Radiative Level Shifts. III. Hyperfine Structure in Hydrogenic Atoms*

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A comprehensive calculation of the second-order quantum-electrodynamic corrections to the hyperfine splitting of S states is presented. The gauge-invariant reduction of the self-energy expression given by Yennie and Erickson is used to systematically verify previous calculations of orders α , $\alpha(Z\alpha)$, $\alpha(Z\alpha)^{2}\ln^{2}(Z\alpha)^{-2}$, and $\alpha(Z\alpha)^{2}\ln(Z\alpha)^{-2}$ relative to the lowest order Fermi splitting E^{F} and to obtain a result for the dominant contribution to order $\alpha(Z\alpha)^2$ for the 1S and 2S levels. The new contribution for the 1S state is

 $(\alpha/\pi)(Z\alpha)^{2}[18.4\pm5]E^{F} = [2.3\pm0.6]\times10^{-6}E^{F},$

where α is the fine-structure constant, $Z\alpha$ is the strength of the Coulomb potential, and the error limits are estimates of uncalculated terms. Our results for n=2 provide a substantial check of Zwanziger's calculation of the hyperfine splittings in the 1S and 2S levels.

1. INTRODUCTION

HE recent measurement of the hyperfine structure of muonium¹ and the persistent discrepancy between theory and precise measurements of the hyperfine structure of hydrogen² have led to renewed interest in the theoretical calculations.³⁻⁶ In this paper, the third in a series on the calculation of radiative level shifts,⁷ we present a comprehensive calculation of the second-order quantum-electrodynamic corrections to the hyperfine splitting of S states. By employing a gauge-invariant reduction of the self-energy expression and computational techniques developed by Erickson and Yennie,7 we are able to systematically verify previous calculations of order α , $\alpha(Z\alpha)$, $\alpha(Z\alpha)^2 \ln^2(Z\alpha)^{-2}$, $\alpha(Z\alpha)^2 \ln(Z\alpha)^{-2}$ relative to the lowest order Fermi formula and obtain a new result for the dominant contribution to order $\alpha(Z\alpha)^2$ for the 1S and 2S levels. $[\ln^2 x \equiv (\ln x)^2.]$ This new contribution is found to be

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 ¹ W. E. Cleland, J. M. Bailey, M. Eckhause, V. W. Hughes, R. M. Mobley, R. Prepost, and J. E. Rothberg, Phys. Rev. Letters 13, 202 (1964).
 ² S. B. Crampton, D. Kleppner, and N. F. Ramsey, Phys. Rev. Letters 11, 338 (1963).
 ³ A. L. Lavzer, Bull. Am. Phys. Soc. 6, 514 (1964); Nuova
- ³ A. J. Layzer, Bull. Am. Phys. Soc. 6, 514 (1961); Nuovo Cimento 33, 1538 (1964).
- ⁴ D. E. Zwanziger, Bull. Am. Phys. Soc. 6, 514 (1961); Nuovo Cimento 34, 77 (1964).
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⁶ Suggestions of new contributions to the hydrogen hyperfine structure have been made by C. K. Iddings (Ref. 5), by S. Fenster, R. Köberle, and Y. Nambu, Phys. Letters 19, 513 (1965) ^{renster, R.} Koberle, and Y. Nambu, Phys. Letters 19, 513 (1965) and, Progr. Theoret. Phys. (Kyoto) Suppl., Extra Number, 250 (1965), and by S. D. Drell and J. D. Sullivan, Phys. Letters 19, 516 (1965) and private communication.
⁷ G. W. Erickson and D. R. Yennie, Ann. Phys. (N. Y.) 35, 271 (1965); 35, 447 (1965). These references are referred to as papers I and II, respectively.

an order of magnitude larger than its nominal order and, in fact, its contribution is twice as large (in the opposite direction) as the contribution of order $\alpha(Z\alpha)^2 \ln(Z\alpha)^{-2}$. If the accuracy of the measurement of the muonium hfs1 (and of the magnetic moment of the muon) is improved, this new term will be important for the accurate determination of the fine-structure constant.

Before presenting the calculations we will briefly review the various contributions to the hyperfine structure of the S-state levels of the hydrogenic atom. The correct covariant treatment of the energy levels of the two-body system proceeds from the Bethe-Salpeter bound-state equation. Its reduction to physical terms is facilitated by the use of four dimensionless parameters: the electron-to-nucleus mass ratio m/M, the ratio of nuclear and atomic sizes R/a_0 , the fine-structure constant α , and the strength of the Coulomb potential $Z\alpha$.

In first approximation $(m/M \rightarrow 0, R/a_0 \rightarrow 0, \alpha \rightarrow 0)$ one may take the electron to obey the Dirac equation with fixed Coulomb and magnetic dipole potentials

$$V = -Z\alpha/r, \quad \mathbf{A} = \mathbf{\mu} \times \mathbf{r}/r^3,$$

where $\mathbf{u} = g(|\mathbf{e}|/2M)\mathbf{I}$ is the nuclear-magnetic dipole operator. To first order in the magnetic moment, but to all orders in $Z\alpha$, the energy separation of the singlet and triplet levels of the nS state is⁸

$$\delta E_n^{(1)} = E_n^F [1 + (Z\alpha)^2 b(n)], \qquad (1.1)$$

where

$$E_n^F = \frac{|e|}{2m} \frac{8\pi}{3} |\boldsymbol{\phi}_n(0)|^2 \langle \boldsymbol{\sigma} \cdot \boldsymbol{y} \rangle \Big|_{(F=1)-(F=0)}$$
(1.2)

is the Fermi energy difference representing the non-

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 $^{{}^{8}\}phi_{n}(r)$ is the nonrelativistic wave function for the nS states. The units are $\hbar = c = 1$, $\alpha = e^2$, where e = -|e| is the charge of the electron. $\mathbf{F} = \mathbf{I} + \mathbf{S}$ is the total spin.

relativistic interaction of the magnetic moment density of the electron (evaluated at the nuclear position) and the nuclear magnetic moment. The term $(Z\alpha)^2 b(n)$ is the Breit relativistic correction,⁹ which is $(\frac{3}{2})(Z\alpha)^2$ $+O(Z\alpha)^4$ and $(17/8)(Z\alpha)^2+O(Z\alpha)^4$ for the 1S and 2S levels, respectively. E_n^F is the lowest order expression for the hyperfine separation and all corrections will be expressed as multiples of it.

At the second level of approximation one continues to treat the nucleus as a fixed point potential $(m/M \rightarrow 0)$ and $R/a_0 \rightarrow 0$) but now considers contributions of radiative corrections of relative order α , α^2 , \cdots , evaluating these terms to first order in the nuclear moment using Dirac states for the electron in Coulomb and magnetic dipole potentials. The functional dependence of the radiative corrections is not analytic in $Z\alpha$ but actually has the form

$$\delta E_{n}^{(2)} = E_{n}^{F} \left\{ \frac{\alpha}{2\pi} - 0.328 \frac{\alpha^{2}}{\pi^{2}} + c_{1}\alpha(Z\alpha) + \frac{\alpha}{\pi} (Z\alpha)^{2} [c_{22} \ln^{2}(Z\alpha)^{-2} + c_{21}(n) \ln(Z\alpha)^{-2} + c_{20}(n)] + \frac{\alpha^{3}}{\pi^{3}} + \frac{\alpha^{2}}{\pi^{2}} Z\alpha + \cdots \right\}, \quad (1.3)$$

i.e., a series in α , $Z\alpha$, and $\ln(Z\alpha)^{-2}$. The first two terms are the corrections to the static magnetic moment of the electron. The other terms arise when binding is taken into account. The term of order $\alpha(Z\alpha)F_n^F$ was found by Kroll and Pollack¹⁰ and Karplus, Klein, and Schwinger¹¹ to be given by

$$c_1 = -\frac{5}{2} + \ln 2$$
.

More recently, Zwanziger¹² calculated the (n=2)-(n=1) difference of the coefficients in the second line of (1.3),

$$\begin{bmatrix} c_{21}(2) - c_{21}(1) \end{bmatrix} \ln(Z\alpha)^{-2} + \begin{bmatrix} c_{20}(2) - c_{20}(1) \end{bmatrix} = (7/2 - 8/3 \ln 2) \ln(Z\alpha)^{-2} - 2.619 + \pi(-0.94 \pm 0.02)$$

and, since then, Layzer³ and Zwanziger⁴ have obtained the separate coefficients of the logarithmic terms,

$$c_{22} = -\frac{2}{3},$$

$$c_{21}(1) = \frac{37}{72} + \frac{4}{15} - \frac{8}{3} \ln 2,$$

$$c_{21}(2) = -\frac{16}{3} \ln 2 + 4 + \frac{1}{72} + \frac{4}{15}.$$

Finally, at the third level of calculation one must consider the effects of a nucleus of finite size and mass. These terms arise in the reduction¹³ of the two-body Bethe-Salpeter equation and correspond physically to recoil, second-order perturbation in the dipole potential, nuclear polarization, etc. The main effect of recoil is conventionally summarized by using the reduced mass instead of the electron mass in evaluating the wavefunction in (1.2). We thus include with E_n^F the over-all correction factor

$$\left(\frac{M}{M+m}\right)^3.\tag{1.4}$$

The remainder of the nuclear corrections¹⁴ beyond those given by (1.4) and its cross terms with (1.3) is nontrivial. For muonium, the additional nuclear correction is

$$\delta E_n^{(3)} = E_n^F \left[-\frac{3\alpha}{\pi} \frac{mM}{M^2 - m^2} \ln \frac{M}{m} \right] \equiv E_n^F \delta_\mu \quad (1.5)$$

to lowest order in α and $Z\alpha$. For hydrogen, one obtains

$$\delta E_n^{(3)} = E_n^F \left[-8.7 \alpha \frac{m}{M} \right]$$
$$= E_n^F \left[-35 \times 10^{-6} \right] \equiv E_n^F \delta_p, \qquad (1.6)$$

assuming photon-proton interactions are described by elastic-scattering form factors. Nuclear-polarization corrections to this assumption have been found to be negligible.5

The total hyperfine splitting of the ground state is then

$$\delta E_{1} = E_{1}^{F} \left(\frac{M}{M+m} \right)^{3} \left\{ 1 + \delta_{\text{nucl}} + \frac{3}{2} (Z\alpha)^{2} + \frac{\alpha}{2\pi} - 0.328 \frac{\alpha^{2}}{\pi^{2}} - \alpha (Z\alpha) \left(\frac{5}{2} - \ln 2\right) + \frac{\alpha}{\pi} (Z\alpha)^{2} \left[-\frac{2}{3} \ln^{2} (Z\alpha)^{-2} + \left(\frac{37}{72} + \frac{4}{15} - \frac{8}{3} \ln 2\right) \times \ln (Z\alpha)^{-2} + c_{20}(1) \right] \right\}, \quad (1.7)$$

where we have neglected terms explicitly third order in the small parameters. We compare δE_1 with experiment in Sec. 7 using the most accurately known physical constants¹⁵ and the dominant part of the c_{20} coefficient.

Because of the interest in obtaining as reliable a theoretical prediction as possible, we shall present a new unified derivation of the $Z\alpha$ expansion of the radiative correction of order α relative to the hyperfine

 ⁹ G. Breit, Phys. Rev. 35, 1447 (1930).
 ¹⁰ N. Kroll and F. Pollack, Phys. Rev. 84, 597 (1951); 86, 876 (1952).

¹¹ R. Karplus, A. Klein, and J. Schwinger, Phys. Rev. 84, 597 (1951). ¹² D. E. Zwanziger, Phys. Rev. 121, 1128 (1960).

¹³ M. M. Sternheim, Phys. Rev. **130**, 211 (1963); W. A. Barker and F. N. Glover, *ibid.* **99**, 317 (1955). ¹⁴ C. Iddings and P. Platzman, Phys. Rev. **113**, 192 (1959) and **115**, 919 (1959); R. Arnowitt, *ibid.* **92**, 1002 (1953); W. Newcomb and E. Salpeter, *ibid.* **97**, 1146 (1955); A. C. Zemach, *ibid.* **104**, 1771 (1956) 1771 (1956)

¹⁵ Phys. Today 17, No. 2, 48 (1964); J. W. M. Dumond and E. R. Cohen, Rev. Mod. Phys. 37, 537 (1965). The errors given in (7.6)-(7.8) are three standard deviations.

formula. The calculation given here has several distinct advantages. First, the calculation retains gauge invariance up to the point of the evaluation of matrix elements. Thus there is no cancellation of spurious gaugevariant terms and the terms that do occur are readily interpretable in physical language. In fact, the calculation proceeds as an expansion in terms of field strengths rather than powers of potentials, and only the first two terms in such a series are required for the coefficients of interest here. Second, the calculation is made quite compact by using an algebraic notation developed in paper I. Finally, we can readily apply the orderdetermining rules discussed in paper II to rigorously identify terms that contribute to a given order, and just as important, rigorously indicate that a given neglected term is of an unimportant higher order in $Z\alpha$.

The calculation will also include an estimate of the size of the $\alpha(Z\alpha)^2 E_n^F$ coefficient $c_{20}(n)$ for n=1 and n=2. We do this for two reasons. In the Lamb shift it is observed that accompanying the $\alpha(Z\alpha)^6 \ln^2(Z\alpha)^{-2}mc^2$ term is a rather large contribution of order $\alpha(Z\alpha)^6mc^2$. Thus, the contribution of order $\alpha(Z\alpha)^2 E_n^F$ might be considerably larger than the nominal order indicates. We will also be able to give a substantial check of Zwanziger's calculation¹² of the ratio of hyperfine splittings in the 1S and 2S levels.

In the next section, we summarize the formal algebraic reduction of the expression for the second-order self-energy correction. In Sec. 3, the calculation procedures are summarized and applied to the evaluation of the lowest order contribution, that of the second-order anomalous magnetic moment. The order-determining rules are given in Sec. 4 and are used to single out the types of terms which contribute to orders of interest. In Sec. 5, the $\alpha(Z\alpha)E_n^F$ terms are identified and calculated. The calculation of the $\alpha(Z\alpha)^2 \ln^2(Z\alpha)^{-2}E_n^F$ and $\alpha(Z\alpha)^2 \ln(Z\alpha)^{-2}E_n^F$ terms (for n=1, 2) is given in Sec. 6, as well as the calculation of the dominant contributions of order $\alpha(Z\alpha)^2 E_n^F$. The results are summarized and discussed in Sec. 7. Appendix A lists the wave functions used in the calculations. Appendix B gives the formal derivation of terms reduced differently in paper I and shows the cancellation of some contributions. The second-order vacuum polarization contribution is calculated in Appendix C. The term giving the dominant contribution to the state dependence of the $\alpha(Z\alpha)^2 E_n^F$ coefficient $c_{20}(n)$ is calculated in Appendix D.

2. REDUCTION OF THE SELF-ENERGY **EXPRESSION**

Quantum-electrodynamic corrections of order α to atomic spectra correspond to two types of Feynman diagrams, the self-energy correction to the bound electron current and vacuum polarization. In effect these radiative corrections modify the electron's magnetic moment and spread its electromagnetic distribution, both effects being directly observable in the hyperfine structure of S states. The vacuum

polarization effect is straightforward to evaluate and will be briefly dealt with in Appendix C.

The starting point for the calculation of the secondorder self-energy correction to the energy of an electron bound in a fixed potential A^{*} is the formal, gaugeinvariant expression,¹⁶ (I-2.1)

$$\Delta E_{n} = \frac{\alpha}{4\pi} \int \frac{d^{4}k/\pi^{2}i}{k^{2} + i\epsilon} \left\langle n \left| \gamma_{\mu} \frac{1}{\mathbf{\Pi} - \mathbf{k} - m + i\epsilon'} \gamma^{\mu} \right| n \right\rangle - \left\langle n \left| \delta m \right| n \right\rangle. \quad (2.1)$$

In accordance with Sec. 1 we are to evaluate ΔE_n to first order in the nuclear magnetic moment $\boldsymbol{\mu}$ in states $|n\rangle$ which satisfy the Dirac equation with Coulomb and magnetic dipole potentials,¹⁷

$$eA^{\nu} = \left(-\frac{Z\alpha}{r}, \frac{e\mathbf{u} \times \mathbf{r}}{r^3}\right). \tag{2.2}$$

The resulting energy difference $\Delta E_n(F=1) - \Delta E_n(F=0)$ will then have the form $\alpha f_n(Z\alpha)E_n^F$.

Observing that ΔE_n depends on the external potential A^{ν} through the operators

$$\Pi^{\nu} \equiv p^{\nu} - eA^{\nu} \equiv (E_n - eA^0, \mathbf{p} - e\mathbf{A})$$
(2.3)

and the Dirac state satisfying

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

it might seem natural to immediately expand the bound electron Green's function and the wave function in powers of A^{ν} to terms linear in μ and the first few terms in $Z\alpha \cong 1/137$. This direct approach fails for several reasons. First, a direct expansion in the potential is manifestly non-gauge-invariant and can lead to "false" expansions in which all terms are of the same order in $Z\alpha$ and which sometime contain spurious lower order terms which ultimately cancel.¹⁸ It will be clear that the natural expansion must be in terms of the gaugeinvariant field strength $F_{\mu\nu} \equiv \partial_{\mu}A_{\nu} - \partial_{\nu}A_{\mu}$. Second, ΔE_n contains terms which involve the nonanalytic $\ln(Z\alpha)^{-2}$.

