

values (0, 1, and 2) of the total spin  $S$ . A preliminary examination indicates that the first-order dispersion energies then depend on a parameter related to  $S$ , somewhat as they depended on  $\sigma$  for doublet atoms in Section II. However, this matter will not be pursued further here.

A point of some interest (especially if approximate theoretically computed values of  $\mu_{mn}$  are to be used in the absence of experimental values) is the relation of  $\mu_{mn}$  to the value of  $\mu_{mn}$  for a one-electron transition. The cases of the bivalent alkaline-earth and Hg-type atoms and of the rare gas atoms when one atom is in its ground state and the other in its  $sp$  or  $p^5s$  resonance state are especially simple. In both cases, a 2-electron approximation should be fairly accurate (see the 1-electron approximation for alkali metal atoms in Sec. VI). In this approximation it is easily shown for the bivalent metal atoms that  $\mu_{mn}$  is  $2^{1/2}$  times as large, hence  $\mu_{mn}^2$  and  $f_{mn}$  are twice as large, as for a similar transition  $p \leftarrow s$  of a single electron. In the case of the rare gas atoms,  $\mu_{mn}^2$  and  $f_{mn}$  are again just twice as

large as for a similar  $s \leftarrow p$  transition of a single electron (*not*, as one might perhaps casually surmise, six times as large because of the six electrons in the  $p^6$  shell). If one uses real AO's and  $\Phi$ 's, as is convenient here,  $\mu_{mn}$  in Eq. (14) corresponds in the bivalent metal case to any *one* of the transitions  $sp_q, {}^1P_q \leftarrow s^2, {}^1S$ , where  $q$  may be  $x, y,$  or  $z$ . All of these give the same value of  $(\mu_{mn}^{(a)})^2$ , each time twice that for the corresponding transition  $p_q, {}^2P_q \leftarrow s, {}^2S$ , because *either* of the two electrons in  $s^2$  can jump. In the rare gas case, one has again three equal  $\mu_{mn}^{(z)}$ 's, of which, for example,  $(\mu_{mn}^{(z)})^2$  corresponds to  $p_x^2 p_y^2 p_z s, {}^1P_z \leftarrow p_x^2 p_y^2 p_z^2, {}^1S$ , with a value twice that for  $p_x^2 p_y^2 s, {}^2S \leftarrow p_x^2 p_y^2 p_z, {}^2P_z$ . It will be noted that for any one  $q$ , only two electrons of  $p^6$  can be active.

In all the foregoing cases, of course, account must be taken of the fact that a fraction of  $\mu_{mn}^2$  is lost from  ${}^1P$  to  ${}^3P_1$ , depending on the energy difference between  ${}^3P$  and  ${}^1P$  and on how strong the spin-orbit coupling in  ${}^3P$  is. This loss can readily be computed by standard methods if one knows the positions of the  ${}^3P_0, {}^3P_1, {}^3P_2,$  and  ${}^1P$  energy levels.

## Theory of the Hyperfine Anomalies of Deuterium, Tritium, and Helium-3<sup>†\*</sup>

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The covariant equation for the three-body deuterium system is discussed, and reduced to a three-dimensional equation for the case of instantaneous two-body interactions. A noncovariant perturbation scheme, based on this three-dimensional equation, was employed to calculate the hyperfine structure (hfs) to order  $\alpha m/M$  (hfs) for  ${}_1\text{H}^2, {}_1\text{H}^3, {}_2\text{He}^3+$ . The results are compared with the experimental values, and shown to be compatible. Final determination of the theoretical values and the adequacy of the theory is shown to depend critically on the determination of a number of experimental quantities, in particular on a more precise measurement of  $\alpha$ , of the nucleon electric and magnetic form factors and associated nucleon polarization, of the presence and magnitude of a two-nucleon spin-orbit potential, and of the singlet  $n$ - $p$  effective range.

