{ Mc/sec } (Z = 1; 2). \tag{4.16a}$$

We estimate the next higher order contributions after (4.5-7) to be at most

$$3\pi Z\alpha \frac{\alpha^2(Z\alpha)^4 m}{\pi^2 n^3} = \pm 0.016; \qquad \pm 0.52 \text{ Mc/sec } (Z = 1; 2) \tag{4.16b}$$

and

$$\frac{\alpha}{\pi} \frac{\alpha^2(Z\alpha)^4 m}{\pi^2 n^3} = \pm 0.001; \qquad \pm 0.01 \text{ Mc/sec } (Z = 1; 2). \tag{4.16c}$$

The reduced mass correction of (4.3) used in some previous calculations (*18*) (see also footnote 7)

$$-3 \frac{m}{M} \frac{4\alpha(Z\alpha)^5 m}{n^3} \left(1 + \frac{11}{128} - \frac{1}{2} \ln 2 + \frac{5}{192}\right) = -0.012; \qquad -0.006; \qquad -0.09 \text{ Mc/sec (H; D; He}^+), \tag{4.17a}$$

has been omitted here for consistency since it is probably cancelled to some extent by the next higher order contribution after (4.9a), estimated to be about

$$+2 \frac{m}{M} \frac{4(Z\alpha)^6 m}{n^3} = +0.010; \quad +0.005; \quad +0.16 \text{ Mc/sec (H; D; He}^+). \tag{4.17b}$$

The reduced mass corrections of (4.5, 6, 7) are of the same nominal order, $\alpha^6 m/M$, as (4.17), but are smaller by a factor of $Z\pi^2$ or more. Terms containing two factors of m/M, such as the term dropped in (4.1b),

$$6 \left(\frac{m}{M}\right)^2 \frac{4\alpha(Z\alpha)^4 m}{3\pi n^3} \ln (Z\alpha)^{-2} = +0.002; \qquad +0.001; \qquad +0.002 \text{ Mc/sec (H; D; He}^+), \tag{4.18}$$

or the self-energy of the nucleus, for which the μ^3/m^2 in $\Delta E(L)$ is replaced by μ^3/M^2, will also cancel each other to some extent and are seen to be smaller than (4.17) by a factor of 2π or more (since the $2(m/M) \ln (Z\alpha)^{-2}$ factor in (4.18) is smaller than the $Z\alpha$ factor in (4.17)). We may reasonably use (4.17b) as a generous upper bound on the magnitude of the sum of all the terms mentioned in this paragraph.

Nuclear structure effects have been taken into account phenomenologically here by the finite size contribution (4.10). For example, the anomalous moment of the proton, besides contributing to the hyperfine structure, contributes[10]

[10] Equation (16) in ref. *17*.

TABLE III

ESTIMATED ERROR LIMITS IN ΔE_{2S}

Source	Eq.	H	D	He^+	D − H
$\alpha^2(Z\alpha)^4$ (see footnote 11)	(4.5)	0.099	0.099	1.59	0
Fine structure constant	(4.20)	0.041	0.041	0.55	0
$\alpha(Z\alpha)^6$ remainder	(4.15)	0.036	0.036	2.31	0
Higher order radiative terms	(4.16)	0.019	0.019	0.74	0
Higher order recoil terms	(4.17)	0.010	0.005	0.16	0.005
Nuclear size uncertainty	(4.10c)	0.004	0.050	0.42	0.054
Nuclear structure		negl.	0.018	0.26	0.018
Total		0.209	0.268	6.03	0.077

$$(1.79)\left(\frac{m}{M}\right)^2 \frac{(Z\alpha)^4 m}{n^3}\delta_{l0} = 0.023 \text{ Mc/sec} \tag{4.19}$$

to the Lamb shift in hydrogen, but also affects electron scattering and thereby is accounted for by the finite size of the proton. We will consider nucleon structure effects to be negligible and will use Salpeter's (*9*, *17*) value of 10% of (4.9) as an estimate of unaccounted-for nuclear structure effects. Their smallness is at least partially verified by the good agreement with experiment for the difference between Lamb shifts in deuterium and hydrogen, which is strictly due to nuclear effects.