Since ΔE_n is gauge-invariant, it is a function of $F^{\mu\nu}$ rather than the potentials. Moreover, since it is defined to vanish for zero field strength, ΔE_n is presumably at least linear in $F^{\mu\nu}$. In fact, after the d^4k integration has been performed, ΔE_n must take the form

$$\Delta E_n = \alpha \langle n | \cdots F^{\mu\nu} \cdots Q_{\mu\nu} \cdots | n \rangle, \qquad (2.5)$$

¹⁶ The notation is that of J. D. Bjorken and S. D. Drell, *Relativistic Quantum Mechanics* (McGraw-Hill Book Company, Inc., New York, 1964). Scalar products of Dirac matrices with four-vectors are denoted $A \equiv \gamma \cdot A \equiv \gamma \cdot A = \gamma^0 A^0 - \gamma \cdot A$ and $\Pi \equiv \gamma \cdot \Pi \equiv \mathbf{p} - e\mathbf{A}.$

¹⁷ To distinguish the operators, wave functions, etc., which correspond to u=0, we will use the subscript c (for Coulomb potential). For the additional parts linear in the nuclear magnetic moment, we use the subscript μ . For example, the wave function in the complete Coulomb and magnetic dipole potential (2.2), $\phi_n = \phi_{nc} + \delta_{\mu} \phi_n$ or $|n\rangle = |n_c\rangle + |n_{\mu}\rangle$, may be split into a part ϕ_{nc} , which satisfies the Dirac equation without \mathbf{u} , plus a "magnetic correction" $\delta_{\mu} \phi_n$. Details of these wave functions are discussed in Appendix A. ¹⁸ H. M. Fried and D. R. Yennie, Phys. Rev. **112**, 1391 (1958).

where, because of the transformation properties of ΔE_n , $Q_{\mu\nu}$ must be an antisymmetric tensor. The tensors available are (1) $\sigma_{\mu\nu} \equiv [\gamma_{\mu}, \gamma_{\nu}]/2i$, which gives the magnetic moment structure $M \equiv e\sigma_{\mu\nu}F^{\mu\nu}/2 = e\sigma \cdot \mathcal{K} - ie\alpha \cdot \mathcal{E}$; (2) $\Pi_{\mu}\gamma_{\nu} - \Pi_{\nu}\gamma_{\mu}$, which gives the "L" structure $\Pi_{\mu} \cdot [\Pi^{\mu}, \Pi]$; and (3) $F_{\mu\nu}$, corresponding to $\mathcal{E}^2 - \mathcal{K}^2$. The \cdots represent interspersed scalar functions which can involve Π , Π^2 , and M, or scalar combinations such as $\Pi_{\mu} \cdots \Pi^{\mu}$.

A systematic reduction of ΔE_n to calculable terms of the above type is given in paper I. The procedure is gauge-invariant and avoids "false" expansions where actual logarithmic dependences exist. In brief the calculation of $\Delta E_n = 0$ for the case of the free electron $(F^{\mu\nu}=0)$ is used as a guide for the corresponding calculation for a bound electron $(F^{\mu\nu}\neq 0)$. The calculations would in fact be identical and the result $\Delta E_n = 0$ would again be obtained were it not for the fact that the components Π_{μ} do not commute with each other. Remainder terms are thus obtained which are at least linear in the commutator $[\Pi^{\mu},\Pi^{\nu}] = -ieF^{\mu\nu}$; these are listed in Table I. Some modifications in the reduction procedure of paper I are made in Table I which simplify the hyperfine calculations. The new derivations are given in Appendix B.

The double bar \parallel "symmetric insertion" notation used in Table I is a convenient algebraic device for combining several similar terms. For example, I_{L3} is actually the sum of three terms obtained by successively replacing each of the three 1/D factors by $1/D^2$. The $\parallel (1/D^2)$ notation indicates $\parallel (1/D) \parallel (1/D)$, i.e., two consecutive insertions. In I_{M1} , the insertion of $\parallel (1/D)$ into $(1/D_1)$ gives $(1/D_1^2)$. In I_{LM} one is to form terms by replacing each 1/D by (1/D)M(1/D). The reader is referred to Sec. I-2 for the full development of this notation.

The content of the terms in Table I can perhaps best be understood if we calculate them to lowest order in $F^{\mu\nu}$ (only the I_L and I_M terms are required) while approximating each denominator as

$$D_0 = z^2 m^2 + K - k^2 + z(1-z)H.$$
(2.6)

Then, as indicated in later sections, ΔE_n reduces to the sum of two important forms

$$\Delta E_n(L) = -\frac{2\alpha}{3\pi m^2} \left\langle n \left| \mathbf{p} \cdot \left(\ln \frac{m^2}{H} + \frac{11}{24} \right) \left[\mathbf{p}, e \mathbf{A} \right] \right| n \right\rangle,$$
$$\Delta E_n(M) = \frac{\alpha}{2\pi} \left(-\frac{e}{2m} \right) \left\langle n \left| \frac{1}{2} \sigma_{\mu\nu} F^{\mu\nu} \right| n \right\rangle. \tag{2.7}$$

If we had retained the terms involving **p** in the denominators, then the expressions would be modified by "form-factor" functions of \mathbf{p}^2 . These serve to suppress relativistic regions of the matrix-element integration $|\mathbf{p}| \gtrsim m, r \lesssim 1/m$.

The terms $\Delta E_n(L)$ and $\Delta E_n(M)$ give, respectively, corrections to the bound-state energy due to the charge distribution and static anomalous magnetic moment of

TABLE I. The Erickson-Yennie reduction of the one-photon selfenergy expression $\Delta E_n = \frac{\alpha}{4\pi} \int_0^1 dz \int_0^1 d\lambda^2 \int_0^\infty dK \int_F \frac{d^4k}{\pi^2 i} \langle n | I - I_{bm} | n \rangle$ to calculable gauge-invariant terms.

The mass-renormalized operator $I-I_{\delta m}$ is the sum of the following terms ^a
$I_{L1} = 8(1-z^2)z^3m^2 \frac{1}{D_{\lambda}} \frac{1}{D_{\lambda}} \frac{1}{D_{\lambda}} [\Pi^{\nu}, \Pi] \frac{1}{D_{\lambda^2}} \left \frac{1}{D_{\lambda}} \right $
$I_{L2} = -4z(1-z)\Pi_{\nu} \frac{1}{D} [\Pi^{\nu}, \Pi] \frac{1}{D} \left \frac{1}{D^2} \right $
$I_{L3} = -4z^{2}(1-z)\frac{1}{D}\prod_{r}\frac{1}{D}\prod_{r}(\Pi^{r},\Pi^{r})\frac{1}{D}\left \frac{1}{D}\right $
$I_{L4} = -4z^3 \frac{1}{D} \left[\Pi_{\nu, \tau} \frac{1}{D} \left[\Pi^{\nu, \tau}, \Pi \right] \frac{1}{D} \right] \frac{1}{D}$
$I_{M1} = 2(1+z)m\frac{1}{D}z^2M\frac{1}{D_1} \left \frac{1}{D^2} \right $
$I_{M2} = -4m \frac{1}{D} \frac{1}{D} \left \frac{1}{D^2} \right $
$I_{LM} = -2z[I_{L3} + I_{L4}] \left \frac{M}{D} \right $
$I_{a1} = 4(1-z^2)z^3m\frac{1}{D_{\lambda}}\left[\Pi_{\nu},\Pi\right]\frac{1}{D_{\lambda}}\left[\Pi^{\nu},\Pi\right]\frac{1}{D_{\lambda}^2}\left \left \frac{1}{D_{\lambda}}\right \right $
$I_{a2} = -4z^3 m \frac{1}{D} \begin{bmatrix} \Pi_{\nu}, \Pi \end{bmatrix} \frac{1}{D} \begin{bmatrix} \Pi^{\nu}, \Pi \end{bmatrix} \frac{1}{D} \left \left \frac{1}{D^2} \right \right $
$I_{b} = 4(1-z^{2})z^{3}m \left\{ \frac{1}{D_{\lambda}}\Pi_{r} \left[\frac{1}{D_{\lambda}}, \Pi \right] \left[\Pi^{r}, \Pi \right] \frac{1}{D_{\lambda}^{2}} \right\}$
$+ \left[\frac{1}{D_{\lambda}}, \boldsymbol{\Pi}\right] \boldsymbol{\Pi}_{\boldsymbol{r}} \frac{1}{D_{\lambda}} [\boldsymbol{\Pi}^{\boldsymbol{r}}, \boldsymbol{\Pi}] \frac{1}{D_{\lambda}^{2}} + \frac{1}{D_{\lambda}} \boldsymbol{\Pi}_{\boldsymbol{r}} \frac{1}{D_{\lambda}} [\boldsymbol{\Pi}^{\boldsymbol{r}}, \boldsymbol{\Pi}] \left[\boldsymbol{\Pi}, \frac{1}{D_{\lambda}^{2}}\right] \right\} \left \left \frac{1}{D_{\lambda}} \right \frac{1}{D_{\lambda}} \left[\frac{1}{D_{\lambda}} \right] \right \frac{1}{D_{\lambda}} \left[\frac{1}{D_{\lambda}} \right] \frac{1}{D_{\lambda}} \frac{1}{D_{\lambda}} \left[\frac{1}{D_{\lambda}} \right] \frac{1}{D_{\lambda}} \frac{1}{D_$
$I_{c} = 4(1+z)z^{3}m\lambda \frac{1}{D_{\lambda}}\Pi_{\nu}\frac{1}{D_{\lambda}}\left\{\left(k-\lambda z\Pi\right)_{\mu},\left[\Pi^{\mu},\Pi^{\nu}\right]\right\}\frac{1}{D_{\lambda}^{2}}\left \left \frac{1}{D_{\lambda}}\right \right $
$I_{d} = 4z^{2} \left\{ \frac{1}{D} \left[\Pi_{\mu}, D \right] \left(\frac{1}{D} \left[\Pi^{\mu}, \Pi \right] \frac{1}{D} \right] \left \frac{1}{D} \right) \right\}$
$-\frac{1}{D} \begin{bmatrix} \Pi^{\mu}, \Pi \end{bmatrix} \frac{1}{D} \begin{bmatrix} \Pi_{\mu}, D \end{bmatrix} \frac{1}{D^2} \bigg\} \bigg \bigg \frac{1}{D}$
$I_{e} = -4z^{2}(\boldsymbol{k} - z\boldsymbol{\Pi}) \frac{1}{D} [\boldsymbol{\Pi}_{\mu}, \boldsymbol{\Pi}] \frac{1}{D} [\boldsymbol{\Pi}^{\mu}, \boldsymbol{\Pi}] \frac{1}{D} \bigg \bigg \frac{1}{D^{2}}$
Notation: $D = r^2 m^2 + K = (h - r \Pi)^2 + r(1 - r) H = r^2 M$
$D_{\lambda} = z^{2}m^{2} + K - (k - \lambda z \Pi)^{2} + z(1 - z)H$
$D_1 = z^2 m^2 + K - (k - z\Pi)^2 + z(1 - z)H$
$M = \Pi^2 - \Pi^2 = e\sigma_{\mu\nu}F^{\mu\nu}/2$

 $H \equiv m^2 - \Pi^2$

^a The terms labeled I_{LM} , I_c , I_d , I_e correspond to a different arrangement of the terms labeled I_c , I_d , I_e , I_f in paper I. The new derivations are given in Appendix B. the electron.¹⁹ The quantity H in $\Delta E_n(L)$ is the Dirac Hamiltonian

$$H \equiv m^{2} - \Pi^{2} = 2m [\mathbf{p}^{2}/2m + V + \epsilon_{n}] - [e\sigma_{\mu\nu}F^{\mu\nu}/2 + \mathbf{p} \cdot e\mathbf{A} + e\mathbf{A} \cdot \mathbf{p}] + [\mathbf{A}^{2} - V^{2} - 2\epsilon_{n}V - \epsilon_{n}^{2}]. \quad (2.8)$$

Note that *H* vanishes acting on the state $|n\rangle$ and depends on *n* through the binding energy $\epsilon_n \equiv m - E_n > 0$. The $\ln(m^2/H)$ term arises in connection with the infrared behavior of the photon; the binding of the electron serves to cut off what would be a logarithmically divergent d^4k integration in the case of the free electron. Employing a sum over states, this term gives the famous Bethe sum for the Lamb shift and is of order of magnitude $(4\alpha Z\alpha/3m^2) \ln(Z\alpha)^{-2} |\phi_n(0)|^2$.

The terms proportional to \boldsymbol{u} in $\Delta E_n(L)$ will be shown to be of orders

$$\alpha(Z\alpha)E_n^F$$
, $\alpha(Z\alpha)^2 \lceil \ln^2(Z\alpha)^{-2}, \ln(Z\alpha)^{-2}, 1 \rceil E_n^F$.

The quadratic logarithm term arises from the confluence of the "infrared" photon integration with an integration over the electron's coordinates which could diverge logarithmically were it not for the form-factor cutoff in the relativistic integration region. The terms linear in $\boldsymbol{\mathfrak{y}}$ in $\Delta E_n(M)$ give the anomalous moment correction $(\alpha/2\pi)E_n^F$ plus terms of order

$$\alpha(Z\alpha)E_n^F$$
, $\alpha(Z\alpha)^2[\ln(Z\alpha)^{-2},1]E_n^F$.

Other contributions to order $\alpha(Z\alpha)E_n^F$ are found to arise from the parts of I_L , I_M , and I_{LM} which are quadratic in $F^{\mu\nu}$. The remaining terms only contribute to order $\alpha(Z\alpha)^2E_n^F$ or higher.

3. CALCULATION PROCEDURES AND THE LOWEST ORDER MAGNETIC MOMENT CORRECTION

We shall first discuss in a general manner the procedures used to reduce the terms I(D) of ΔE_n to a calculable form. The essential problem is that the denominators D and D_1 involve momenta and potentials in a rather complicated way; hence, we must resort to expansions. The following is a useful reduction sequence:

- (i) Neglect $z^2 M$ in each denominator: $I(D) \rightarrow I(D_1)$;
- (ii) "Shift" $(k \lambda z \Pi)^2$ to $k^2 \colon I(D_1) \to I(D_0);$
- (iii) Take $H \doteq 0$ in those denominators next to the wave functions.

For each step we must later consider the resulting error or correction terms. One of the most useful results of Paper II is a simple rule which indicates rigorously the orders in $Z\alpha$ and $\ln Z\alpha$ to which a given term may contribute. In the next section we review the notation involved and extend the rule to situations where hyperfine operators or hyperfine wave functions are involved. Suffice it to say for the present that the reduction sequence is chosen so that the correction terms to steps (i) and (ii) are almost invariably higher order than the original term; the order is never decreased. "Outside" denominators (acting on wave functions) are now functions of H alone so there is no error in performing step (iii). After these steps any "inside" denominators still retain their dependence on H. A possible calculation procedure is to insert a complete set of Dirac states and evaluate the matrix element numerically, as in the Bethe sum term. For the hyperfine radiative corrections we shall find that the sumover-states calculation can be postponed by approximating $H \rightarrow \mathbf{p}^2$ in the inside denominators, the error being a small contribution of order $\alpha(Z\alpha)^2 E_n^F$. With such a procedure we can write the entire denominator as a function of p alone, and the matrix element can be evaluated analytically in the momentum representation.

The application of the standard steps (i), (ii), (iii) to the I_M terms is straightforward. After performing step (i) by neglecting z^2M in each denominator, we set aside for future investigation the correction term

$$I_{M1-M} \equiv 2(1+z)m \frac{1}{D} z^2 M \frac{1}{D_1} z^2 M \frac{1}{D_1} \left| \left| \frac{1}{D^2} \right| \right|$$
(3.1)

and similar terms from I_{M2} . It will prove convenient to write the results of step (i) in the form²⁰

$$I_{M}(D_{1}) = [2(1+z)-4]z^{2}m\frac{1}{D_{1}}[M_{\mu}+2\mathbf{p}\cdot e\mathbf{A}]\frac{1}{D_{1}}\Big|\Big|\frac{1}{D_{1}^{2}} + [2(1+z)-4]z^{2}m\frac{1}{D_{1}}[M_{c}-2\mathbf{p}\cdot e\mathbf{A}]\frac{1}{D_{1}}\Big|\Big|\frac{1}{D_{1}^{2}}, \quad (3.2)$$

where

$$M_{\mu} = e \boldsymbol{\sigma} \cdot \boldsymbol{\mathcal{K}}, \quad M_{c} = -i e \boldsymbol{\alpha} \cdot \boldsymbol{\mathcal{E}}.$$
 (3.3)

We shall postpone discussion of the higher order terms in the second line of (3.2) until Sec. 6. For step (ii), we shift $D_1 \rightarrow D_0$ and again set aside the correction terms, which may be written as an expansion in powers of $D_1-D_0=2zk\cdot\Pi-z^2\Pi^2$. After step (ii), all of the denominators D_0 are next to the wave functions, and thus automatically become simply $D_{00}=z^2m^2+K-k^2$.

¹⁹ The operators in $\Delta E_n(L)$ and $\Delta E_n(M)$ can be interpreted as the nonrelativistic limit $(\mathbf{q}^2 \ll m^2)$ of the order α renormalized bound-electron current in interaction with the external potential. The $\ln(m^2/H)$ term shows that the Dirac component of this current depends in an essential way on the external potential.

²⁰ This separation avoids introducing a spurious divergence due to relativistic wave functions when $D_1 \rightarrow D_0$.

After this, we need only evaluate²¹

$$\Delta E_{n}(M_{\mu}) \equiv \frac{\alpha}{4\pi} \int_{0}^{1} dz \ 2(-1+z) \int_{0}^{\infty} dK$$

$$\times \int \frac{d^{4}k}{\pi^{2}i} \frac{1}{D_{00}^{2}} \left| \left| \frac{1}{D_{00}^{2}} \langle n_{c} \right| M_{\mu} + 2\mathbf{p} \cdot e\mathbf{A} \right| n_{c} \rangle$$

$$= \frac{\alpha}{2\pi} \left\langle n_{c} \left| \frac{-1}{2m} (M_{\mu} + 2\mathbf{p} \cdot e\mathbf{A}) \right| n_{c} \right\rangle$$

$$= \frac{\alpha}{2\pi} \langle n_{c} \right| - \gamma \cdot e\mathbf{A} | n_{c} \rangle$$

$$= \frac{\alpha}{2\pi} \delta E_{n}^{(1)}, \qquad (3.4)$$

where $\delta E_n^{(1)}$ is the Fermi energy including the Breit relativistic wave-function corrections. $\Delta E_n(M_{\mu})$ is the energy shift corresponding to the electron's anomalous magnetic moment of order α .

4. IDENTIFICATION OF CONTRIBUTING TERMS

In order to calculate ΔE_n to a specific order in $Z\alpha$ (and in fact, $\ln Z\alpha$) it is clear that because of the complexity of the terms I(D) and their many possible expansions in terms of unbounded operators, a simple method is needed to determine the order of magnitude of the neglected terms. A rigorous analysis of the structure of the matrix elements and the parametric integrations of ΔE_n has yielded such an order-determining rule (Sec. II-5). This rule of order is most simply understood applied to a term I_K of ΔE_n which has already been reduced to a nonrelativistic matrix element by performing the Dirac algebra and approximating the relativistic states as Pauli-Schrödinger wave functions. We also suppose that the denominators of I_K do not involve the external potential A^* .