### I. INTRODUCTION

THE hyperfine splitting of hydrogen has been calculated to order  $\alpha^2$  (hfs) in the relativistic and radiative corrections,<sup>1</sup>  $\alpha m/M$  in the mass corrections,<sup>2</sup> and  $(r$ -nucleus)/ $a_0$  in the structure corrections.<sup>3</sup> These orders are of comparable magnitude, and the following formula for the  $\text{H}^1$  hfs is good to a few ppm:

$$\begin{aligned} \Delta\nu_{\text{H}} = & (16/3)\alpha^2 c R_{\infty} (\mu_p/\mu_e) \{1+m/M\}^{-3} \\ & \times \{1+\alpha/2\pi+0.386\alpha^2/\pi^2\}^2 \{1+3\alpha^2/2\} \\ & \times \{1-\alpha^2(5/2-\ln 2)\} \{1-35(\pm 3.5)\times 10^{-6}\} \\ & \times \{1-\Delta\}, \end{aligned} \quad (1)$$

where  $R_{\infty}$  is the rydberg constant for a nucleus of infinite mass;  $\mu_p$  is the magnetic moment of the proton;  $\mu_e$  the magnetic moment of the electron; the first bracket is the reduced mass correction<sup>4</sup>; the second bracket is the ratio of the magnetic moment of the electron to the Bohr magneton; the third bracket is the relativistic Breit correction; the fourth bracket is the radiative correction of Kroll and Pollock<sup>1</sup>; the fifth bracket is the mass correction and the nucleon structure correction; the sixth bracket includes all other possible

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<sup>1</sup> G. Breit, Phys. Rev. **46**, 1447 (1930); C. M. Sommerfield, Phys. Rev. **107**, 328 (1957); N. Kroll and F. Pollock, Phys. Rev. **86**, 876 (1952).

<sup>2</sup> W. A. Newcomb and E. E. Salpeter, Phys. Rev. **97**, 1146 (1955); R. A. Arnowitt, Phys. Rev. **92**, 1002 (1953).

<sup>3</sup> A. C. Zemach, Phys. Rev. **104**, 1771 (1956); C. K. Iddings and P. M. Platzman, Phys. Rev. **113**, 192 (1959).

<sup>4</sup> G. Breit and R. E. Meyerott, Phys. Rev. **72**, 1023 (1947).

corrections, to be discussed in this section. The reduced mass correction depends in a trivial way on the nuclear mass, whereas the succeeding three brackets concern the electron in the external Coulomb field and do not depend on the nuclear mass or structure. The entire expression through the fourth bracket is denoted by  $E^F$ , and the hyperfine anomaly for heavier elements is defined with respect to the variation of the fifth and sixth bracket with nuclear species:

$$(\Delta\nu/\Delta\nu_{\text{H}})_{\text{exp}} = (E^F/E_{\text{H}}^F)(1-\delta), \quad (2)$$

with  $\delta \equiv$  hyperfine anomaly.

The mass and structure corrections arise from the exchange of one or two transverse photons of high momentum ( $k > m$ ) in the Bethe-Salpeter perturbation theory, with the zero-order two-body interaction taken to be the instantaneous Coulomb interaction. There are three types of corrections: one proportional to  $\ln(M/m) \sim 7$ ; a second, nonlogarithmic, of order unity, arising from the lower limit of the covariant perturbation integrals; and a third large term to which all momenta (but primarily those for which  $m < k < M$ ) contribute, arising from the finite size of the proton. The corrections of order unity are expected to be 10–15% as large as those of order  $\ln(M/m)$ . This is the case even in H<sup>1</sup>, despite the almost complete fortuitous cancellation of the  $\ln(M/m)$  terms. The logarithmic terms come entirely from retardation and recoil corrections to the zero-order hyperfine operator. Furthermore, the contribution from negative energy proton intermediate states does not depend on the detailed wave function of these states. These considerations enabled Newcomb and Salpeter<sup>5</sup> to develop a noncovariant method which gives the logarithmic terms, and hence about 90% of the mass correction. The proton structure corrections<sup>3</sup> can also be derived from either a three-dimensional approach or a covariant one, with results which agree within 20%.<sup>6</sup> These calculations have been based on an exponential form factor<sup>7</sup> as determined by the Stanford experiments.