The uncertainty (4.11c) in the fine structure and other physical constants is seen by (4.14) to make the Lamb shift uncertain by 39 ppm, or

$$\pm 0.041; \qquad \pm 0.55 \text{ Mc/sec} \tag{4.20}$$

for $Z = 1, 2$. This and the contributions of the quoted uncertainties in the coefficient[11] in (4.5) and the nuclear radii in (4.10c) are added in Table III to the estimated bounds of the omitted terms. The results are roughly on a par with the error limits quoted for the measurements, which are three times the standard deviation plus an estimated uncertainty (of the order of the standard deviation) for corrections. That is, both the experimental and theoretical uncertainties represent absolute limits of error, many times larger than the expected error.[11]

The final results are compared with the measurements (*25*, *26*) in Table IV. Except for hydrogen, the differences between experiment and theory are seen

[11] The presumed rigorous upper and lower bounds giving the uncertainty in the coefficient in (4.5) have been found to be violated for some of the individual integrals in that calculation (private communication from Max Soto) and therefore do not meet our criterion of being an absolute limit of error. However, rather than dropping the whole term and adding perhaps twice its magnitude to the uncertainties, we use the quoted values in the expectation that exact calculations will be completed soon (private communication from Max Soto) and in the hope that their results will be favorable, as noted in the text.

TABLE IV

LAMB SHIFT ($2S_{1/2}$–$2P_{1/2}$) (Mc/sec)

	H	D	D − H	He^+
Theory	1057.643 ± 0.21	1058.906 ± 0.27	1.263 ± 0.08	14040.48 ± 6.0
Experiment	1057.77 ± 0.10[a]	1059.00 ± 0.10[a]	1.23 ± 0.15[a]	14040.2 ± 4.5[b]

[a] Reference *25*.

[b] Reference *26*.

to be less than one quarter of the combined error limits, a very satisfactory result. (As in an earlier comparison (*18*), there is fortuitously an essentially exact agreement for ionized helium.) For hydrogen, the difference is less than half the combined error limits, still a satisfactory comparison. The comparison would be improved even further with an increase in the $\alpha^2(Z\alpha)^4$ coefficient in (4.5) within its quoted limits.[11] In fact, with an optimum result for that coefficient, all differences between theory and experiment could be brought to within one-fifth of the combined error limits (even with the large uncertainty due to that coefficient removed from the error limits).[12]

For completeness, we have listed other Lamb shifts (*27–32*) in Table V, although their accuracy is not as great as those in Table IV. It might be noted that the lowest order Lamb shift calculation for two-electron atoms (*30*) is quiet similar to that presented here, while the calculation for $Z = 80$ involves quite a different type of approximation (*32*) since $Z\alpha \approx 0.6$.

APPENDIX

For the integral in Eq. (3.41) we use the nonrelativistic S-state wave functions in the momentum representation,

$$\phi_{nS}^{\mathrm{NR}}(p) = \frac{(2\beta)^{5/2}}{2\pi} \frac{1}{(p^2 + \beta^2)^2} C_{n-1}^1\left(\frac{p^2 - \beta^2}{p^2 + \beta^2}\right), \tag{A1}$$

where C_{n-1}^1 is a Gegenbauer polynomial. It is convenient to use the variable

$$\zeta = 2 \cot^{-1} p/\beta, \tag{A2}$$

for which

$$2\beta \int_0^\infty \frac{dp}{p^2 + \beta^2} f\left(\frac{p^2 - \beta^2}{p^2 + \beta^2}\right) = \int_0^\pi d\zeta\, f(\cos\zeta), \tag{A3}$$

[12] *Note added in proof*: In a recent paper, Robiscoe (*33*) reports a new measurement of the Lamb shift in H. His result is 1058.07 ± 0.10 Mc/sec, which disagrees with Lamb value (25) by 0.3 Mc/sec, and with the theoretical value by 0.4 Mc/sec, which is outside the combined errors of theory and experiment. Robiscoe states that these discrepancies cannot be regarded as firmly established until his value has been confirmed by an independent measurement.