The content of any term I_K in terms of $Z\alpha$ and $\ln Z\alpha$ will then be characterized by the following three quantities: the "nominal order" of the matrix element as determined by assigning each operator factor in the numerator its nonrelativistic expectation value; the degree *i* of "infrared" divergence of the *z* integration at $z \to 0$ which would occur if each denominator of I_K were replaced by $D_{00} \equiv z^2 m^2 + K - k^2$; and the degree *e* of "electron" divergence at $|\mathbf{p}| \to \infty (\mathbf{r} \to 0)$, which would occur in the momentum space (position space) evaluation of the matrix element if the denominators in I_K were D_{00} .²²

$$\int_0^\infty dK \int_F \frac{d^4k}{\pi^2 i} \frac{1}{[K-k^2+A]^2} \left| \left| \frac{1}{D^{2+n}} = \frac{1}{A} \right| \left| \frac{1}{A^n} \right|,$$

in which A is positive-definite.

If both the z integration and matrix element integration converge for $I_K(D_{00})$ (i.e., i < 0, e < 0) then the effective range of integration is determined by the nonrelativistic wave functions, and the dominant order of I_K will be just the nominal order. If both i and e are zero (i.e., logarithmic behavior in both photon and electron integrations) then the dominant order of I_K is the nominal order multiplied by $\ln^2(Z\alpha)$. For the cases i<0, e=0 or i=0, e<0, a single $\ln Z\alpha$ factor is obtained. If either i or e is greater than zero then the dominant order of I_K is m factors of $(Z\alpha)^{-1}$ larger than the nominal order, where m is the larger of 2i and e. The dominant order also has a $\ln Z\alpha$ factor if in addition 2i=e<0.

It is straightforward to apply these rules to determine which orders a given term in Table I contributes to the hyperfine structure. One first drops the operator dependence of the denominators, returning later to determine the orders contained in the neglected terms (which are never of lower order). After performing the γ algebra and taking the nonrelativistic wave functions,²³ we can look for dependence on the magnetic dipole moment u in two places. Either the operator itself has magnetic dependence or the linear dependence on $\boldsymbol{\mu}$ comes from the wave functions. In the former case the operator $e\mathbf{A} = -ie\mathbf{\mu} \times [\mathbf{p}, 1/r]$ contributes the factor $E_n^F/Z\alpha$ to the nominal order. For the other case we note in Appendix A that $\delta_{\mu}\phi_n(r)$, the magnetic correction to the nonrelativistic Coulomb wave function, coincides asymptotically with $[E_1^F/2(Z\alpha)^4m^2]V\phi_n(r)$ at small r. Accordingly, for the purposes of determining the dominant order, the magnetic wave function correction is equivalent to a factor $E_n^F/(Z\alpha)^2$ for determining the nominal order and equivalent to an extra 1/r acting on the Coulomb wave function for determining e. As a convenient notation we list the indices of a term in the form $_{2i}N_e$, where N represents the nominal order $(Z\alpha)^N$, counting 1 for each power of $Z\alpha$ and 4 for E_n^F ; eA thus can be counted as $[\mathbf{p}, V]$, and $\delta_{\mu} \phi_n$ as $V \phi_n$.

We emphasize that the rule of order determines rigorously only the dominant order of a term. Contributions from the nonasymptotic parts of the wave functions give higher order terms; a contribution of order $\alpha(Z\alpha)^2 \ln^2(Z\alpha)^{-2}E_n^F$ does not preclude contributions of order $\alpha(Z\alpha)^2 \ln(Z\alpha)^{-2}E_n^F$; etc.

We can make the observation that the nominal order is always even since integration symmetry requires an even power of momentum \mathbf{p} in the numerator; consequently, from the rule of order, actual contributions can involve $\ln Z\alpha$ or $\ln^2 Z\alpha$ factors only when accompanying even powers in $Z\alpha$. We also observe that the contributions of leading order of those terms which

²¹ We use the integration identity (I-2.33c)

²² The index *i* may be determined for each term of the polynomial in *z* contained in I_K simply by noting that if $I_K(D_{00})$ has *n* denominators, then 2(n-3) powers of 1/z remain after the d^4k and dK integrations.

The index e is given by the formula

 $e = n_p + n_{1/r} - 3 - w$,

where the first two terms give the number of operators \mathbf{p} and 1/r in the numerator structure and w is the effective power of r of the wave functions near the origin. For nonrelativistic Coulomb S states, w=0, 1, 2 is the number of wave functions acted directly upon by \mathbf{p} .

upon by \mathbf{p} . ²³ This approximation usually yields a correction term of relative order $(\mathbb{Z}\alpha)^2$. See Sec. II-5.

have $e \ge 0$ and $e \ge 2i$ depend on the asymptotic wave functions and hence are "state-independent"; the entire $1/n^3$ dependence is absorbed in the definition of E_n^F .

Now, with the advantage of the order determining rules, we can sort out those terms of Table I which contribute to the orders of interest. The search can be narrowed considerably by noting that except for I_L and I_M all terms have $i \leq 0$, are explicitly quadratic in the field strength, and always have nominal order N at least 8 when they contribute to the hyperfine splitting of S states. We also note that the quadratic terms $I_{a,b,c,d,e}$ have numerator structures containing either magnetic wave functions (and effectively three powers of 1/r so that N-e=6+w) or an odd number of γ matrices (which bring in the small components of a wave function so that N-e=5+w, with $w \ge 1)^{24}$; in either case these terms have $N-e \ge 6$ and only contain state-independent $(\alpha/\pi)(Z\alpha)^2 E_n^F$ contributions. Such terms will not be calculated in this paper. Their contributions will actually be quite small due to several parametric integrations (z,λ,u) , each giving a numerical factor less than 1.

The quadratic term I_{LM} has the structure

$$\frac{1}{D}\prod_{\nu}\frac{1}{D}[\prod_{\nu},\Pi]\frac{1}{D}\Big|\Big|\frac{1}{D}\Big|\Big|\frac{M}{D}$$

We obtain a w=0 contribution when the left hand D^{-1} is replaced by $D^{-1}MD^{-1}$. This term has N-e=5, so we obtain a contribution to order $\alpha(Z\alpha)E_n^F$. All terms of this order are calculated in Sec. 5.

Almost all of the contributions to orders of interest come from I_L and I_M , the terms which contain structures linear in the field strength.

The full content of the I_L numerator is

$$\Pi^{\mu} \cdot [\Pi_{\mu}, \Pi] = \mathbf{p} \cdot [\mathbf{p}, \gamma_0 V] - \mathbf{p} \cdot [\mathbf{p}, \mathbf{\gamma} \cdot e\mathbf{A}] + E_n \cdot [V, \mathbf{\gamma} \cdot \mathbf{p}] - \mathbf{p} \cdot [e\mathbf{A}, \mathbf{\gamma} \cdot \mathbf{p}] - V \cdot [V, \mathbf{\gamma} \cdot \mathbf{p}] - e\mathbf{A} \cdot [\mathbf{p}, V\gamma_0]. \quad (4.1)$$

The first two numerators in (4.1) yield terms (denoted by I_{Lc} and $I_{L\mu}$, respectively) which have nominal order N=6, indices $i \leq 0$, e=1, 0 and hence contributions of order

$$\alpha(Z\alpha)E_n^F$$
, $\alpha(Z\alpha)^2[\ln^2(Z\alpha)^{-2},\ln(Z\alpha)^{-2},\mathbf{1}]E_n^F$.

The terms given by the third line of (4.1) are transformed in Appendix B to forms quadratic in $F^{\mu\nu}$. These terms, together with those from the fourth line of (4.1), therefore give negligible state-independent $\alpha(Z\alpha)^2 E_n F$ contributions, of the same type as $I_{a,b,c,d,e}$.

The dominant contribution of I_M is characterized by

$$_{2i}N_e = -24_{-1} : \alpha E_n^F$$

for $I_{M\mu}$ and by

$$_{2i}N_e = -26_{0,-1} : \alpha(Z\alpha)^2 [\ln(Z\alpha)^{-2}, 1]E_n^F$$

for I_{Mc} (with a magnetic wave function).

We should emphasize that careful consideration must be given to the correction terms obtained in reducing the denominators and wave functions of I_M and I_L to calculable forms. The reduction procedure given in Sec. 5 shows that contributions to order $\alpha(Z\alpha)E_n^F$ also arise from first-order expansions of M in the denominators of I_L and from the first-order magnetic form-factor correction (i.e., expansion of \mathbf{p}^2 in the denominators) of I_M . The systematic analysis of Sec. 6 shows that contributions of order $\alpha(Z\alpha)^2 \ln(Z\alpha)^{-2}E_n^F$ are found in the expansion of V in the denominators of $I_{L\mu}$ and I_{Lc} , the expansion of M_c in the denominators of $I_{L\mu}$, and form-factor plus relativistic wave-function corrections to I_M .

5. THE $\alpha(Z\alpha)E_n^F$ RADIATIVE CORRECTIONS

We now proceed to a specific, self-contained calculation of the contributions of order $\alpha(Z\alpha)E_n^F$. We leave the systematic analysis of higher order corrections for Sec. 6.

It is clear from the order-determining rules that $\alpha(Z\alpha)E_n{}^r$ contributions occur only when $N_e=6_1, 8_3, 10_5$, etc. (with 2i < e). The condition $N-e=n_{1/r}+3+w=5$ is met only by $n_{1/r}=1$, w=1 or $n_{1/r}=2$, w=0; i.e., only one or two operators 1/r (either from V, eA, or $\delta_\mu\phi_n$), each acting on a Coulomb wave function. Moreover, since $e \ge 1$, the electron integration is in the relativistic region $p \gg \beta$, so that only the asymptotic wave functions (A2) and (A5) are required. We thus may limit our search to terms which (after reduction of the Dirac algebra and angular integration) have numerator structures of the form

$$V(\mathbf{p}^2)^n V$$
 or $V(\mathbf{p}^2)^{n+1}$ $(n=1,2,\cdots)$

evaluated between asymptotic nonrelativistic Coulomb wave functions. [In fact, this observation provides a simple over-all technique for calculating the desired contributions to the $\alpha(Z\alpha)E_n^F$ order.] The only terms found to yield such structures are I_{Le} , $I_{L\mu}$, I_M , and I_{LM} , since the numerator structure of the neglected terms always involve an "isolated" V, i.e., an operator 1/rnot acting upon a wave function. In addition, the evaluation of the contributing terms is simplified by selecting only the operator arrangements with potentials at the outside and by employing only the asymptotic part of the wave functions. The other numerator arrangements and the nonasymptotic parts of the wave functions contribute to higher orders and are considered in Sec. 6.

The dominant order of the I_{Lc} and $I_{L\mu}$ terms is $\alpha(Z\alpha)E_n^F$, but contributions to this order also occur in the reduction of their denominators to calculable form. The exact reduction procedure we use to obtain these terms is fairly arbitrary, and, in fact, several procedures

²⁴ Actually, I_d and I_e have canceling w=0 contributions. This is demonstrated in the second part of Appendix B.

have been used to check the results of this section. The systematic reduction used here follows the sequence (i), (ii), (iii) of Sec. 3 and has the feature of preserving gauge invariance up to the final step. Only at the final stage will we select the terms linear in the nuclear magnetic moment.

Let us thus start with the structures I_{Lc} and $I_{L\mu}$ and (i) expand the magnetic moment operator M from the denominators (and denote the correction terms as I_{L-M}). In each outside denominator we (ii) "shift" the k term:

$$(k - \lambda z \Pi)^2 \rightarrow k^2$$
, $D_{(\text{outside})} \rightarrow D_1$

(and denote the correction terms as I_{L-p}), so that (iii) $D_{1(\text{outside})} \doteq D_{00}$. Thus, besides the correction terms I_{L-M} and I_{L-p} , the term I_L reduces to a form with outside denominators

$$D_{00} = z^2 m^2 + K - k^2 \tag{5.1}$$

and inside denominators

$$D_{\lambda} = z^2 m^2 + K - (k - \lambda z \Pi)^2 + z(1 - z)H \qquad (5.2)$$

 $(\lambda = 1 \text{ except in } I_{L1}).$

We now proceed to extract the leading order by making the following valid approximations (i.e., leaving corrections of higher order). We simplify the inside denominators by letting

$$(k - \lambda z \Pi)^2 \rightarrow k_0^2 - (\mathbf{k} - \lambda z \mathbf{p})^2 \equiv (k - \lambda z \mathbf{p}')^2$$
 (5.3)
and

$$H \rightarrow \mathbf{p}^2$$
. (5.3')

The neglected terms cannot be order $\alpha(Z\alpha)E_n^F$ since the expanded potentials do not act on the wave functions. The resulting inside denominators

$$D_{\lambda 1} = z^2 m^2 + K - (k - \lambda z p')^2 + z(1 - z) \mathbf{p}^2 \qquad (5.4)$$

may be combined with the outside denominators by a parametric integration. The denominator combining formula in terms of symmetric insertions is

$$\frac{1}{D_{\lambda 1}} \frac{1}{D_{00}} \left| \left| \left(\frac{1}{D_{\lambda 1}}\right)^{l} \left(\frac{1}{D_{00}}\right)^{r} \left(\frac{1}{D}\right)^{l} \right. \right. \\ \left. = \int_{0}^{1} du \left(\frac{1}{D_{\lambda u}}\right)^{2} \left| \left| \left(\frac{u}{D_{\lambda u}}\right)^{l} \left(\frac{1-u}{D_{\lambda u}}\right)^{r} \left(\frac{1}{D_{\lambda u}}\right)^{l} \right. \right|$$
where

$$\left|\left|\frac{1}{D}\right| = \left|\left|\frac{1}{D_{\lambda 1}}\right| + \left|\left|\frac{1}{D_{00}}\right|\right|\right|$$
(5.6)

and

$$D_{\lambda u} \equiv u D_{\lambda 1} + (1-u) D_{00}$$

= $z^2 m^2 + K - (k - u \lambda z p')^2$
+ $u z (1-z) \mathbf{p}^2 + u (1-u) \lambda^2 z^2 \mathbf{p}^2$. (5.7)

We now selectively calculate terms linear in **u**. The required $\alpha(Z\alpha)E_n^F$ structure arises from the I_{Lc} terms when we take the magnetic asymptotic S-wave part of the left-hand wave functions:

$$\delta_{\mu}\phi_n \longrightarrow C_{\mu}\phi_n V ,$$

where

$$C_{\mu} \equiv \frac{2}{3} \frac{|e|}{m} \frac{\langle \boldsymbol{\sigma} \cdot \boldsymbol{y} \rangle}{Z\alpha} = \frac{m E_n^F}{2Z\alpha\beta^3}.$$
 (5.8)

Thus, in nonrelativistic approximation we obtain the following reduced structure:

$$I_{Lc-\delta\phi}: C_{\mu}\left(\phi_{n}, V\frac{1}{D_{00}}\mathbf{p} \cdot \frac{1}{D_{\lambda 1}}\mathbf{p}V\frac{1}{D_{00}}\phi_{n}\right) \left| \left| \frac{1}{D} \right| \right|$$
(5.9)

For $I_{L\mu}$, which only couples large to small components, we effectively have the numerator structure

$$\frac{\boldsymbol{\sigma} \cdot \mathbf{p}}{2m} \mathbf{p} \cdot \mathbf{p} \cdot \boldsymbol{\sigma} \cdot |\boldsymbol{e}| \mathbf{A} = \frac{\mathbf{p}^2}{2m} \mathbf{p} \cdot |\boldsymbol{e}| \mathbf{A} + \frac{\mathbf{p}^2}{2m} i\boldsymbol{\sigma} \cdot \mathbf{p} \times |\boldsymbol{e}| \mathbf{A}, \quad (5.10)$$

where $\mathbf{p} \cdot e\mathbf{A} \doteq 0$ for S states and $\mathbf{A} = -\mathbf{\mu} \times \nabla(1/r)$ $=i\mathbf{u}\times[\mathbf{p},V]/Z\alpha$. Keeping only the term with V to the right and performing the angular average, (5.10) becomes

$$\frac{-|e|}{Z\alpha} \langle \boldsymbol{\sigma} \cdot \boldsymbol{y} \rangle \frac{2}{3} \frac{\mathbf{p}^2}{2m} \mathbf{p}^2 V \qquad (5.11)$$

and is to be taken between nonrelativistic Coulomb states. Finally, if we replace \mathbf{p}^2 with -2mV acting on the left-hand wave function (which is valid in the asymptotic limit), then we obtain the same structure as $I_{Lc-\delta_{\mu}\phi}$ in (5.9).

We now return to the contributions I_{L-M} and I_{L-p} obtained in the reduction of I_L . The same steps through (5.3) applied to these terms do not give corrections of order $\alpha(Z\alpha)E_n^F$. The I_{L-M} contribution to $\alpha(Z\alpha)E_n^F$ is obtained only when M is expanded from the left-hand outside denominator of I_L . The $I_{Lc-M\mu}$ terms (with $M_{\mu} \rightarrow C_{\mu} V \mathbf{p}^2$) then give the structure

$$I_{Lo-M\mu}: z^2 C_{\mu} \left(\phi_n, \frac{1}{D_{00}} V \mathbf{p}^2 \frac{1}{D_{\lambda 1}} \mathbf{p} \cdot \frac{1}{D_{\lambda 1}} \mathbf{p} V \frac{1}{D_{00}} \phi_n \right) \left| \left| \frac{1}{D} \right| \right|$$
(5.12)

The analysis for $I_{L\mu-Mc}$ is similar; we easily find that it gives the same $\alpha(Z\alpha)E_n^F$ structure as (5.12). (Note that the I_{L1} denominators yield no I_{L1-M} corrections to this order.)