When Eq. (1) is evaluated, using the latest values of the physical constants as given by Dumond and Cohen,<sup>8</sup>

<sup>5</sup> W. A. Newcomb, Ph.D. thesis, Cornell University, 1952 (unpublished); W. A. Newcomb and E. E. Salpeter, Phys. Rev. **97**, 1146 (1955).

<sup>6</sup> The covariant calculation also removes the logarithmic divergence in the double-Pauli term. This is to be expected since the form factor spreads out the moment into a finite region.

<sup>7</sup> R. Hofstadter, Revs. Modern Phys. **28**, 214 (1956); D. R. Yennie, M. M. Levy, and D. G. Ravenhall, Revs. Modern Phys. **29**, 144 (1957); M. R. Yearian and R. Hofstadter, Phys. Rev. **110**, 552 (1958); **111**, 934 (1958); R. Hofstadter, M. R. Yearian, and F. Bumiller, Revs. Modern Phys. **30**, 482 (1958); A. M. Sessler and R. L. Mills, Phys. Rev. **110**, 1453 (1958).

<sup>8</sup> J. W. M. Du Mond and E. R. Cohen, *Handbuch der Physik*, edited by S. Flügge (Springer-Verlag, Berlin, 1957), Vol. 35, Part 1, p. 1; J. W. M. Du Mond and E. R. Cohen, Phys. Rev. Letters **1**, 291 (1958); see also S. M. Koenig, A. G. Prodell, and P. Kusch, Phys. Rev. **88**, 191 (1952).

one obtains:

$$\begin{aligned} (\Delta\nu_{\text{H}})_{\text{theor}} &= (1420.40094 \pm 14 \text{ ppm})(1-\Delta'), \\ \Delta' &= (35 \pm 3.5) \times 10^{-6} + \Delta. \end{aligned} \quad (2)$$

$\Delta'$  is the sum of the structure correction and  $\Delta$ . This is to be compared with<sup>9</sup>

$$(\Delta\nu_{\text{H}})_{\text{exp}} = 1420.40573. \quad (3)$$

If we equate Eq. (2) and Eq. (3), we obtain:

$$(38.5 \pm 23.5) \times 10^{-6} = -\Delta. \quad (4)$$

There is thus a discrepancy between theory and experiment, which can range from 15 to 60 ppm.<sup>10</sup> The interpretation that is given to this discrepancy will significantly affect the meaning of the results for the heavier nuclei that are considered in this paper. There are three possible sources for this discrepancy: (1) The value of  $\alpha$  may actually lie outside the maximum error allowed by Dayhoff, Triebwasser, and Lamb.<sup>11</sup> A re-determination of  $\alpha$  would be of great help in this connection. (2) The form factor may differ considerably from an exponential. It cannot yet be ruled out that a highly singular form factor exists, which would give rise to a value for  $\langle r_{\text{em}} \rangle$  which differs considerably from  $\langle r_{\text{em}}^2 \rangle^{1/2}$ . (3) Nucleon polarization terms may yield an additional correction  $\Delta$  of the proper sign and magnitude. The form factor calculations consider the proton merely as an extended charge distribution, and do not take into account possible excitation of this distribution during the exchange of two or more (virtual) photons. Drell and Ruderman<sup>12</sup> have estimated the size of this contribution, and have found that it gives a correction of the order of  $\frac{1}{2}\%$  of the main Coulomb and magnetic scattering. Such a correction to the over-all scattering may represent a non-negligible correction to the hfs, which is itself already only a small part of the total electron-proton interaction. Iddings and Platzman,<sup>13</sup> using dispersion relations, have calculated the contribution of intermediate states containing one meson. They find a correction of  $<1$  ppm. Thus it seems unlikely that the hfs discrepancy can be accounted for by polarization of the  $\pi$ -meson cloud. One cannot, of course, rule out such a possibility, or exclude more complicated mesonic effects.