TABLE V

OTHER LAMB SHIFTS

	RF measurements (Mc/sec)			
	$D(n = 3)$[a]	$D(n = 4)$[a]	$D(n = 3; j = 3/2)$[a]	$H(n = 3)$[b]
Experiment	$315.30 \pm .80$	133.0 ± 10	5.0 ± 10	313.6 ± 5.7
Theory	315.34	133.16	5.3	314.7

	Optical measurements (cm^{-1})[c]			
	$D(1S)$	$D(2S)$	$D(3S)$	$T(2S)$
Experiment	$0.26_2 \pm 0.03_8$	0.0369 ± 0.0016	$0.0083^{+0.002}_{-0.003}$	$0.037^{+0.002}_{-0.004}$
Theory	0.273	0.0353	0.0105	0.035

	He^+ $(n = 2)$	He^+ $(n = 3)$	He^+ $(n = 4)$	He^+ $(4S)$	H^{4+} $(4P)$
Experiment	0.48_0	0.140 ± 0.005	0.05_9	0.056 ± 0.003	0.011 ± 0.003
Theory	0.468	0.140	0.059	0.058	0.001

	Ionization energy for two-electron atoms (cm^{-1})		
	He $(1\,^1S)$[d]	He $(2\,^1S)$[d]	He $(2\,^3S)$[d]
Experiment	198 310.82 ± 0.15	32 033.26 ± 0.03	38 454.73 ± 0.05
Theory	198 310.685 ± 0.005	32 033.214 ± 0.014	38 454.718 ± 0.009
(L. S.)	(−1.341)	(−0.104)	(−0.109)

	Li^+ $(1\,^1S)$[d]	Li^+ $(2\,^1S)$[e]	Li^+ $(2\,^3S)$[d]
Experiment	610 079.4 ± 3	118 704.82 ± 0.15	134 044.19 ± 0.10
Theory	610 079.61	118 704.88	134 044.12
(L. S.)	(−7.83)	(−0.69)	(−1.14)

	Absorption edge for the K electron in Hg (Ry)[f]
Experiment	6107.7 ± .6
Theory	6099
(L. S.)	(−38)

[a] Reference *27*.
[b] Reference *28*.
[c] Reference *29*.
[d] Reference *30*.
[e] Reference *31*.
[f] Reference *32*.

$$C_{n-1}^{1}\left(\frac{p^2-\beta^2}{p^2+\beta^2}\right)=\frac{\sin n\zeta}{\sin\zeta}\,, \tag{A4}$$

$$\ln\frac{(Z\alpha)^2m^2}{p^2+\beta^2}=2\ln\frac{n}{2}-2\sum_{r=1}^{\infty}\frac{\cos r\zeta}{r}\,, \tag{A5}$$

$$\begin{aligned}\int d\Omega\,\frac{\mathbf{p}\cdot(\mathbf{p}-\mathbf{p}')}{(\mathbf{p}-\mathbf{p}')^2}&=2\pi\left[1+\frac{p^2-p'^2}{4pp'}\ln\left(\frac{p+p'}{p-p'}\right)^2\right]\\&=2\pi\left[1+\frac{1}{\cot\frac{1}{2}\zeta\cot\frac{1}{2}\zeta'}\left(\frac{1}{\sin^2\frac{1}{2}\zeta}-\frac{1}{\sin^2\frac{1}{2}\zeta'}\right)\right.\\&\qquad\left.\cdot\sum_{s=1}^{\infty}\frac{\sin s\zeta\sin s\zeta'}{s}\right],\end{aligned} \tag{A6}$$

and the integral becomes

$$\begin{aligned}L_{nS}^{(0)}&=\frac{1}{4\pi^2\beta^3}\int d^3p\,\phi_{nS}^{\mathrm{NR}}(p)\int d^3p'\,\phi_{nS}^{\mathrm{NR}}(p')\ln\frac{(Z\alpha)^2m^2}{p^2+\beta^2}\frac{\mathbf{p}\cdot(\mathbf{p}-\mathbf{p}')}{(\mathbf{p}-\mathbf{p}')^2}\\&=\frac{1}{\pi^2}\int_0^{\pi}d\zeta\sin n\zeta\int_0^{\pi}d\zeta'\sin n\zeta'\left[2\ln\frac{n}{2}-2\sum_{r=1}^{\infty}\frac{\cos r\zeta}{r}\right]\\&\qquad\cdot\left\{\cot\tfrac{1}{2}\zeta\cot\tfrac{1}{2}\zeta'+\left(\frac{1}{\sin^2\frac{1}{2}\zeta}-\frac{1}{\sin^2\frac{1}{2}\zeta'}\right)\sum_{s=1}^{\infty}\frac{\sin s\zeta\sin s\zeta'}{s}\right\}.\end{aligned} \tag{A7}$$