Contributions to order $\alpha(Z\alpha)E_n^F$ from I_{L-p} are obtained for the shift of only the left-hand denominators of I_L ; specifically we have the structure

where we have selected only that part of the shift which contributes to the order of interest here. Selection of the parts linear in \boldsymbol{u} lead to the identical structures for The matrix elements for I_{M-p} are $I_{Lc-p-\delta_{\mu}\phi}$ and $I_{L\mu-p}$:

$$(2)C_{\mu}\left(\phi_{n},\frac{1}{D_{00}}V(2\mathbf{k}\cdot\lambda z\mathbf{p}-\lambda^{2}z^{2}\mathbf{p}^{2})\right)$$

$$\times\frac{1}{D_{\lambda1}}\mathbf{p}\cdot\frac{1}{D_{\lambda1}}\mathbf{p}V\frac{1}{D_{00}}\phi_{n}\right)\left|\left|\frac{1}{D}\right|\right|.$$
(5.14)

After combining denominators with the u integration (5.5), we may integrate the **k** term by parts according to (I-2.46),

$$\left|\left|\frac{\mathbf{k}}{D_{\lambda u}} \doteq \right|\right| \frac{\lambda z u \mathbf{p}}{D_{\lambda u}}, \qquad (5.15)$$

so we have the effective replacement

$$2\mathbf{k} \cdot \lambda z \mathbf{p} - \lambda^2 z^2 \mathbf{p}^2 \doteq \lambda^2 z^2 \mathbf{p}^2 (2u - 1). \qquad (5.16)$$

We now turn to I_{LM} and note that its structure is the same as I_{L3-M} and I_{L4-M} in lowest order, differing only by the replacement of z^2M with -2zM. [We shall see that the total $\alpha(Z\alpha)E_n^F$ contribution of I_{LM} and all the I_{L3} , I_{L4} -derived terms actually cancel.]

Finally, we note that the only contribution to order $\alpha(Z\alpha)E_n^F$ obtained in the reduction of I_M in Sec. 3 is the shift correction

$$\left(\phi_{n}, \frac{1}{D_{00}}(2\mathbf{k} \cdot z\mathbf{p} - z^{2}\mathbf{p}^{2})\frac{1}{D_{1}}z^{2}M\frac{1}{D_{1}}\phi_{n}\right) \left| \left| \frac{1}{D^{2}}, (5.17) \right| \right|$$

plus a similar term for shifting the right-hand denominator. To extract the $\alpha(Z\alpha)E_n^F$ contribution of the term (5.17), we take $M \to M_{\mu} \to C_{\mu} \mathbf{p}^2 V$, shift the right-hand denominator $D_1 \rightarrow D_{00}$, and integrate by parts as in (5.16).

In order to obtain the total $\alpha(Z\alpha)E_n^F$ contribution, we must evaluate the detailed structures of I_L , I_M , and I_{LM} as given in Table I. The matrix elements for I_{Lc} and $I_{L\mu}$ are

$$2C_{\mu}\left(\phi_{n}, V \frac{\mathbf{p}^{2}}{D_{00}D_{\lambda 1}}V\phi_{n}\right) \times \left| \left| \left[\frac{4(1-z^{2})z^{3}m^{2}}{D_{00}^{2}D} - \frac{4z(1-z)}{D^{2}} - \frac{4z^{2}(1-z)}{D_{00}D} - \frac{4z^{3}}{D_{00}^{2}} \right] \right|_{(1)}$$

$$(5.18)$$

The matrix elements for I_{L-p} , I_{L-M} , and I_{LM} are

$$2C_{\mu}\left(\phi_{n}, V\frac{\mathbf{p}^{4}}{D_{00}D_{\lambda 1}}V\phi_{n}\right)\left|\left|\left\{\frac{4\left(1-z^{2}\right)z^{3}m^{2}\left(2u-1\right)\lambda^{2}z^{2}}{D_{\lambda 1}D_{00}^{2}D}\right.\right.\right.\right.$$

$$\left.-\left[\frac{4z^{2}\left(1-z\right)}{D_{11}D_{00}D}+\frac{4z^{3}}{D_{00}^{2}D_{11}}\right]\left[z^{2}\left(2u-1\right)+z^{2}-2z\right]\right\}.$$
(5.19)
(3)

$$2C_{\mu} \left(\phi_{n}, V \frac{\mathbf{p}^{2}}{D_{00}D_{11}} V \phi_{n} \right) \\ \times \left| \left| \frac{\left[2(1+z)m - 4m \right](-2m)(2u-1)z^{4}}{D_{00}D^{2}} \right| \right| \right|$$
(5.20)

After we combine denominators using (5.5), all of the terms have the form

$$\frac{\alpha}{4\pi} \int_0^1 du \int_0^1 dz \int_0^1 d\lambda^2 \int_0^\infty dK \int_F \frac{d^4k}{\pi^2 i} \times 2C_\mu \left(\phi_n, V \frac{(\mathbf{p}^2)^{\rho+1}}{D_{\lambda u^2}} V \phi_n\right) \left| \left| \frac{P(z, u)}{(D_{\lambda u})^{r+1}} \right|, \quad (5.21)$$

where $\rho, \tau = 0, 1, 2$, and the parameter λ is 1 except in the I_{L1} -derived terms.

The dK and d^4k integrations may be done immediately as in Ref. 21 after shifting by $u\lambda zp'$ (which is a c number in momentum space). There are now τ denominators, each of the form

$$z^{2}m^{2} + [u(1-u)\lambda^{2}z^{2} + uz(1-z)]\mathbf{p}^{2} \equiv a^{2}\mathbf{p}^{2} + z^{2}m^{2}. \quad (5.22)$$

The matrix-element integration is easily performed in momentum space using the asymptotic form

$$V\phi_n \rightarrow -\frac{1}{\mathbf{p}^2} \left[\left(\frac{2}{\pi} \right)^{1/2} Z \alpha \phi_n(0) \right];$$
 (5.23)

for example,

$$\int_{0}^{\infty} \frac{dp}{a^{2}\mathbf{p}^{2} + z^{2}m^{2}} = \frac{\pi}{2} \frac{1}{azm}.$$
 (5.24)

We then obtain a common factor

$$\begin{bmatrix} \frac{\alpha}{4\pi} \end{bmatrix} \begin{bmatrix} 4\pi \end{bmatrix} \begin{bmatrix} \frac{2}{\pi} (Z\alpha)^2 |\phi_n(0)|^2 \end{bmatrix} \begin{bmatrix} 2C_\mu \end{bmatrix} \begin{bmatrix} \frac{\pi}{2} & \frac{1}{m} \end{bmatrix}$$
$$= \frac{\alpha}{\pi} (Z\alpha) E_n^F, \quad (5.25)$$

multiplying λ , z, u parametric integrals of the same form as (II-5.46). The separate integrals and their values are listed in Table II.

The total contribution is

$$\alpha(Z\alpha)E_n^F[-13/4+\ln 2]. \tag{5.26}$$

Combining this with the vacuum polarization result (C9)

$$\alpha(Z\alpha)E_n^F[\frac{3}{4}], \qquad (5.27)$$

we obtain the total radiative correction

$$\alpha(Z\alpha)E_n^F\left[-\frac{5}{2}+\ln 2\right],\tag{5.28}$$

thus confirming the results of Kroll and Pollack¹⁰ and Karplus, Klein, and Schwinger.¹¹

or

TABLE II. $\alpha(Z\alpha)E_n^F$ coefficients. Integration $\frac{1}{\pi}\int_0^1 \frac{dz}{\sqrt{z}}\int_0^1 \frac{du}{\sqrt{u}}\int_0^1 d\lambda^2$ of the tabulated integrands.^a

Term	Integrand	Integral		
I_{L1}	$2(1-z^2)(1-u)^2$	$1/2 + \ln 2$		
	$\times [1-z+\lambda^2 z(1-u)]^{-1/2}$			
$I_{L1-M,p}$	$z(1-z^2)\lambda^2(2u-1)(1-u)^2$	$5/8 - \ln 2$		
	$\times [1-z+\lambda^2 z(1-u)]^{-3/2}$			
I_{L2}	$-4(1-z)[1-uz]^{-1/2}$	$2 - 8 \ln 2$		
I_{L3}	$-4z(1-z)(1-u)[1-uz]^{-1/2}$	$-13/4+4 \ln 2$		
$I_{L3-M, p}$	$4(1-z)z(1-u)(1-uz)[1-uz]^{-3/2}$	$13/4 - 4 \ln 2$		
I_{L4}	$-4z^2(1-u)^2[1-uz]^{-1/2}$	$3/2 - 3 \ln 2$		
$I_{L4-M, p}$	$4z^2(1-u)^2(1-uz)[1-uz]^{-3/2}$	$- 3/2 + 3 \ln 2$		
I_{M-p}	$-2z(1-z)(1-2u)(1-u)[1-uz]^{-1/2}$	$-51/8+9 \ln 2$		
Total		$-13/4 + \ln 2$		

^a Evaluated in II-(B. 8-13).

6. THE HIGHER ORDER RADIATIVE CORRECTIONS TO THE HYPERFINE STRUCTURE

We have anticipated in Secs. 2 and 4 the presence of radiative corrections of order

$$\begin{array}{l} \alpha(Z\alpha)^2 \ln^2(Z\alpha)^{-2}E_n{}^F, \quad \alpha(Z\alpha)^2 \ln(Z\alpha)^{-2}E_n{}^F, \\ \quad \text{and} \quad \alpha(Z\alpha)^2E_n{}^F. \end{array}$$

The specific sources of logarithmic terms may be found using the order-determining rule given in Sec. 4. Contributing terms can only have indices

$$_{2i}N_e = {}_06_0 \quad \text{for} \quad \alpha(Z\alpha)^2 \ln^2(Z\alpha)^{-2}E_n{}^F$$

$$_{2i}N_e = {}_{0}6_e(e<0), \quad _{2i}6_0(i<0), \quad _{2}8_2, \quad _{4}10_4, \cdots$$

for $\alpha(Z\alpha)^2 \ln(Z\alpha)^{-2}E_n^F.$

Thus, all terms but those derived from I_L and I_M are eliminated from consideration since they are at least quadratic in the field strength with $N \ge 8$, $i \le 0$.

Contributions to the nonlogarithmic order, $\alpha(Z\alpha)^2 E_n^F$, are legion and arise from all terms of Table I. As pointed out in Sec. 4, contributions from terms quadratic in the field strength with $i \leq 0$ are of the size of a small fraction times $(\alpha/\pi)(Z\alpha)^2 E_n^F$ and do not contribute to the ratio $8\delta E_2/\delta E_1$. As in the corresponding Lamb shift calculation of terms of order $\alpha(Z\alpha)^6mc^2$, we will only estimate a bound on the total magnitude of such terms. We will, however, calculate explicitly the terms of order $\alpha(Z\alpha)^2 E_n^F$ which accompany the logarithmic contributions; as in the Lamb shift calculation, we expect such terms to have coefficients much larger than unity. This is indeed the case, so these terms give the dominant contribution to the $\alpha(Z\alpha)^2 E_n^F$ coefficient. With the exception of one small term, which must be calculated by a sum-over-states method, we will also be able to obtain the total $\alpha(Z\alpha)^2 E_n^F$ "statedependent" contribution to the (n=2)/(n=1) hyperfine splitting ratio.

The most interesting higher order contributions

arise from the I_L terms, and we start our calculations there. We first take seven steps in succession which reduce the I_L terms to a convenient calculable form. After the calculation of the final form, we will return to carefully consider in reverse sequence the contribution of the neglected terms of each step.

As in Sec. 3 we first reduce the denominators of the I_L terms through the steps (i), (ii), (iii). The denominators acting on the wave functions

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

may be combined with the inside denominators

$$D_0 = z^2 m^2 + K - k^2 + z(1-z)H$$

with a parametric u integration. Carrying out the dK and d^4k integrations²¹ and using the specific form of the I_L terms, we obtain as in Sec. I-3:

$$\Delta E_n(L) = -\frac{\alpha}{\pi} \int_0^1 du \int_0^1 dz \times P(z,u) \left\langle n \left| \prod_{r=1}^n [\Pi^r, \Pi] \right| n \right\rangle, \quad (6.1)$$

where

$$P(z,u) = -2(1-z^2)u(1-u) + (1-z) + z(1-z)(1-u) + z^2(1-u)^2$$

and

$$\Delta = zm^2 + u(1-z)H. \tag{6.2}$$

Continuing the reduction sequence, we

(iv) take nonrelativistic forms:

$$H \to H_{NR} = \mathbf{p}^2 + 2mV + \beta^2, \quad |n\rangle \to |n\rangle_{NR}; \quad (6.3)$$

(v) neglect the Coulomb potential in H_{NR} :

$$\Delta_{NR} \rightarrow \Delta_0 = zm^2 + u(1-z)(\mathbf{p}^2 + \beta^2); \qquad (6.4)$$

and (vi) neglect all numerator structures in I_L but I_{Lc} :

$$\Pi_{\mu} \cdot \left[\Pi^{\mu}, \Pi \right] \to \mathbf{p} \cdot \left[\mathbf{p}, V \right] \gamma_0. \tag{6.5}$$

The matrix element, to first order in the magnetic moment, is thus reduced to

$$\begin{pmatrix} \delta_{\mu}\phi_{n}, \mathbf{p} \cdot \frac{1}{\Delta_{0}} [\mathbf{p}, V]\phi_{n} \end{pmatrix} + \begin{pmatrix} \phi_{n}, \mathbf{p} \cdot \frac{1}{\Delta_{0}} [\mathbf{p}, V]\delta_{\mu}\phi_{n} \end{pmatrix}$$

$$= \begin{pmatrix} \delta_{\mu}\phi_{n}, \frac{1}{\Delta_{0}} [\mathbf{p} \cdot , [\mathbf{p}, V]]\phi_{n} \end{pmatrix}$$

$$+ \begin{pmatrix} \phi_{n}, \mathbf{p} \cdot \left[\frac{1}{\Delta_{0}}, [\mathbf{p}, V]\right]\delta_{\mu}\phi_{n} \end{pmatrix}, \quad (6.6)$$

where $|\phi_n\rangle$ is the nonrelativistic Coulomb wave function: $H_{NR}|\phi_n\rangle=0$. As the final step, we

(vii) neglect the second matrix element in (6.6).

We now can concentrate on calculating the first term of (6.6), which we designate $I_{Lc-\delta_{\mu}\phi}$. It is perhaps the most interesting term considered in this section in that it is the sole source of the double logarithm contribution. We may write the matrix element either in momentum space, or what will prove more convenient, in position space:

$$\begin{pmatrix} \delta_{\mu}\phi_{n}, \frac{1}{\Delta_{0}} [\mathbf{p} \cdot, [\mathbf{p}, V]]\phi_{n} \end{pmatrix}$$

$$= \frac{-Z\alpha}{2\pi^{2}} \int d^{3}p \frac{\delta_{\mu}\phi_{n}(p)}{\Delta_{0}(p)} \int d^{3}p'\phi_{n}(p')$$

$$= -Z\alpha\phi_{n}(0) \frac{1}{u(1-z)} \int d^{3}r \,\delta_{\mu}\phi_{n}(r) \frac{e^{-\beta r/y}}{r}, \quad (6.7)$$

where

$$y^{2} \equiv \frac{u(1-z)\beta^{2}}{zm^{2}+u(1-z)\beta^{2}} = \frac{(1-z)\omega}{z+(1-z)\omega}, \qquad (6.8)$$

with

 $\omega \equiv u\beta^2/m^2.$

The required S-wave magnetic wave functions for n=1 and n=2 are given in Appendix A. The energy shift corresponding to $I_{Lc-\delta_{\mu}\phi}$ is then

$$\Delta E_n(L_c - \delta_\mu \phi) = \frac{\alpha}{\pi} (Z\alpha)^2 E_n F \frac{2m^2}{\beta^2} \int_0^1 \frac{du}{u} \int_0^1 \frac{dz}{1-z} \times P(z, u) \int_0^\infty s^2 ds \ \delta_\mu \phi_n(s) \frac{e^{-s/y}}{s}, \quad (6.9)$$

where, for n = 1 and 2,

$$\delta_{\mu}\phi_{n}(s) \equiv 2e^{-s} \left[\frac{-1}{2ns} + (\ln 2s + \gamma - 1) + (2 - n) \left(-\frac{3}{2} + s \right) + (n - 1) \frac{1}{4} - (n - 1)s \left(\ln 2s + \gamma - \frac{13}{4} + \frac{s}{2} \right) \right], \quad (6.10)$$

in terms of the dimensionless radial variable

$$s \equiv \beta r.$$
 (6.11)

The radial integral for the leading term of $\delta_{\mu}\phi_n(s)$ is

$$\frac{-2}{2n} \int_0^\infty ds \ e^{-s} e^{-s/y} = \frac{-1}{n} \frac{y}{1+y} = \frac{-y}{n} + \frac{1}{n} \frac{y^2}{1+y}.$$
 (6.12)

If we express y in terms of z and β as in (6.8) and use the $Z\alpha \rightarrow 0$ limit of the first part of (6.12),

$$y = \left[\frac{u(1-z)\beta^2}{zm^2 + u(1-z)\beta^2}\right]^{1/2} \xrightarrow{Z_{\alpha \to 0}} \frac{\beta}{m} \left[\frac{u(1-z)}{z}\right]^{1/2}, \quad (6.13)$$

in the z and u integrations of (6.9), we obtain a result purely of order $\alpha(Z\alpha)E_n^F$, which has already been included in the calculations of Sec. 5. The correction to (6.13) is found, using (II-5.52), to be

$$-\frac{\alpha}{\pi} (Z\alpha)^{2} E_{n}^{F} \frac{2m^{2}}{n\beta} \int_{0}^{1} \frac{du}{\sqrt{u}} \int_{0}^{1} \frac{dz}{\sqrt{z}} \\ \times \left\{ \frac{1}{[zm^{2} + u(1-z)\beta^{2}]^{1/2}} - \frac{1}{[zm^{2}]^{1/2}} \right\} P(z,u) \\ = \frac{\alpha}{\pi} (Z\alpha)^{2} E_{n}^{F} \left[\frac{4}{-n} \right] \int_{0}^{1} du P(0,u) \\ + 0[\alpha(Z\alpha)^{3} E_{n}^{F}]. \quad (6.14)$$