The unsatisfactory state of affairs in H<sup>1</sup> will bear directly on the situation in the heavier nuclei.

<sup>9</sup> P. Kusch, Phys. Rev. **100**, 1188 (1955).

<sup>10</sup> It is interesting to note that before the introduction of the structure correction, there seemed to be no discrepancy. There were, however, uncomfortable logarithmic divergences in the final result.

<sup>11</sup> E. S. Dayhoff, S. Triebwasser, and W. E. Lamb, Jr., Phys. Rev. **89**, 106 (1953).

<sup>12</sup> S. D. Drell and M. A. Ruderman, Phys. Rev. **106**, 561 (1957).

<sup>13</sup> C. K. Iddings and P. M. Platzman, Phys. Rev. **115**, 919 (1959).

II. hfs OF DEUTERIUM

A. Covariant Equation

The three-body Bethe-Salpeter equation is<sup>14</sup>  
 $i\psi(x_1'x_2'x_3')$

$$= \int dx_1 dx_2 dx_3 dx_4 dx_5 dx_6 K_+^a(1'4)K_+^b(2'5) \times K_+^c(3'6)\bar{G}(456; 123)\psi(x_1x_2x_3), \quad (7)$$

where the kernel  $\bar{G}$  is the sum of all irreducible interaction diagrams. We assume the absence of three-body forces, and take the three-body interactions to be compounded of two-body interactions. We further assume that we can choose a Lorentz frame in which the main part of the two-body interaction can be represented by an instantaneous interaction  $\bar{G}_{ij}$  which will be taken to be the zero-order interaction.  $\bar{G}_{ij}$  depends only on the relative coordinates of  $i$  and  $j$ , and can be written, e.g., for  $i, j=1, 2$ , as:

$$\bar{G}_{12}(x_4x_5x_6; x_1x_2x_3) = \bar{G}_{12}(x_4-x_5)\delta(x_4-x_1) \times \delta(x_5-x_1)\delta(x_6-x_3)\delta(x_3-x_3')\delta(t_4-t_5). \quad (8)$$

The total kernel is the sum of the three basic interactions, and all other interactions:

$$\bar{G} = \bar{G}_{12} + \bar{G}_{23} + \bar{G}_{31} + \bar{G}_\Delta. \quad (9)$$

$\bar{G}_\Delta$  will be treated as a perturbation. Multiplication of Eq. (7) by  $(i\nabla_i' - m_i)$ , where  $\nabla \equiv \gamma \cdot \partial / \partial x$ , leads to the integro-differential equation

$$i(i\nabla_1' - m_1)(i\nabla_2' - m_2)(i\nabla_3' - m_3)\psi(x_1'x_2'x_3') = (i\nabla_3' - m_3) \int dx_1 dx_2 \bar{G}_{12}(x_1-x_3)\psi(x_1x_2x_3') + \dots \quad (10)$$

The Fourier transform of Eq. (10) gives the basic equation in momentum space. To make the energy dependence clearer, we multiply by  $\gamma_4^1 \gamma_4^2 \gamma_4^3$  and denote  $\gamma_4^1 \gamma_4^2 \gamma_4^3 \bar{G}$  by a letter without a bar. The equation is

$$-i\mathcal{L}\chi(p_1p_2p_3) = [\epsilon_3 - H_3(p_3)] \int dk_{12} G_{12}(-k_{12}) \times \chi(p_1+k_{12}, p_2-k_{12}, p_3) + \dots, \quad (11)$$

where

$$\mathcal{L} \equiv [\epsilon_1 - H_1(p_1)][\epsilon_2 - H_2(p_2)][\epsilon_3 - H_3(p_3)], \quad (12)$$

$$p_i = (\mathbf{p}_i, \epsilon_i),$$

$$H_i(\mathbf{p}_i) = \alpha^i \cdot \mathbf{p}_i + \beta_i m_i.$$

$k_{ij}$  is the momentum exchanged in the instantaneous interaction between  $i$  and  $j$ . The motion of the center of mass has been separated out in Eq. (11), being represented by a monochromatic exponential with mo-