With the integrals

$$\frac{1}{\pi}\int_0^{\pi}d\zeta'\sin n\zeta'\cot\tfrac{1}{2}\zeta'=1, \tag{A8}$$

$$\frac{1}{\pi}\int_0^{\pi}d\zeta'\sin n\zeta'\sin s\zeta'=\tfrac{1}{2}\delta_{ns}\,, \tag{A9}$$

$$\frac{1}{\pi}\int_0^{\pi}d\zeta'\sin n\zeta'\frac{\sin s\zeta'}{\sin^2\frac{1}{2}\zeta'}=2\min(n,s), \tag{A10}$$

we get

$$\begin{aligned}L_{nS}^{(0)}&=\frac{1}{\pi}\int_0^{\pi}d\zeta\sin n\zeta\left[2\ln\frac{n}{2}-2\sum_{r=1}^{\infty}\frac{\cos r\zeta}{r}\right]\\&\qquad\cdot\left\{\cot\tfrac{1}{2}\zeta+\frac{\sin n\zeta}{2n\sin^2\frac{1}{2}\zeta}-2\sum_{s=1}^{\infty}\min(n/s,1)\sin s\zeta\right\}.\end{aligned} \tag{A11}$$

Finally, with the previous integrals and the more general integrals

$$\frac{1}{\pi}\int_0^{\pi}d\zeta\sin n\zeta\cos r\zeta\cot\tfrac{1}{2}\zeta=\left\{\begin{array}{ll}1 & r<n\\ \tfrac{1}{2} & r=n\\ 0 & r>n\end{array}\right\}, \tag{A12}$$

$$\frac{1}{\pi}\int_0^{\pi} d\zeta \sin n\zeta \cos r\zeta \sin s\zeta = \tfrac{1}{4}\left[\delta_{r-n+s} + \delta_{r-s+n} - \delta_{r-n-s} - \delta_{r+n+s}\right] \tag{A13}$$

$$\frac{1}{\pi}\int_0^{\pi} d\zeta \sin n\zeta \cos r\zeta \frac{\sin n\zeta}{\sin^2 \frac{1}{2}\zeta} = \begin{Bmatrix} 2n - r & 0 \leqq r \leqq 2n \\ 0 & r \geqq 2n \end{Bmatrix}, \tag{A14}$$

we find

$$\begin{aligned} L_{ns}^{(0)} &= 2\ln\frac{n}{2}\left\{1 + \frac{2n}{2n} - \frac{2n}{2n}\right\} - 2\left\{\sum_{r=1}^{n-1}\frac{1}{r} + \frac{1}{2n} + \sum_{r=1}^{2n}\frac{2n-r}{2nr}\right. \\ &\quad \left. - 2\left[\sum_{s=1}^{n-1}\frac{1}{4}\left(\frac{1}{n-s} - \frac{1}{n+s}\right) + \frac{1}{4}\left(\frac{-1}{2n}\right)\right.\right. \\ &\quad \left.\left. + \sum_{s=n+1}^{\infty}\frac{n}{s}\frac{1}{4}\left(\frac{1}{s-n} - \frac{1}{s+n}\right)\right]\right\} \\ &= 2\ln\frac{n}{2} - 2\sum_{r=1}^{n}\frac{1}{r} + \frac{1}{n} - 2\sum_{r=1}^{2n}\frac{1}{r} + 2\frac{2n}{2n} + \sum_{t=1}^{n-1}\frac{1}{t} \\ &\quad - \sum_{t=n+1}^{2n}\frac{1}{t} + \sum_{t=1}^{n}\frac{n}{t(t+n)} \\ &= 2\ln\frac{n}{2} + 2 - 4\left(1 + \frac{1}{3} + \frac{1}{5} + \cdots + \frac{1}{2n-1}\right). \end{aligned} \tag{A15}$$

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