The contribution of the $y^2/(1+y)$ part of (6.12) is

$$\frac{\alpha}{\pi}(Z\alpha)^{2}E_{n}^{F}\frac{2m^{2}}{n}\int_{0}^{1}du\int_{0}^{1}\frac{dzP(z,u)}{zm^{2}+u(1-z)\beta^{2}}\frac{1}{1+y},\quad(6.15)$$

which diverges logarithmically at $z \sim 0$ if we set $Z\alpha = 0$ in the integrand. The logarithmic contribution is found by taking $1/(1+y) \rightarrow 1$; the result is

$$\frac{\alpha}{\pi} (Z\alpha)^{2} E_{n}^{F} \left[\frac{2}{n}\right] \int_{0}^{1} du \\ \times \left\{ P(0,u) \ln \frac{m^{2}}{u\beta^{2}} + \int_{0}^{1} dz \frac{P(z,u) - P(0,u)}{z} \right\}, \quad (6.16)$$

in which we have included the nonlogarithmic contribution of P(z,u) - P(0,u) and have dropped terms of order $\alpha(Z\alpha)^3 E_n^F$. The contribution of the remainder, which converges for $Z\alpha=0$, is found by transforming from a z integration to a y integration (II-B.6c),

$$\frac{\alpha}{\pi} (Z\alpha)^{2} E_{n}^{F} \frac{2m^{2}}{n} \int_{0}^{1} du \int_{0}^{1} \frac{dy^{2} P(z,u)}{y^{2}m^{2} + u(1-y^{2})\beta^{2}} \left[\frac{1}{1+y} - 1\right]$$
$$\xrightarrow{Z\alpha \to 0} \frac{\alpha}{\pi} (Z\alpha)^{2} E_{n}^{F} \left[\frac{2}{n}\right] \int_{0}^{1} du P(0,u) \left[-2\ln 2\right]. \quad (6.17)$$

The total contribution of the leading term of $\delta_{\mu}\phi_n(s)$ to the orders of interest is then easily found to be

$$\frac{\alpha}{\pi} (Z\alpha)^2 E_n F \frac{4}{3n} \left[\ln \left(\frac{n}{Z\alpha} \right)^2 + \frac{11}{24} + 2 - 2 \ln 2 \right]. \quad (6.18)$$

For the next part of $\delta_{\mu}\phi_n(s)$ the relevant radial integration is

$$2\int_{0}^{\infty} ds \ e^{-s/y} e^{-s} (\ln s + \gamma - 1) = \frac{-2y^2}{(1+y)^2} \ln \frac{1+y}{y}, \quad (6.19)$$

and we thus must evaluate

$$-\frac{\alpha}{\pi}(Z\alpha)^{2}E_{n}{}^{F}[4]\int_{0}^{1}du\int_{0}^{1}dz$$

$$\times \frac{P(z,u)}{z+(1-z)\omega}\frac{1}{(1+y)^{2}}\ln\frac{1+y}{y}.$$
 (6.20)

Let us consider first the P(0,u) term, which exhibits an infrared divergence at $z \sim 0$ when $\omega = 0$. We make the separation

$$\frac{1}{(1+y)^2} \ln \frac{1+y}{y} = \ln \frac{1}{y} + \ln(1+y) - \frac{2y+y^2}{(1+y)^2} \ln \frac{1+y}{y}.$$
 (6.21)

Then by changing variables to $x = (1-\omega)(1-z)$, the z integration of the $\ln 1/y$ term has the form

$$\int_{0}^{1} \frac{dz}{z + (1 - z)\omega} \ln \frac{1}{y}$$

$$= -\frac{1}{2} \frac{1}{1 - \omega} \int_{0}^{1 - \omega} \frac{dx}{1 - x} \ln \left(\frac{x}{1 - x} \frac{\omega}{1 - \omega} \right)$$

$$= \frac{1}{4} \ln^{2} \frac{1}{\omega} + \frac{\pi^{2}}{12} + 0(\omega), \qquad (6.22)$$

and gives the double logarithm $-\frac{2}{3}(\alpha/\pi)(Z\alpha)^2 E_n F$ $\times \ln^2(Z\alpha)^{-2}$ radiative correction to the hyperfine structure. For the remainder of the function (6.21), the z integration is convergent for $\omega \sim 0$. Changing variables again from dz to dy^2 , the integration for $\omega = 0$ is

$$\int_{0}^{1} 2dy \left[\frac{1}{y} \ln(1+y) - \frac{2+y}{(1+y)^{2}} \ln \frac{1+y}{y} \right]$$

= $-\ln^{2} 2 - \ln 2 - 1.$ (6.23)

Performing the u integration with P(0,u), we then obtain the contribution

$$-\frac{\alpha}{\pi}(Z\alpha)^{2}E_{n}{}^{F}\left[\frac{2}{3}\ln^{2}\left(\frac{n}{Z\alpha}\right)^{2}+\frac{13}{9}\ln\left(\frac{n}{Z\alpha}\right)^{2}+\frac{89}{54}+\frac{2}{9}\pi^{2}-\frac{8}{3}(\ln^{2}2+\ln^{2}2+1)\right].$$
 (6.24)

For the remainder of the polynomial, we notice the z integration is convergent for $\omega \sim 0$ and

$$\int_{0}^{1} du \int_{0}^{1} dz \frac{P(z,u) - P(0,u)}{z + (1 - z)\omega} \frac{1}{(1 + y)^{2}} \ln \frac{1 + y}{y}$$
$$= \int_{0}^{1} du \int_{0}^{1} dz \frac{P(z,u) - P(0,u)}{z}$$
$$\times \left[\frac{1}{2} \ln \frac{1}{\omega} + \frac{1}{2} \ln \frac{z}{1 - z} + 0(\sqrt{\omega}) \right], \quad (6.25)$$

which gives the additional contribution

$$\frac{\alpha}{\pi} (Z\alpha)^2 E_n F \left[\frac{7}{36} + \frac{5}{6} \ln \left(\frac{n}{Z\alpha} \right)^2 \right].$$
(6.26)

We proceed in much the same manner for the remaining parts of $\delta_{\mu}\phi_n(s)$. After the radial integration we have the contribution

$$\begin{aligned} \frac{\alpha}{4\pi} (Z\alpha)^2 E_n^{\ F} \int_0^1 du \int_0^1 \frac{dz \ P(z,u)}{z + (1-z)\omega} \frac{1}{(1+y)^2} \\ & \times \left\{ \ln 2 + (n-2) \left[\frac{3}{2} - \frac{2y}{1+y} \right] + (n-1) \left[\frac{1}{4} + \frac{2y}{1+y} \left(\ln \frac{1+y}{y} - \ln 2 + \frac{7}{4} - \frac{3}{2} \frac{y}{1+y} \right) \right] \right\} \\ &= 4 \frac{\alpha}{\pi} (Z\alpha)^2 E_n^{\ F} \int_0^1 du \left\{ P(0,u) \left[\left(\ln \frac{1}{\omega} - 2 \int_0^1 dy \frac{2+y}{(1+y)^2} \right) \left(\ln 2 + \frac{3}{2}(n-2) + \frac{1}{4}(n-1) \right) \right. \\ & \left. - 4 \int_0^1 \frac{dy}{(1+y)^3} \left((n-2) - (n-1) \left(\ln \frac{1+y}{y} - \ln 2 + \frac{7}{4} - \frac{3}{2} \frac{y}{1+y} \right) \right) \right] \\ &+ \int_0^1 dz \frac{P(z,u) - P(0,u)}{z} \left[\ln 2 + \frac{3}{2}(n-2) + \frac{1}{4}(n-1) \right] \right\} \\ &= \frac{8}{3} \frac{\alpha}{\pi} (Z\alpha)^2 E_n^{\ F} \left\{ \left[\ln \left(\frac{n}{Z\alpha} \right)^2 - \frac{13}{24} - 2 \ln 2 \right] \left[\ln 2 + \frac{3}{2}(n-2) + \frac{1}{4}(n-1) \right] - \frac{3}{2}(n-2) + \frac{31}{8}(n-1) \right\} \end{aligned}$$
(6.27)

for n=1 and n=2.

(6.26), and (6.27), we obtain

$$\Delta E_n (L_c - \delta_\mu \phi) = \frac{\alpha}{\pi} (Z\alpha)^2 E_n^F \times \left[-\frac{2}{3} \ln^2 (Z\alpha)^{-2} + \left(\frac{8}{3} \ln 2 - \frac{59}{18}\right) \ln (Z\alpha)^{-2} + \left(-\frac{8}{3} \ln^2 2 + \frac{59}{9} \ln 2 - \frac{2}{9} \pi^2 + \frac{1151}{108}\right) \right]$$

and

$$\times \left[-\frac{2}{3} \ln^2(Z\alpha)^{-2} + \frac{13}{18} \ln(Z\alpha)^{-2} + \left(-\frac{2}{9} \pi^2 + \frac{1385}{108} \right) \right] (6.28)$$

for n = 1 and n = 2, respectively.

We now return to consider the terms neglected in steps (i) through (vii). In step (vii) we ignored the second matrix element in (6.6), whose contribution can be written in momentum space as

$$\frac{\alpha}{\pi} (Z\alpha)^{2} E_{n}{}^{F} \int_{0}^{1} du \int_{0}^{1} dz \frac{P(z,u)}{z+(1-z)\omega} \frac{1}{\pi^{4}} \int \frac{d^{3}t'}{(t'^{2}+1)^{2}} \\ \times \int \frac{d^{3}t}{t^{2}+1} \frac{\mathbf{t}' \cdot (\mathbf{t}-\mathbf{t}')}{(\mathbf{t}-\mathbf{t}')^{2}} \left[\frac{1}{1+y^{2}t'^{2}} - \frac{1}{1+y^{2}t^{2}} \right], \quad (6.29)$$

where, so far, we have only included the contribution from the asymptotic parts of the wave functions $\phi_n(p')$ and $\delta_{\mu}\phi_n(p)$ as given in (A2) and (A5). The d^3t' , d^3t integrals can be put in the form of the integrals given in Appendix B of paper II. The result is

$$\frac{\alpha}{\pi} (Z\alpha)^{2} E_{n}^{F} \int_{0}^{1} du \int_{0}^{1} dz \frac{P(z,u)}{z + (1 - z)\omega} \frac{1}{(1 + y)^{2}}$$
$$= \frac{\alpha}{\pi} (Z\alpha)^{2} E_{n}^{F} \left[\frac{2}{3} \ln \frac{n^{2}}{(Z\alpha)^{2}} - \frac{2}{3} - \frac{4}{3} \ln 2 + \frac{13}{18} - \frac{5}{12} + O(Z\alpha) \right]. \quad (6.30)$$

The contribution from the nonasymptotic parts of the wave functions is most easily calculated in position space. This is done in Appendix D, and we find the additional contributions

$$\frac{\alpha}{\pi} (Z\alpha)^2 E_n^{\ F} \left[\frac{19}{3}, \frac{8}{27} \right]$$
(6.31)

for n=1 and n=2, respectively.

The terms dropped in step (vi) involve all the various numerator structures of I_L (4.1) except I_{Lc} . The analysis of Appendix B shows that, except for $I_{L\mu}$, all of these depend quadratically on the field strength and

Combining the contributions of Eqs. (6.18), (6.24), hence may be disregarded here. The $I_{L\mu}$ matrix element,

$$-\left\langle n \left| \mathbf{p} \cdot \frac{1}{\Delta_0} [\mathbf{p}, \mathbf{\gamma} \cdot e\mathbf{A}] \right| n \right\rangle_{NR}, \qquad (6.32)$$

however, is very important. The γ matrix brings in small components so we have

$$-\left(\phi_{n},\mathbf{p}\cdot\frac{1}{\Delta_{0}}\left[\mathbf{p},\left\{\frac{\boldsymbol{\sigma}\cdot\mathbf{p}}{2m},\,\boldsymbol{\sigma}\cdot e\mathbf{A}\right\}\right]\phi_{n}\right)$$
$$\doteq-\frac{1}{2m}\left(\phi_{n},\frac{1}{\Delta_{0}}\mathbf{p}\cdot\left[\mathbf{p},M_{\mu}\right]\phi_{n}\right).\quad(6.33)$$

For S states, the $\mathbf{p} \cdot M_{\mu} \mathbf{p}$ contribution vanishes upon angular integration.²⁵ The contribution from step (vi) may be written in momentum space as

$$\Delta E_{n}(L_{\mu}) = -\frac{\alpha}{\pi} \int_{0}^{1} du \int_{0}^{1} dz$$
$$\times P(z, u) \left(-\frac{1}{2m} \right) C_{\mu} \frac{-Z\alpha}{2\pi^{2}} (2\pi)^{3/2} \phi_{n}(0)$$
$$\times \int d^{3}p \mathbf{p}^{2} \phi_{n}(p) \frac{1}{zm^{2} + u(1-z)(\mathbf{p}^{2} + \beta^{2})}, \quad (6.34)$$

or, with the use of the wave equation

$$\mathbf{p}^{2}\boldsymbol{\phi}_{n} = \begin{bmatrix} -2mV - \beta^{2} \end{bmatrix} \boldsymbol{\phi}_{n}, \qquad (6.35)$$

may be written in position space as

$$\Delta E_{n}(L_{\mu}) = \frac{\alpha}{\pi} E_{n}^{F} \int_{0}^{1} du \int_{0}^{1} dz \frac{P(z,u)}{u(1-z)} \int_{0}^{\infty} r \, dr \, e^{-\beta r/y} (2mV + \beta^{2}) \frac{\phi_{n}(r)}{\phi_{n}(0)} \,. \quad (6.36)$$

The radial integrations are similar to, but easier than those in $I_{Lc-\delta_{\mu}\phi}$, and yield

$$\Delta E_n(L_{\mu}) = \frac{\alpha}{\pi} E_n^F \int_0^1 du \int_0^1 dz \frac{P(z,u)}{u(1-z)} \\ \times \left\{ -2n \frac{y}{1+y} + \frac{y^2}{(1+y)^2} \\ -(n-1) \left[-2n \frac{y^2}{(1+y)^2} + 2\frac{y^3}{(1+y)^3} \right] \right\}$$
(6.37)

for n=1, 2. As in (6.12), the leading term proportional

²⁵ It is easy to see this for the S-wave part of M_{μ} . For the D-wave part, note that after integration, the matrix element must be linear in $\boldsymbol{\sigma} \cdot \boldsymbol{y}$, the only scalar. The coefficient of $\boldsymbol{\sigma} \cdot \boldsymbol{y}$ may be obtained by choosing the two vectors $\boldsymbol{\sigma}$ and \boldsymbol{y} to be parallel to each ordering the two vectors $\boldsymbol{\sigma}$ and \boldsymbol{y} to be parallel to bilance by choosing the two vectors $\mathbf{\sigma}$ and $\mathbf{\mu}$ to be parallel to each coordinate axis in turn and then averaging over the three directions. Since $\mathbf{\sigma}$ and $\mathbf{\mu}$ appear linearly in the matrix element (6.33), the *D*-wave part of M_{μ} gives no contribution: $\mathbf{\sigma} \cdot \mathbf{q}\mathbf{\mu} \cdot \mathbf{q} - \frac{1}{3}\mathbf{\sigma} \cdot \mathbf{\mu} \mathbf{q}^2 \doteq \frac{1}{3}\mathbf{\sigma} \cdot \mathbf{\mu} (q_x^2 + q_y^2 + q_x^2) - \frac{1}{3}\mathbf{\sigma} \cdot \mathbf{\mu} \mathbf{q}^2 = 0.$

to -2ny contributes a result purely of order $\alpha(Z\alpha)E_n^F$, which has been included in Sec. 5, plus a remainder of order $\alpha(Z\alpha)^2 E_n^F$, identical to (6.14). As in (6.15), the terms

$$[2n+1-(n-1)(-2n)]y^{2} = (2n^{2}+1)y^{2} \quad (6.38)$$

yield a contribution of order $\alpha(Z\alpha)^2 E_n^F \ln(Z\alpha)^{-2}$ just like (6.16), with $\lfloor 2/n \rfloor$ replaced by $\lfloor 2+1/n^2 \rfloor$. The remaining terms, of order y^3 , are like (6.17) and yield

$$\frac{\alpha}{\pi} E_n{}^F \int_0^1 du \int_0^1 \frac{dy^2 P(z,u)}{y^2 m^2 + u(1-y^2)\beta^2} \frac{\beta^2}{y^2} \\ \times \left\{ \frac{-2ny^3}{1+y} + \left[1 + 2n(n-1) \right] y^2 \left[\frac{1}{(1+y)^2} - 1 \right] \right. \\ \left. - (n-1) \frac{2y^3}{(1+y)^3} \right\} \\ \xrightarrow{Z \alpha \to 0} \frac{\alpha}{\pi} (Z\alpha)^2 E_n{}^F \int_0^1 du \ P(0,u) \\ \times \left[-2\left(2 + \frac{1}{n^2}\right) \ln 2 - \frac{1}{n^2} - (n-1)\left(\frac{2}{n} + \frac{3}{2n^2}\right) \right]. \quad (6.39)$$

The total contribution to the orders of interest for n=1, 2 is thus easily found to be

$$\Delta E_n(L_{\mu}) = -\frac{\alpha}{\pi} (Z\alpha)^2 E_n^F \left\{ \frac{2}{3} \left(2 + \frac{1}{n^2} \right) \left[\ln \left(\frac{n}{2Z\alpha} \right)^2 + \frac{11}{24} \right] + \frac{8}{3n} - \frac{2}{3n^2} - (n-1) \left(\frac{4}{3n} + \frac{1}{n^2} \right) \right\}.$$
 (6.40)

The terms neglected in step (v) are given by replacing $1/\Delta$ in (6.1) with

$$\frac{1}{\Delta_{NR}} - \frac{1}{\Delta_0} = -2mu(1-z)\frac{1}{\Delta_{NR}}V\frac{1}{\Delta_0}.$$
 (6.41)

This does give a logarithmic contribution 282. Continuing the expansion of V gives no logarithm, but rather an infinite series of state-dependent $\alpha(Z\alpha)^2 E_n^F$ terms. We only consider here the matrix elements

$$-\left\langle n \left| p_{i} \frac{1}{\Delta_{0}} u(1-z) 2m V \frac{1}{\Delta_{0}} [p_{i}, V] \gamma_{0} \right| n \right\rangle_{NR} + \left\langle n \left| p_{i} \frac{1}{\Delta_{0}} u(1-z) 2m V \frac{1}{\Delta_{0}} [p_{i}, \gamma \cdot e\mathbf{A}] \right| n \right\rangle_{NR}. \quad (6.42)$$