mentum four-vector  $(0,0,0,E)$  where

$$E = \epsilon_1 + \epsilon_2 + \epsilon_3 \quad (13)$$

is the total energy of the system. In particular, we seek the ground state of the bound system, for which

$$E < m_1 + m_2 + m_3. \quad (14)$$

For this state, we can consider only those components of the wave function in which pairs of particles propagate together in negative energy states. This is due to the instantaneous character of the interaction, which guarantees that if we want the state at all times to contain three particles (i.e., has  $N_+ - N_- = 3$ ) then we can only have at any time states in which both interacting particles propagate together along their time-ordered world lines. If we introduce the free Casimir projection operators, we then have the result that any solution can be written as the sum of four components,  $+++$ ,  $+-$ ,  $-+-$ , and  $--+$ . Now let  $\varphi$  be a function defined by

$$\varphi(p_1p_2p_3) = \mathcal{L}\chi(p_1p_2p_3), \quad (15)$$

and let  $\mathcal{G}_{ij}$  be an integral operator which operates only on the three space components of the momentum vectors, such that

$$\mathcal{G}_{12}f(p_1p_2p_3) \equiv \int d\mathbf{k}_{12} G_{12}(-\mathbf{k}_{12}) \times f(\mathbf{p}_1 + \mathbf{k}_{12}, \mathbf{p}_2 - \mathbf{k}_{12}, \epsilon_1, \epsilon_2, \mathbf{p}_3, \epsilon_3). \quad (16)$$

The first integral on the right-hand side of Eq. (11) is then

$$\mathcal{G}_{12} \int d\lambda_{12} \varphi(\mathbf{p}_1, \epsilon_1 + \lambda_{12}, \mathbf{p}_2, \epsilon_2 - \lambda_{12}, \mathbf{p}_3, \epsilon_3) \times [\epsilon_1 + \lambda_{12} - H_1]^{-1} [\epsilon_2 - \lambda_{12} - H_2]^{-1}. \quad (17)$$

The four integrals arising from Eq. (17) when  $\varphi$  is expressed as the sum of its four components, are each functions of  $\epsilon_3$  alone. Thus the integral as a whole is a function of  $\epsilon_3$ , and the remaining integrals on right-hand side of Eq. (11) are functions of  $\epsilon_1$  and  $\epsilon_2$ , respectively. We can therefore write

$$\varphi = f_1(\epsilon_1) + f_2(\epsilon_2) + f_3(\epsilon_3), \quad (18)$$

where the  $f$ 's are known functions. We further define the auxiliary functions

$$\varphi_i(\epsilon_i) = f_i(\epsilon_i) - f_i(E_i), \quad i=1, 2, 3 \quad (19)$$

$$\varphi_i(E_i) = 0,$$

$$\varphi_0 = \sum_{i=1}^3 f_i(E_i), \quad (20)$$

where

$$E_i = +(\mathbf{p}_i^2 + m_i^2)^{1/2}, \quad (21)$$

so that Eq. (18) becomes

$$\varphi = \varphi_0 + \sum_{i=1}^3 \varphi_i(\epsilon_i). \quad (22)$$

<sup>14</sup>The nonrelativistic limit has been treated in the following paper: G. Wentzel, Phys. Rev. **89**, 684 (1953).

In all of the above expressions only the energy dependence has been shown explicitly, the dependence on the  $\mathbf{p}_i$  being understood.  $\varphi_0$  is a function of the spatial components alone. Inserting Eq. (22) into the right-hand side of Eq. (11), we can perform the integration over the fourth variable; if we indicate nonvanishing components by the use of projection operators, we obtain<sup>15</sup>:

$$\begin{aligned} \varphi = & 2\pi(\Lambda_{+++} + \Lambda_{--+}) \mathcal{G}_{12}(\Lambda_{+++} - \Lambda_{--+}) \\ & \times [E - \epsilon_3 - H_1 - H_2]^{-1} (\varphi_0 + \varphi_3) \\ & + 2\pi(\Lambda_{+++} + \Lambda_{+-}) \mathcal{G}_{13}(\Lambda_{+++} - \Lambda_{+-}) \\ & \times [E - \epsilon_2 - H_1 - H_3]^{-1} (\varphi_0 + \varphi_2) \\ & + 2\pi(\Lambda_{+++} + \Lambda_{+-}) \mathcal{G}_{23}(\Lambda_{+++} - \Lambda_{+-}) \\ & \times [E - \epsilon_1 - H_2 - H_3]^{-1} (\varphi_0 + \varphi_1). \end{aligned} \quad (23)$$