For I_{Lc-V} , the first line of (6.42), the required e=2structure is obtained by taking the asymptotic magnetic wave function on the left and the asymptotic form

$$-[p_i, V]\phi_n \to p_i \frac{n(2\beta)^{5/2}}{2\pi \mathbf{p}^2 2m}$$
(6.43)

on the right. We thus obtain the logarithmic con- The e=2 structure is obtained by asymptotic steps

tribution

$$-\frac{\alpha}{\pi} \int_{0}^{1} du \int_{0}^{1} dz P(z,u)u(1-z) \\ \times \left[\left(\frac{-C_{\mu}}{2m} \right) \left(\frac{n(2\beta)^{5/2}}{2\pi} \right)^{2} - Z\alpha}{2\pi^{2}} \right] \\ \times \int \frac{d^{2}p}{\mathbf{p}^{2}\Delta_{0}(\mathbf{p}^{2})} \int \frac{d^{3}p'}{\mathbf{q}^{2}} \frac{\mathbf{p} \cdot \mathbf{p}'}{\mathbf{p}'^{2}\Delta_{0}(\mathbf{p}'^{2})} \\ = -\frac{\alpha}{\pi} (Z\alpha)^{2} E_{n}^{F} \left[\frac{2}{3} \ln \frac{n^{2}}{(Z\alpha)^{2}} - \frac{5}{12} + O(Z\alpha) \right] \\ \times [4 \ln 2 - 2]. \quad (6.44)$$

For $I_{L\mu-V}$, the second line of (6.42), we obtain the e=2structure by taking the 1/r in $\mathbf{A} = -\mathbf{\mu} \times \nabla(1/r)$ acting on the right-hand wave function, and $\sigma \cdot \mathbf{p}/2m$ (from the small components) only on the left. Using the asymptotic wave functions, we then have

$$-\frac{\alpha}{\pi} \int_{0}^{1} du \int_{0}^{1} dz P(z,u)u(1-z)$$

$$\times \left[\left(\frac{-Z\alpha}{2\pi^{2}} \right) \left(\frac{n(2\beta)^{5/2}}{2\pi} \right)^{2} \left(\frac{e}{iZ\alpha} \frac{1}{2m} \right) \right]$$

$$\times \int \frac{d^{3}p}{\mathbf{p}^{4}\Delta_{0}(\mathbf{p}^{2})} \mathbf{\sigma} \cdot \mathbf{p} \int \frac{d^{3}p'}{\mathbf{q}^{2}} \frac{\mathbf{p} \cdot \mathbf{p}'}{\Delta_{0}(\mathbf{p}'^{2})\mathbf{p}'^{2}} \mathbf{\sigma} \cdot \mathbf{y} \times \mathbf{p}'. \quad (6.45)$$

By combining the σ matrices and using the trick noted in footnote 25, the momentum integrations may be simplified to the form

$$\int \frac{d^3 p}{\mathbf{p}^4 \Delta_0(\mathbf{p}^2)} \int \frac{d^3 p'}{\mathbf{q}^2} \frac{\mathbf{p} \cdot \mathbf{p}'}{\Delta_0(\mathbf{p}'^2)\mathbf{p}'^2} \frac{2}{3} \mathbf{\sigma} \cdot \mathbf{\mu} \mathbf{p} \cdot \mathbf{p}'$$
$$= \frac{\pi^4}{u(1-z)} \frac{1}{zm^2 + u(1-z)\beta^2} [4 \ln 2 - \frac{3}{2}]_3^2 \mathbf{\sigma} \cdot \mathbf{\mu} \quad (6.46)$$

and hence $I_{L\mu-V}$ yields the logarithmic contribution

$$-\frac{\alpha}{\pi}(Z\alpha)^{2}E_{n}{}^{F}\left[\frac{2}{3}\ln\frac{n^{2}}{(Z\alpha)^{2}}-\frac{5}{12}+O(Z\alpha)\right] \times \left[4\ln 2-\frac{3}{2}\right]. \quad (6.47)$$

In step (iv) we will not consider the corrections to the nonrelativistic approximation of the wave functions since the neglected terms are of order 082 and higher. In the reduction of $H \rightarrow H_{NR}$, the logarithmic indices $_{28_2}$ are obtained from the first-order expansion of $M_{\mu}+M_{c}+2\mathbf{p}\cdot e\mathbf{A}$; however, only the $I_{L\mu-Mc}$ structure contributes for S states after the angular integrations are performed. The contributing matrix element is

$$-\left\langle n \left| p_{i} \frac{1}{\Delta_{0}} u(1-z) M_{c} \frac{1}{\Delta_{0}} [p_{i}, \mathbf{\gamma} \cdot c\mathbf{A}] \right| n \right\rangle. \quad (6.48)$$

similar to those used for the $I_{L\mu-V}$ matrix element. In momentum space we thus have the logarithmic contribution

$$-\frac{\alpha}{\pi} \int_{0}^{1} du \int_{0}^{1} dz P(z,u)u(1-z)$$

$$\times \left[\frac{-e}{2miZ\alpha} \left(\frac{n(2\beta)^{5/2}}{2\pi}\right)^{2} - \frac{Z\alpha}{2\pi^{2}}\right]$$

$$\times \int \frac{d^{3}p}{\Delta_{0}(\mathbf{p}^{2})} \frac{1}{\mathbf{p}^{4}} \int \frac{d^{3}p'}{\mathbf{q}^{2}} \frac{\mathbf{p} \cdot \mathbf{p}'}{\Delta_{0}(\mathbf{p}'^{2})\mathbf{p}'^{2}} \boldsymbol{\sigma} \cdot \mathbf{q} \boldsymbol{\sigma} \cdot (\mathbf{u} \times \mathbf{p}'). \quad (6.49)$$

The momentum integrals reduce to

$$\int \frac{d^3 p}{\Delta_0(\mathbf{p}^2)} \frac{1}{\mathbf{p}^4} \int \frac{d^3 p}{\mathbf{q}^2} \frac{\mathbf{p} \cdot \mathbf{p}'}{\Delta_0(\mathbf{p}'^2)\mathbf{p}'^2} \frac{2}{3} \boldsymbol{\sigma} \cdot \boldsymbol{\mu}(\mathbf{p} - \mathbf{p}') \cdot \mathbf{p}' \quad (6.50)$$

and we thus obtain the $I_{L\mu-Mc}$ contribution

$$\frac{\alpha}{\pi} (Z\alpha)^2 E_n^{F} \left[\frac{2}{3} \ln \frac{n^2}{(Z\alpha)^2} - \frac{5}{12} + O(Z\alpha)^2 \right] \left[-\frac{1}{2} \right]. \quad (6.51)$$

This completes the calculation of the logarithmic and dominant $\alpha(Z\alpha)^2 E_n^F$ contributions of the I_L terms, since the corrections to steps (i), (ii), (iii) do not yield such contributions. The I_M terms, the only other source of logarithmic orders, are easier to discuss since *i* is negative. Following a modification of the reduction sequence outlined in Sec. 3, we shall approximate $D \rightarrow D_1$, expand D_1 in powers of *H*, and shift the *k* integration by everything but *z***p**. All of the neglected terms can be rearranged to show quadratic dependence on the field strength. Since *i* is zero or negative, we will not consider them further. The remaining structure is

$$\frac{\alpha}{4\pi} \int_{0}^{1} dz \, 2(-1+z) z^{2} m \left\langle n \left| \frac{1}{z^{2} m^{2} + K - k_{0}^{2} + (\mathbf{k} - z\mathbf{p})^{2}} M \right. \right. \\ \left. \left. \left. \left. \left. \left. \frac{1}{z^{2} m^{2} + K - k_{0}^{2} + (\mathbf{k} - z\mathbf{p})^{2}} \right| n \right\rangle \right| \left| \frac{1}{D^{2}} \right| \left. \left. \left. \left(6.52 \right) \right. \right. \right. \right. \right. \right.$$

In momentum space the momenta following M are denoted as usual by \mathbf{p}' . The denominators can be combined with a parametric u integration in the form

$$D_{u} \equiv uD + (1-u)D' = z^{2}m^{2} + K - k_{0}^{2} + (\mathbf{k} - z\mathbf{p}_{u})^{2} + z^{2}u(1-u)\mathbf{q}^{2}, \quad (6.53)$$

where

$$\mathbf{p}_u = u\mathbf{p} + (1-u)\mathbf{p}',$$

 $\mathbf{q}^2 = (\mathbf{p} - \mathbf{p}')^2.$

In momentum space we may shift the d^4k integration by the *c* number $z\mathbf{p}_u$, perform the dK, d^4k , and dz integrations, and obtain

$$\Delta E_n(M) = \int_0^1 du \frac{\alpha}{2\pi} \left(-\frac{1}{2m} \right) \\ \times \left\langle n \left| \frac{1}{1+u(1-u)\mathbf{q}^2/m^2} M \right| n \right\rangle. \quad (6.54)$$

Let us first look at the M_{μ} contribution for nonrelativistic large components only. For S states $M_{\mu} \rightarrow C_{\mu} \mathbf{q}^2 V$, and we have the momentum-space expression

$$\Delta E_n(M_\mu)_{NRLC} = \frac{\alpha}{2\pi} \left(-\frac{1}{2m} \right) C_\mu \left(-\frac{2\alpha}{2\pi^2} \right)$$

$$\times \int_0^1 du \int d^3p \int d^3p' \frac{\phi_n(p)\phi_n(p')}{1+a^2\mathbf{q}^2}, \quad (6.55)$$
where
$$a^2 = \frac{u(1-u)}{m^2}.$$

We transform to coordinate space by using the Fourier transform

$$\frac{1}{1+a^2\mathbf{q}^2} = \frac{1}{(2\pi)^3} \frac{2\pi^2}{a^2} \int d^3r \ e^{-i\mathbf{q}\cdot\mathbf{r}} \frac{e^{-r/a}}{r} \qquad (6.56)$$

so that the $p,\,p^\prime$ integrations may be done immediately and yield

$$\Delta E_n(M_\mu)_{NRLC} = \frac{\alpha}{2\pi} \frac{1}{2m} C_\mu$$
$$\times Z\alpha \int_0^1 du \int d^3 r \phi_n^2(r) \frac{e^{-r/a}}{ra^2}. \quad (6.57)$$

Since $r \sim a \sim 1$ here, we may use the expansion of the wave function about $\beta r = 0$,

$$\phi_n(r) = \phi_n(0) \bigg[1 - Z\alpha mr + \frac{1}{3} \bigg(1 + \frac{1}{2n^2} \bigg) (Z\alpha mr)^2 + O(Z\alpha mr)^3 \bigg], \quad (6.58)$$

to obtain the power series

$$\Delta E_{n}(M_{\mu})_{NRLC} = \frac{\alpha}{2\pi} E_{n}^{F} \int_{0}^{1} du \int_{0}^{\infty} dx \ xe^{-x} \left\{ 1 - 2Z\alpha x [u(1-u)]^{1/2} + \left[1 + \frac{2}{3} \left(1 + \frac{1}{2n^{2}} \right) \right] (Z\alpha x)^{2} u(1-u) + O(Z\alpha)^{3} \right\}$$
$$= E_{n}^{F} \left[\frac{\alpha}{2\pi} - \frac{\alpha}{4} Z\alpha + \frac{\alpha}{6\pi} \left(5 + \frac{1}{n^{2}} \right) (Z\alpha)^{2} + O(Z\alpha)^{3} \right]. \quad (6.59)$$

The first term is again the contribution of the static anomalous moment. The second term is part of the $I_{M\mu-p}$ contribution already considered in Sec. 5.

The additional contributions to $\Delta E_n(M_\mu)$ arising from the use of complete relativistic wave functions, rather than the nonrelativistic large components, are most easily obtained if M_μ is divided into two parts,²⁰

$$M_{\mu} = (M_{\mu} + 2\mathbf{p} \cdot e\mathbf{A}) + (-2\mathbf{p} \cdot e\mathbf{A}). \qquad (6.60)$$

The relativistic wave-function corrections to the first $\alpha(Z\alpha)^2 E_n^F$ is term may be taken from Breit⁹ if we neglect the denominator structure [an error of order $\alpha(Z\alpha)^4 E_n^F$] and recall

$$-(1/2m)\langle n_c | M_{\mu} + 2\mathbf{p} \cdot e\mathbf{A} | n_c \rangle = \langle n_c | -\mathbf{\gamma} \cdot e\mathbf{A} | n_c \rangle. \quad (6.61)$$

One finds the contributions

$$\frac{\alpha}{\pi} (Z\alpha)^2 E_n {}^F \left[\frac{3}{4}; \frac{17}{16} \right]$$
(6.62)

for n=1 and n=2, respectively. The contribution of the second term, $-2\mathbf{p} \cdot e\mathbf{A}$, to the S-state hfs arises from the small components, which can be taken as $\mathbf{\sigma} \cdot \mathbf{p}/2m$ acting on the nonrelativistic wave function ϕ_n . In momentum space we thus obtain

$$\frac{\alpha}{2\pi} \frac{-1}{2m} \int_0^1 du \int d^3 p \, \phi_n(p) \frac{-\boldsymbol{\sigma} \cdot \mathbf{p}}{2m}$$
$$\times \frac{1}{2\pi^2} \int d^3 p' \frac{1}{1+a^2 \mathbf{q}^2} \frac{-2e}{i} \frac{\mathbf{p} \cdot \mathbf{y} \times \mathbf{q}}{\mathbf{q}^2} \frac{\boldsymbol{\sigma} \cdot \mathbf{p}'}{2m} \phi_n(p'). \quad (6.63)$$

In position space the operator structure is written

$$\frac{1}{1+a^2\mathbf{q}^2} \frac{\mathbf{p} \cdot \mathbf{y} \times \mathbf{q}}{\mathbf{q}^2}$$
$$= \frac{1}{4\pi} \int d^3 r \, e^{-i\mathbf{q} \cdot \mathbf{r}} \frac{\mathbf{p} \cdot \mathbf{y} \times \mathbf{r}}{i\mathbf{r}} \frac{d}{d\mathbf{r}} \left(\frac{1-e^{-r/a}}{\mathbf{r}}\right) \quad (6.64)$$

and the spin structure for S states is

$$\frac{\boldsymbol{\sigma} \cdot \boldsymbol{\mu} \times \mathbf{r}}{ir} \frac{\boldsymbol{\sigma} \cdot \mathbf{r}}{r} = \boldsymbol{\sigma} \cdot \frac{\boldsymbol{\mu} \times \mathbf{r}}{r} \frac{\mathbf{r}}{r} - \frac{2}{3} \boldsymbol{\sigma} \cdot \boldsymbol{\mu} \qquad (6.65)$$

so we have simply

$$\frac{\alpha}{\pi} E_n F \frac{-1}{4m^2} \int_0^1 du \int_0^\infty dr \, r \left(\frac{d}{dr} \frac{\phi_n(r)}{\phi_n(0)}\right)^2 \frac{d}{dr} \left(\frac{1-e^{-r/a}}{r}\right). \quad (6.66)$$

The asymptotic part of the wave function, . .

$$\frac{d}{dr}\frac{\phi_n(r)}{\phi_n(0)} \sim -Z\alpha m \ e^{-\beta r} \tag{6.67}$$

(which is exact for n=1), yields a result of order $\alpha(Z\alpha)^2 E_n^F \ln Z\alpha$,

$$\frac{\alpha}{\pi}(Z\alpha)^{2}E_{n}^{F}\frac{-1}{4}\int_{0}^{1}du\left[\ln\frac{2a\beta}{1+2a\beta}+\frac{1}{1+2a\beta}\right]$$
$$=\frac{\alpha}{\pi}(Z\alpha)^{2}E_{n}^{F}\left[-\frac{1}{4}\ln\frac{2Z\alpha}{n}+O(Z\alpha)\right].$$
(6.68)

For n=2, the additional contribution of order

$$\frac{\alpha}{\pi} (Z\alpha)^{2} E_{n}^{F} \frac{-1}{4} \int_{0}^{1} du \int_{0}^{\infty} dr \, r e^{-2\beta r} \left[\left(1 - \frac{\beta r}{2} \right)^{2} - 1 \right] \frac{d}{dr} \left(\frac{1}{r} \right)$$
$$= \frac{\alpha}{\pi} (Z\alpha)^{2} E_{n}^{F} \frac{-1}{4} \left[\frac{1}{2} - \frac{1}{16} \right]. \quad (6.69)$$

For n = 1 and n = 2, we thus have the total contribution

$$\Delta E_n (M_{\mu} - \phi_{\text{Rel}}) = -\frac{\alpha}{\pi} (Z\alpha)^2 E_n^F \times \left[-\frac{1}{8} \ln \left(\frac{2Z\alpha}{n} \right)^2 + \frac{3}{4} + \frac{13}{64} (n-1) \right]. \quad (6.70)$$

Finally, $M_c = -\alpha \cdot [\mathbf{p}, V]$ contributes to the above orders as it connects large and small components (which we take in their nonrelativistic limit). To first order in the magnetic moment we thus have

$$\Delta E_n(M_c) = \frac{\alpha}{2\pi} \frac{1}{2m} \frac{-Z\alpha}{2\pi^2} \int_0^1 du \int d^3 p \int d^3 p'$$
$$\times 2 \left[\phi_n(p) \frac{1}{1 + a^2 q^2} \frac{\sigma \cdot q}{q^2} \delta_\mu \chi_n(p') + \phi_n(p) \frac{-\sigma \cdot p}{2m} \frac{1}{1 + a^2 q^2} \frac{\sigma \cdot q}{q^2} \delta_\mu \phi_n(p') \right], \quad (6.71)$$

where, ignoring higher order relativistic modifications, the magnetic contribution to the small component is

$$\delta_{\mu}\chi_{n}(p) = \frac{-\boldsymbol{\sigma}\cdot\boldsymbol{e}\mathbf{A}}{2m}\boldsymbol{\phi}_{n}(p) + \frac{\boldsymbol{\sigma}\cdot\mathbf{p}}{2m}\delta_{\mu}\boldsymbol{\phi}_{n}(p). \quad (6.72)$$

The contribution from the first term of (6.72) in position space is

$$\frac{\alpha}{2\pi} \frac{-e}{2m^2} (-Z\alpha) \int_0^1 du \int d^3 \mathbf{r}$$
$$\times \phi_n(\mathbf{r}) \frac{\partial}{\partial \mathbf{r}} \left(\frac{1-e^{-r/a}}{r}\right) \frac{\mathbf{\sigma} \cdot \mathbf{r}}{ir} \frac{\mathbf{\sigma} \cdot \mathbf{\mu} \times \mathbf{r}}{r^3} \phi_n(\mathbf{r}), \quad (6.73)$$

where the S-state hfs is obtained from

$$\frac{\boldsymbol{\sigma} \cdot \mathbf{r}}{ir} \frac{\boldsymbol{\sigma} \cdot \mathbf{y} \times \mathbf{r}}{r^3} \doteq \frac{2}{3} \frac{\boldsymbol{\sigma} \cdot \mathbf{y}}{r^2}.$$
 (6.74)

Integrating by parts and proceeding as in (6.68) and (6.69), we obtain for n=1 and n=2

$$\frac{\alpha}{\pi}(Z\alpha)^{2}E_{n}^{F}\left[\frac{1}{Z\alpha}\int_{0}^{1}\frac{du}{2ma}+\ln\frac{2Z\alpha}{n}+1+\frac{5}{8}(n-1)+O(Z\alpha)\right],\quad(6.75)$$

$$-\frac{\alpha}{2\pi} \frac{1}{2m^2} \frac{-Z\alpha}{2\pi^2} \int_0^1 du \int d^3 p \int d^3 p' \phi_n(p) \frac{1}{1+a^2 q^2} \frac{\sigma \cdot q \sigma \cdot q}{q^2} \delta_\mu \phi_n(p')$$

$$= \frac{\alpha}{\pi} \frac{Z\alpha}{4m^2} \int_0^1 du \int d^3 r \phi_n(r) \frac{e^{-r/a}}{ra^2} \delta_\mu \phi_n(r)$$

$$= \frac{\alpha}{\pi} (Z\alpha)^2 E_n^F \int_0^1 du \int_0^\infty \frac{r dr}{a^2} e^{-r/a} [1-Z\alpha mr + O((Z\alpha mr)^2)] \left[\frac{-1}{2Z\alpha mr} + \ln 2\beta r + \gamma - 2 + \frac{3}{2}(n-1) + O(Z\alpha mr) \right]$$

$$= \frac{\alpha}{\pi} (Z\alpha)^2 E_n^F \left[\frac{-1}{Z\alpha} \int_0^1 \frac{du}{2ma} + \ln \frac{2Z\alpha}{n} - 2 + \frac{3}{2}(n-1) + \frac{1}{2} + O(Z\alpha) \right]$$
(6.76)

for n=1 and n=2. The total contribution is thus

$$\Delta E_n(M_c) = -\frac{\alpha}{\pi} (Z\alpha)^2 E_n^F \times \left[\ln \left(\frac{2Z\alpha}{n} \right)^2 - \frac{5}{2} + \frac{17}{8} (n-1) + O(Z\alpha) \right]. \quad (6.77)$$

We have thus found that the total contribution of the I_M terms to the orders $\alpha(Z\alpha)^2 E_n^F$ and $\alpha(Z\alpha)^2 E_n^F \times \ln Z\alpha$ is

$$\Delta E_n(M) = \frac{\alpha}{\pi} (Z\alpha)^2 E_n^F \times \left[\frac{7}{8} \ln \left(\frac{2Z\alpha}{n} \right)^2 - \frac{3}{4} + \frac{141}{64} (n-1) \right]. \quad (6.78)$$

7. SUMMARY

The sum of the I_L and I_M contributions calculated in Sec. 6 and of the vacuum polarization terms calculated in Appendix C, together with the lower-order terms calculated in Secs. 3 and 5 may be written as

$$\Delta E_{n} = \frac{\alpha}{\pi} E_{n}^{F} \left\{ \frac{1}{2} + \pi \left(\ln 2 - \frac{5}{2} \right) Z\alpha - \frac{2}{3} (Z\alpha)^{2} \ln^{2} \left(\frac{2n}{Z\alpha} \right)^{2} \right. \\ \left. + \left[\frac{37}{72} + \frac{4}{15} + \frac{7}{2} (n-1) \right] (Z\alpha)^{2} \ln \left(\frac{n}{2Z\alpha} \right)^{2} \right. \\ \left. + \left[\frac{22}{3} \ln 2 - \frac{2}{9} \pi^{2} + 18 - \frac{457}{2700} \right. \\ \left. - \left(4 + \frac{2993}{8640} \right) (n-1) \right] (Z\alpha)^{2} \right\}$$
(7.1)

for n=1 and n=2. The numerical values of the various contributions to the coefficients are listed in Table III.

As anticipated from the Lamb-shift calculation of

order $\alpha(Z\alpha)^{6}mc^{2}$, the $(\alpha/\pi)(Z\alpha)^{2}E_{n}{}^{F}$ coefficient accompanying the $\ln^{2}(Z\alpha)^{-2}$ contribution (second line in Table III) is quite large, +16.63. We should thus have a good estimate of the total coefficient since the other $(\alpha/\pi)(Z\alpha)^{2}E_{n}{}^{F}$ coefficients are small (they only add up to +1.73 even though all except the smallest are positive) and most of the uncalculated coefficients are expected to be even smaller. Let us discuss the various uncalculated terms.

The largest number of uncalculated contributions to order $(\alpha/\pi)(Z\alpha)^2 E_n^F$ are the terms quadratic in the field strength. These are separately rather small since the parametric (z,λ,u) integrations each give factors smaller than 1 and the momentum integration does not give the factor π occurring in the $\alpha(Z\alpha)E_n^F$ coefficient, as in (5.24). The terms would not be expected to add together to give a large coefficient since none of the other calculated coefficients for either the hfs or the Lamb shift are larger than their largest single contribution. It seems quite conservative to put an estimated bound of ± 1 on the total of the $(\alpha/\pi)(Z\alpha)^2 E_n^F$ coefficients from terms quadratic in the field strength.

The only other uncalculated state-independent coefficients of $(\alpha/\pi)(Z\alpha)^2 E_n{}^F$ are from the shift correction terms labeled L-p in Table III. These terms are seen to contribute an extremely small amount (4%) to the $\alpha(Z\alpha)E_n{}^F$ coefficient in Table III and are also found to give only small contributions to the $\alpha(Z\alpha)^5mc^2$ and $\alpha(Z\alpha)^6 \ln(Z\alpha)^{-2}mc^2$ coefficients in the Lamb shift.⁷ We will estimate their contribution to order $(\alpha/\pi)(Z\alpha)^2E_n{}^F$ to be negligible.

The largest uncalculated terms are anticipated to be the contributions of the nonsymptotic parts of the wave functions in the second term in the V expansion of I_L . This is because the first term in the V expansion yields the entire contribution of order $\alpha(Z\alpha)^2 \ln^2(Z\alpha)^{-2}E_n^F$ and the dominant contributions of orders $\alpha(Z\alpha)^2 \ln(Z\alpha)^{-2}E_n^F$ and $\alpha(Z\alpha)^2E_n^F$, both for the state-independent and state-dependent coefficients, when the nonasymptotic parts of the wave functions are used. To estimate the size of the contributions of the

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Term	Eq. No.				$\times (Z\alpha)^2 \ln (Z\alpha)^{-2}$		$\times (Z\alpha)^2$	
		$\times 1$	$\times \pi Z \alpha$	$\times (Z\alpha)^2 \ln^2(Z\alpha)^{-2}$	n = 1	(n=2)-(n=1)	n = 1	(n=2)-(n=1)
$L_{\epsilon} - \delta_{}\phi - \text{asym}$	(5.9), (6.18), (6.30)	0	-1.18	0	+2.00	-0.67	+0.14	+1.13
$L_{c} - \delta_{u} \phi - \text{nonasym}$	(6.24), (6.26), (6.27), (6.31)	0	0	-0.67	-2.76	+2.82	+16.63	-7.34
$L_c - \delta_{} \phi - V - asym$	(6.44)	0	0	0	-0.52	0	+0.32	-0.71
$L_{\sigma} - \delta_{\mu}\phi - V - nonasym$		0	0	0	0	0	not calc.	not calc.
$L_c - \delta_{\mu\phi} - V - V$		0	0	0	0	0	not calc.	not calc.
$L_{\rm m} - {\rm asym}$	(5.9), (5.11), (6.40)	0	-1.18	0	+2.00	-1.17	+0.14	+1.40
$\tilde{L}_{}^{\mu}$ -nonasym	(6.40)	0	0	0	0	+0.67	0	-0.61
$L_{\mu}^{\mu} - V - asym$	(6.47)	0	0	0	-0.85	0	+0.53	-1.18
$L_{\mu}^{\mu} - V - nonasym$		0	0	0	0	0	not cale.	not calc.
$L^{\mu}_{\mu} - V - V$		0	0	0	0	0	not calc.	not calc.
$\overline{L}^{\mu}_{-\phi}$	(5.14)	0	-0.07	0	0	0	not cale.	0
$\overline{L} - M$	(6.51)	0	0	0	-0.33	0	+0.21	-0.46
M	(3.4), (5.17), (6.78)	0.50	-0.14	0	-0.88	0	+0.46	+0.99
Quadratic in F		0	0	0	0	0	not calc.	0
Vac. Pol.	(C9)	0	+0.75	0	+0.27	0	-0.08	-0.33
Total		0.50	-1.81	-0.67	-1.07	+1.65	18.36 + n.c. = +18.36 ± 5 ^a	-7.11 + n.c. = -5.57 ± 0.06^{t}
Coefficient of $E_{-}F$ for $Z = 1$		1161	-96.21	-7.98	-1.30	+2.01	+2.27+0.62	-0.69 ± 0.01
	•	ppm	ppm	ppm	ppm	ppm	ppm	ppm

TABLE III. $(\alpha/\pi)E_n^F$ coefficients.

^a Estimated limit of uncalculated terms. ^b Result of complete numerical calculation in Ref. 15.

nonasymptotic parts in the second term in the V expansion, we combine them with the contributions of the remaining terms in the V expansion to give the only uncalculated state-dependent coefficients. (The calculation of the remaining terms in the V expansion requires a sum-over-states method.) Comparing the total calculated state-dependent coefficient with the complete numerical results of Zwanziger¹² in Table III, we see that only

$$\frac{(-5.57 \pm 0.06) - (-7.11)}{5.57} \cong \frac{1}{4}$$

of the state-dependent coefficient has been uncalculated. Taking about the same fraction of the calculated stateindependent coefficient, ± 18.36 , we estimate about ± 4 for the corresponding uncalculated contributions to the $(\alpha/\pi)(Z\alpha)^2 E_n^F$ coefficient. Adding this to the ± 1 for terms quadratic in the field strength, we estimate

$$|c_{20}(1) - 18.36| < 5,$$
 (7.2)

as listed in Table III.

Having used the precision of Zwanziger's result to estimate the size of our uncalculated terms, let us reverse the procedure and note that our calculated terms provide a good check of the sign and magnitude of Zwanziger's (n=2)-(n=1) difference. Such a check is particularly desirable since the Lamb shift statedependent coefficients are quite small and one might thereby expect the hfs state-dependent coefficient to be similarly small. This is not found to be the case, either for the $\alpha(Z\alpha)^2 \ln(Z\alpha)^{-2} E_n^F$ coefficient or (especially) the $\alpha(Z\alpha)^2 E_n^F$ coefficient. The reason for the large coefficients is seen to be that the $\delta_{\mu}\phi_n(r)$ (the "magnetic correction" parts of the wave functions), unlike the Coulomb wave functions, are strongly state-dependent near r=0, apart from the state-independent divergent leading term $-1/2Z\alpha mr$ in (A3). This was particularly seen in the calculations in Appendix D.

Using the value

$$c_{20}(1) = 18.36 \pm 5 \tag{7.3}$$

in Eq. (1.7) with²⁶

.

 $\delta_p =$

$$E_{1}^{F} = \frac{10}{3} \alpha^{2} c R_{\infty}^{\mu_{p}}$$

= 1421.102 \pm 0.039 \frac{Mc}{sec} (\pm 27.4 ppm) (7.4)

and

$$(-35\pm3)\times10^{-6},$$
 (7.5)

where15

$$\alpha^{-1} = 137.0388 \pm 0.0019 \ (\pm 13.7 \text{ ppm}),$$
 (7.6)

$$c = 2.997 \ 925 \times 10^{10} \pm 3 \times 10^4 \ \text{cm/sec}$$

(±0.9 ppm), (7.7)

(

$$R_{\infty} = 109\ 737.31 \pm 0.03\ \mathrm{cm}^{-1}\ (\pm 0.3\ \mathrm{ppm}),$$
 (7.8)

$$\mu_p/\mu_0 = 0.001\ 521\ 032\ 5,\tag{7.9}$$

we obtain 26

$$\delta E_1(H; \text{theor}) = 1420.345 \pm 0.044 \text{ Mc/sec}$$

$$\pm 31 \text{ ppm}$$
) (7.10)

for the ground-state hfs in hydrogen. This disagrees with the experimental value²

$$\delta E_1(H; \exp) = 1420.405\ 751\ 800 \pm 28 \times 10^{-9}$$

_____ Mc/sec (7.11)

²⁶ The error intervals quoted for the numbers used for the theoretical values of δE_1 represent estimated absolute limits of error rather than a standard deviation or expected error. Thus, we use three standard deviations for the E_1^F error limit of ± 27.4 ppm (which is almost entirely due to the uncertainty in α) and add this to $\pm 5(Z\alpha)^2 = \pm 0.6$ ppm from $c_{20}(1)$ and to ± 3 ppm from δ_p or ± 13 ppm from μ_{μ}/μ_p to get the ± 31 ppm in (7.10) and (7.12) or the ± 41 ppm in (7.15). Smaller error intervals quoted elsewhere (Refs. 1, 4, 14) are obtained by using one or two standard deviations for the uncertainty in α .

 by^{26}

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$$\frac{\delta E_1(H; \exp) - \delta E_1(H; \text{theor})}{\delta E_1(H)} = 43 \pm 31 \text{ ppm}.$$
 (7.12)

This discrepancy makes the hydrogen hfs measurement unsuitable for determining α .

For muonium, we may take²⁷

$$\mu_{\mu}/\mu_{p} = 3.183 \ 38 \pm 0.000 \ 04 \ (\pm 13 \ \text{ppm}),^{28} \ (7.13)$$

and δ_{μ} as in (1.5) with

$$M_{\mu}/m_e = 206.765$$
, (7.14)

and obtain²⁶

 $\delta E_1(M; \text{theor}) = 4463.16 \pm 0.18 \text{ Mc/sec}$ $(\pm 41 \text{ ppm})$ (7.15)

which agrees quite well with experiment,¹

$$\delta E_1(M; \exp) = 4463.15 \pm 0.06 \text{ Mc/sec}$$

(±13 ppm).²⁸ (7.16)

If, instead, we use the experimental values to determine the fine-structure constant, we obtain²⁸

$$\alpha^{-1} = 5131.2210 (\mu_{\mu}/\mu_{p}\delta E_{1})^{1/2} = 137.0390 \pm 0.0012$$

(±9 ppm), (7.17)

which agrees quite well with the value (7.6) obtained from the fine-structure separation of the $2P_{3/2} - 2P_{1/2}$ levels in deuterium.29

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APPENDIX A: WAVE FUNCTIONS USED IN THE CALCULATIONS

The 1S and 2S nonrelativistic Schrödinger wave functions for the electron in a Coulomb field are

$$\phi_1(\mathbf{r}) = \phi_1(0) e^{-\beta \mathbf{r}},$$

$$\phi_2(\mathbf{r}) = \phi_2(0) e^{-\beta \mathbf{r}} (1 - \beta \mathbf{r}) , \qquad (A1)$$

where

with

$$|\phi_n(0)|^2 = \beta^3 / \pi,$$

$$\beta \equiv \beta(n) \equiv Z \alpha m / n.$$

The asymptotic form of these wave functions in momentum space is

$$\phi_n(\mathbf{p}) \sim \frac{n(2\beta)^{5/2}}{2\pi} \frac{1}{(\mathbf{p}^2 + \beta^2)^2}. \quad (\mathbf{p}^2 \gg \beta^2) \qquad (A2)$$

²⁷ D. P. Hutchinson, J. Menes, G. Shapiro, and A. M. Patlach, Phys. Rev. 131, 1351 (1963).
²⁸ The error intervals in (7.13) and (7.15) are estimated error

$\pm 9 \text{ ppm} \leq \pm \frac{1}{2} [(\pm 13 \text{ ppm})^2 + (\pm 13 \text{ ppm})^2]^{1/2},$

The S-wave part of the first-order magnetic dipole perturbation to the above wave functions is^{12,30}

$$\times \left[\frac{-1}{2\beta r} + (\ln 2\beta r + \gamma - 1) - \frac{3}{2} + \beta r \right]$$

$$\delta_{\mu} \phi_{2}(r) = 2(Z\alpha)^{2} m C_{\mu} \phi_{n}(0) e^{-\beta r}$$

$$\times \left[\frac{-1}{4\beta r} + (\ln 2\beta r + \gamma - 1) + \frac{1}{4} - \beta r \left(\ln 2\beta r + \gamma - \frac{13}{4} \right) - \frac{1}{2} (\beta r)^{2} \right], \quad (A3)$$

where $\gamma = 0.577^+$ is Euler's constant and

 $\delta_{\mu}\phi_1(r) = 2(Z\alpha)^2 m C_{\mu}\phi_n(0) e^{-\beta r}$

$$E_n^F = 2Z\alpha\beta^3 C_{\mu}/m = 4 |e| \langle \boldsymbol{\sigma} \cdot \boldsymbol{y} \rangle \beta^3/3m. \qquad (A4)$$

The asymptotic form of these wave functions in momentum space is³⁰

$$\delta_{\mu}\phi_{n}(\mathbf{p})\sim C_{\mu}V\phi_{n}(\mathbf{p})=-C_{\mu}\frac{\mathbf{p}^{2}+\beta^{2}}{2m}\phi_{n}(\mathbf{p}).\quad(\mathbf{p}^{2}\gg\beta^{2})\quad(A5)$$

APPENDIX B

In this appendix we account for the difference in form of the terms I_{LM} , I_c , I_d , and I_e of Table I and the terms I_c , I_d , I_e , and I_f of paper I. We first note that the term I_c of Table I can be identified with the contribution of the second part of (I-2.48) before the latter is reduced to the terms I_c and I_d of paper I. Second, instead of transforming the term (I-2.71)

$$I_{0} \equiv 2z\gamma_{\mu}(\boldsymbol{k} - \boldsymbol{z}\boldsymbol{\Pi}) \frac{1}{D} \left[\boldsymbol{\Pi}^{\mu}, \boldsymbol{\Pi}\right] \frac{1}{D} \left| \left| \frac{1}{D^{2}} \right| \right|$$
(B1)

into the terms I_e and I_f of paper I, we take an approach more convenient to the hyperfine structure calculations.

We first note that if γ_{μ} is anticommuted past $(\mathbf{k} - \mathbf{z} \mathbf{\Pi})$ and commuted past D^{-1} we obtain the magnetic moment structure

$$\gamma_{\mu} [\Pi^{\mu}, \mathbf{\Pi}] = 2M, \qquad (B2)$$

and thus rewrite I_0 as the sum of the terms

$$I_0' = 2z(k - z\Pi) \frac{1}{D} (-2M) \frac{1}{D} \left| \left| \frac{1}{D^2} \right| \right|$$
 (B3)

$$H_0'' = 4z(k_{\mu} - z\Pi_{\mu}) \frac{1}{D} [\Pi^{\mu}, \Pi] \frac{1}{D} \left| \left| \frac{1}{D^2} \right| \right|$$
 (B4)

$$I_{e} = -2z(\boldsymbol{k} - z\boldsymbol{\Pi}) \left[\gamma_{\mu}, \frac{1}{D} \right] \left[\Pi^{\mu}, \boldsymbol{\Pi} \right] \frac{1}{D} \left| \left| \frac{1}{D^{2}} \right| \right|$$
(B5)

We next use an integration-by-parts identity (I-2.46)

$$\left| \left| \frac{k_{\nu}}{D} \doteq \right| \right| \frac{z \Pi_{\nu}}{D}$$
 (B6)

³⁰ S. J. Brodsky, thesis, University of Minnesota, 1964 (unpublished).

limits, while the error interval in (7.16) is one standard deviation. The error interval in (7.17),

is essentially one standard deviation. ²⁹ E. S. Dayhoff, S. Triebwasser, and W. E. Lamb, Jr., Phys. Rev. 89, 106 (1953).

to reduce the term

$$I_{0}' = -4z(\mathbf{k} - z\mathbf{\Pi})\frac{1}{D} \bigg| \bigg| \frac{M}{D^{3}} \doteq -4z^{2} \bigg(\gamma_{\mathbf{r}} \frac{1}{D} \Pi^{\mathbf{r}} \frac{1}{D} - \mathbf{\Pi} \frac{1}{D^{2}} \bigg) \bigg| \bigg| \frac{M}{D^{2}}$$
$$= -4z^{2} \bigg(\bigg[\gamma_{\mathbf{r}}, \frac{1}{D} \bigg] \Pi^{\mathbf{r}} \frac{1}{D} - \bigg[\mathbf{\Pi}, \frac{1}{D} \bigg] \frac{1}{D} \bigg) \bigg| \bigg| \frac{M}{D^{2}}. \tag{B7}$$

Note that commutators of M occur when we apply the identity

$$\begin{bmatrix} A, \frac{1}{D} \end{bmatrix} \left\| \frac{B}{D} = -\frac{1}{D} \begin{bmatrix} A, D \end{bmatrix} \frac{1}{D} \right\| \frac{B}{D} + \frac{1}{D} \begin{bmatrix} A, B \end{bmatrix} \frac{1}{D}.$$
 (B8)

Thus,

$$I_{0}' = 4z^{2} \left(\frac{1}{D} \begin{bmatrix} \gamma_{\nu}, D \end{bmatrix} \frac{1}{D} \prod_{\nu} \frac{1}{D} - \frac{1}{D} \begin{bmatrix} \mathbf{\Pi}, D \end{bmatrix} \frac{1}{D^{2}} \right) \left| \left| \frac{M}{D^{2}} - 4z^{2} \left(\frac{1}{D} \begin{bmatrix} \gamma_{\nu}, M \end{bmatrix} \frac{1}{D} \prod_{\nu} \frac{1}{D} - \frac{1}{D} \begin{bmatrix} \mathbf{\Pi}, M \end{bmatrix} \frac{1}{D^{2}} \right) \right| \left| \frac{1}{D^{2}} \right|.$$
(B9)

The subsequent reduction of the first line in I_0' is just like that of (I-2.61) and yields I_{LM} of Table I.

We write the second line of I_0' as

$$-4z^{2}\frac{1}{D}([\gamma_{r},M]\Pi^{r}-[\Pi,M])\frac{1}{D^{2}}\Big|\Big|\frac{1}{D}$$
$$-4z^{2}\frac{1}{D}[\gamma_{r},M]\frac{1}{D}[\Pi^{r},D]\frac{1}{D^{2}}\Big|\Big|\frac{1}{D} \quad (B10)$$

and combine it with

$$I_{0}^{\prime\prime} \doteq 4z^{2} \frac{1}{D} \begin{bmatrix} \Pi^{\mu}, \Pi \end{bmatrix}, \Pi_{\mu} \end{bmatrix} \frac{1}{D^{2}} \left| \left| \frac{1}{D} + 4z^{2} \frac{1}{D} \begin{bmatrix} \Pi^{\mu}, D \end{bmatrix} \frac{1}{D^{2}} \right| \left| \frac{\begin{bmatrix} \Pi^{\mu}, \Pi \end{bmatrix}}{D^{2}}, \quad (B11)$$

where (B6) and (B8) have been used again. The sum of the first terms of (B10) and (B11) vanishes,

$$-[\gamma_{\nu},M]\Pi^{\nu}+[\Pi,M]+[[\Pi^{\mu},\Pi],\Pi_{\mu}]$$

= $\frac{1}{2}\gamma_{\mu}\gamma_{\nu}\gamma_{\lambda}[[\Pi^{\mu},\Pi^{\lambda}],\Pi^{\nu}]=0, \quad (B12)$

as in (I-2.73). The sum of the second terms of (B10) and (B11) becomes I_d in Table I when the identity

$$[\boldsymbol{\gamma}_{\boldsymbol{\nu}}, \boldsymbol{M}] = 2[\boldsymbol{\Pi}_{\boldsymbol{\nu}}, \boldsymbol{\Pi}] \tag{B13}$$

is used. Thus, we have shown

$$I_0 = I_{LM} + I_d + I_e,$$
 (B14)

as required. The terms I_d and I_e turn out to have cancelling w=0contributions (w is defined in footnote 22). In I_d we note

$$\begin{bmatrix} \Pi_{\mu}, D \end{bmatrix} = \begin{bmatrix} \Pi_{\mu}, 2zk \cdot \Pi - z\Pi^2 \end{bmatrix}$$
$$= 2zk {}_{\rho} \begin{bmatrix} \Pi_{\mu}, \Pi^{\nu} \end{bmatrix} - z\Pi \begin{bmatrix} \Pi_{\mu}, \Pi \end{bmatrix} - z \begin{bmatrix} \Pi_{\mu}, \Pi \end{bmatrix} \Pi. \quad (B15)$$

The last two forms give w=0 contributions to I_d when **II** s between the commutators:

$$I_{d}(w=0) = -4z^{3} \left\{ \frac{1}{D} [\Pi_{\mu}, \Pi] \Pi \frac{1}{D^{2}} [\Pi^{\mu}, \Pi] \frac{1}{D} + \frac{1}{D} [\Pi_{\mu}, \Pi] \Pi \frac{1}{D} [\Pi^{\mu}, \Pi] \frac{1}{D^{2}} - \frac{1}{D} [\Pi^{\mu}, \Pi] \frac{1}{D} \Pi [\Pi_{\mu}, \Pi] \frac{1}{D^{2}} \right\} \left\| \left| \frac{1}{D} \right| . \quad (B16)$$

Similarly I_e gives w=0 contributions when the $||k^r \doteq || z \Pi^r$ insertion is performed on the middle D^{-1} :

$$I_{e}(w=0) = -4z^{3}\gamma_{r}\frac{1}{D}[\Pi_{\mu},\Pi]\frac{1}{D}\Pi^{r}\frac{1}{D}[\Pi^{\mu},\Pi]\frac{1}{D}\Big|\Big|\frac{1}{D}.$$
(B17)

If we anticommute the γ^{ν} in (B17) through the $D^{-1}[\Pi_{\mu},\Pi]D^{-1}$, and ignore commutators with D^{-1} (which are higher order since they are cubic in the field strength), we see that (B16) and (B17) cancel. The remainder containing the anticommutator

$$\gamma_{\nu}, [\Pi_{\mu}, \Pi_{\mu}] = 2[\Pi_{\mu}, \Pi_{\nu}]$$
(B18)

has an odd number of γ matrices in the numerator, bringing in the small components of the wave function so that $w \ge 1$.

We also wish to demonstrate that only the $I_{L\mu}$ and I_{Lc} structures of the I_L numerator (4.1) contribute to nominal order N=6. A representative matrix element for the terms in the third line of (4.1) is

$$\left\langle n \left| \frac{1}{D} p^{\mu} \frac{1}{D} \left[eA_{\mu}, (m - \Pi) \right] \frac{1}{D} \right| n \right\rangle \right\| \left| \frac{1}{D} \right\rangle.$$
(B19)

This is clearly zero (since $m-\Pi$ vanishes acting on either wave function) except for commutators of Π with the denominators or with the operator $p^{\mu} = (E_n, \mathbf{p})$. The commutator with the denominators may be written

$$\frac{1}{D} \frac{1}{p^{\mu}} \frac{1}{D} e^{A}_{\mu} \frac{1}{D} \left| \left| \frac{[D, \Pi]}{D} \right| \right| \frac{1}{D}$$
$$\doteq -2z^{2} \frac{1}{D} p^{\mu} \frac{1}{D} e^{A}_{\mu} \frac{1}{D} \left| \left| \frac{[\Pi^{\nu}, \Pi]}{D} \right| \left| \frac{\Pi}{D}, \quad (B20)\right|$$

where we have used the identity

$$[D,\mathbf{\Pi}] = 2z[\Pi^{\nu},\mathbf{\Pi}]k, \qquad (B21)$$

and the equivalence (B6). The contributions of (B20) are of order $\alpha(Z\alpha)^2 E_n^F$ ($_08_2$) and higher. The term from the commutator of Π with p^{μ} is also easily seen to be of higher order, as are the terms in the fourth line of (4.1).

APPENDIX C: THE VACUUM-POLARIZATION CORRECTIONS TO THE HYPERFINE STRUCTURE

The energy shift due to vacuum polarization³¹ is given to order α by

$$\Delta E_n(VP) = \langle n | \gamma \cdot eA^{VP} | n \rangle, \qquad (C1)$$

^{at} R. Serber, Phys. Rev. 48, 49 (1935); E. Uehling, *ibid.* 48, 55 (1935).

where A_{μ}^{VP} is the induced vacuum-polarization potential

$$A_{\mu}{}^{VP}(\mathbf{q}) = \frac{\alpha}{2\pi} \mathbf{q}^2 \int_0^1 dv \, \frac{2v^2(1-v^2/3)}{4m^2 + \mathbf{q}^2(1-v^2)} A_{\mu}(\mathbf{q}) \,. \quad (C2)$$

Higher order terms at least cubic in the external potential A_{μ} have been ignored. In the calculations of the corrections to the hyperfine structure, relativistic modifications to the wave functions may be ignored with error of order $\alpha(Z\alpha)^{3}E_{n}^{F}$.

For the Coulomb part $\gamma \cdot eA \rightarrow \gamma_0 V$, the hyperfine dependence is taken from the linear magnetic corrections to either wave function. In position space we obtain the contribution

$$\Delta E_n(VP-c) = -\frac{\alpha}{\pi} \frac{Z\alpha}{4m^2} \int_0^1 dv \ 2v^2 (1-v^2/3) \\ \times \int d^3 r \phi_n(r) \frac{e^{-r/a}}{ra^2} \delta_\mu \phi_n(r) , \quad (C3)$$

where

$$\equiv (1 - v^2)/4m^2 \tag{C4}$$

and $\delta_{\mu}\phi_n$ is given in Appendix A. The required integrations are straightforward; the result through order $\alpha(Z\alpha)^2 E_n^F$ is

 a^2

$$\Delta E_{n}(VP-c) = \alpha(Z\alpha)E_{n}^{F}\left[\frac{3}{8}\right] + \frac{\alpha}{\pi}(Z\alpha)^{2}\ln\frac{n}{2Z\alpha}\left[\frac{8}{15}\right] + \frac{\alpha}{\pi}(Z\alpha)^{2}E_{n}^{F}\left[\frac{8}{15}\left(\frac{1}{2}-\frac{3}{2}\delta_{n2}\right) + \frac{8}{9}-\frac{46}{225}\right]. \quad (C5)$$

For the magnetic term, $\gamma \cdot eA \rightarrow -\gamma \cdot eA$, we recall the Coulomb S-wave-function matrix-element identity used in the calculation of $I_{L\mu}$,

$$-\mathbf{q}^{2}\boldsymbol{\gamma}\cdot\boldsymbol{e}\mathbf{A}\doteq 2M_{\mu}(V+\epsilon_{n}). \tag{C6}$$

We thus obtain the contribution

$$\Delta E_n(VP-\mu) = -\frac{\alpha}{\pi} Z \alpha \frac{C_\mu}{4m^2} \int_0^1 2v^2 (1-v^2/3)$$
$$\times \int d^3 r \, \phi_n(r) \frac{e^{-r/a}}{ra^2} \phi_n(r) (V+\epsilon_n) \,. \quad (C7)$$

The result through order $\alpha(Z\alpha)^2 E_n^F$ is

$$\Delta E_n(VP-\mu) = \alpha(Z\alpha)E_n^F \left[\frac{3}{8}\right] + \frac{\alpha}{\pi}(Z\alpha)^2 E_n^F \left[-\frac{10}{15} + \frac{1}{10}\delta_{n2}\right]. \quad (C8)$$

The total contribution of (C5) and (C8) is thus $\Delta E_{\alpha}(VP) = \Delta E_{\alpha}(VP - c) + \Delta E_{\alpha}(VP - u)$

$$= \alpha(Z\alpha)E_{n}^{F}\left[\frac{3}{4}\right] + \frac{\alpha}{\pi}(Z\alpha)^{2}\ln\frac{n}{2Z\alpha}\left[\frac{8}{15}\right] + \frac{\alpha}{\pi}(Z\alpha)^{2}E_{n}^{F}\left[\frac{64}{225} - \frac{7}{10}\delta_{n^{2}}\right].$$
 (C9)

APPENDIX D

To evaluate in position space the contribution of the second term in (6.6), we may perform three integrations over angles and obtain

$$\Delta E_n(vii) = \frac{\alpha}{\pi} (Z\alpha)^2 E_n {}^F \int_0^\infty ds \int_0^\infty ds' \int_{|s-s'|}^{s+s'} ds'' \int_0^1 du \int_0^1 dy$$
$$\times \frac{P(z,u)}{y^2 + (1-y^2)\omega} \delta_\mu \phi_n(s) \chi(s,s',s'',y) \frac{d}{ds'} \phi_n(s'), \quad (D1)$$

where

and

$$s \equiv \beta r$$
, $s' \equiv \beta r'$, and $s''^2 \equiv \beta^2 (\mathbf{r} - \mathbf{r}')^2$, (D2)

$$\delta_{\mu}\phi_n(s) \equiv \delta_{\mu}\phi_n(r)/(Z\alpha)^2 m C_{\mu}\phi_n(0) \tag{D3}$$

[as given in (6.10) for n=1 and 2],

$$\phi_n(s') \equiv \phi_n(r') / \phi_n(0), \qquad (D4)$$

$$\chi(s,s',s'',y) \equiv -\frac{e^{-s''/y}}{y} \frac{s'^2 + s^2 - s''^2 - 2s^3/s'}{s^2}.$$
 (D5)

The asymptotic parts of the wave functions

$$\delta_{\mu}\phi_n(s)\sim -e^{-s}/ns$$
, (D6)

$$\frac{d}{ds'}\boldsymbol{\phi}_n(s') \sim -ne^{-s'}, \qquad (D7)$$

correspond to the asymptotic parts (A5) and (A2) in momentum space and thus yield the contribution (6.30), of order $\alpha(Z\alpha)^2 \ln(Z\alpha)^{-2}E_n{}^F$. For the remainder of (D1) the integrations are convergent for $\omega=0$ $(Z\alpha=0)$ so the contribution of order $\alpha(Z\alpha)^2E_n{}^F$ may be obtained by taking the limit

$$\int_{0}^{1} du \int_{0}^{1} dy \frac{P(z,u)\chi(s,s',s'',y)}{y^{2} + (1-y^{2})\omega} \xrightarrow{Z_{\alpha \to 0}} \frac{2}{3} \int_{0}^{1} \frac{dy}{y^{2}} \chi(s,s',s'',y)$$
$$= -\frac{2}{3} e^{-s''} \left[\frac{1}{s''} + \frac{1}{s''^{2}} \right] \left[\frac{s'^{2} + s^{2} - s''^{2} - 2s^{3}/s'}{s^{2}} \right]. \quad (D8)$$

The s'' integration is now easily done, and we obtain

$$\Delta E_n(vii; \text{nonasym}) = \frac{\alpha}{\pi} (Z\alpha)^2 E_n \int_0^\infty ds$$
$$\times \left[\delta_\mu \phi_n(s) I_n(s) - \left(-\frac{e^{-s}}{ns} \right) \left(-\frac{4}{3} n e^{-s} \right) \right], \quad (D9)$$

where, for n = 1 and 2,

$$I_{n}(s) \equiv \frac{4}{3} e^{-s} \left\{ -n + 2s(n-1) \left[\ln 2s + \gamma + \frac{3}{4} \right] - 2s \left[n + 2s(n-1) \right] \int_{0}^{\infty} dt \ e^{-2st} \ln \frac{1+t}{t} \right\}, \quad (D10)$$

with $t \equiv s'/s$. The final results given in (6.31) may be obtained by performing the s and then the t integrations.

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