We relinquish the constraint Eq. (13), and set  $\epsilon_i = E_i$  in Eq. (23). Then, after solving for these values, we obtain solutions for arbitrary  $\epsilon_i$ . For  $\epsilon_i = E_i$  [using Eq. (19)] Eq. (23) reduces to an equation for  $\varphi_0$ . Defining a new function  $\psi$  by

$$\psi = -[E - H_1 - H_2 - H_3]^{-1} \varphi_0, \quad (24)$$

and introducing the abbreviated notation

$$\mathfrak{M}_{12} = 2\pi(\Lambda_{+++} + \Lambda_{--+}) \mathcal{G}_{12}(\Lambda_{+++} - \Lambda_{--+}), \quad (25)$$

we obtain, for  $\epsilon_i = E_i$ , the relation

$$(E - H_1 - H_2 - H_3)\psi = (\mathfrak{M}_{12} + \mathfrak{M}_{13} + \mathfrak{M}_{23})\psi. \quad (26)$$

As in the two-body case, this differs from the "single-particle theory" three-body relativistic equation by the presence of the projection operators. This three-dimensional equation alone suffices to determine the energy eigenvalue  $E$  of our system, a result independent of the  $\epsilon_i$  dependence of the complete wave function. The  $\varphi_i$  are determined from Eq. (23):

$$\{1 - \mathfrak{M}_{ij}[E - \epsilon_k - H_i - H_j]^{-1}\} \varphi_k = (\epsilon_k - E_k) \mathfrak{M}_{ij}[E - \epsilon_k - H_i - H_j]^{-1} \psi, \quad (26a)$$

$$\varphi_k = (\epsilon_k - E_k) \sum_{n \geq 1} [\mathfrak{M}_{ij}(E - \epsilon_k - H_i - H_j)^{-1}]^n \psi, \quad (26b)$$

where  $i \neq j \neq k$  and each index can assume the values 1, 2, 3.

We can now develop a perturbation expansion for the excluded graphs. Eq. (11) can be written

$$(\mathcal{L}_n - \mathcal{G})\chi_n = 0, \quad (27)$$

where  $\mathcal{G}$  stands for the integral operator with kernel  $G_{12} + G_{13} + G_{23}$ , written explicitly as the right-hand side of Eq. (11). The subscript  $n$  refers to a given eigenstate of energy  $E_n$ . The solution is

$$\chi_n = \mathcal{L}_n^{-1}[-(E_n - H_1 - H_2 - H_3)\psi_n + \sum_i \varphi_i^{*(n)}]. \quad (28)$$

An adjoint function  $\tilde{\chi}_n$  can be defined by

$$\tilde{\chi}_n = [-\psi_n^*(E_n - H_1 - H_2 - H_3) + \sum_i \varphi_i^{*(n)}] \mathcal{L}_n^{-1}, \quad (29)$$

<sup>15</sup> The  $(\varphi_1 + \varphi_2)$  parts of the first term on the right-hand side vanish, as can be seen from the explicit expression for the  $\varphi_i$  given in Eq. (26a). Similarly for the other terms.

where  $\psi_n^*$  is the transposed complex conjugate spinor to  $\psi_n$ , and the operators in Eq. (29) operate back on the spinors. For another energy  $E_\Delta \neq E_n$ , let  $\mathcal{L}_\Delta$  be the expression represented by Eq. (12) having total energy  $E_\Delta$ , and let

$$\chi_n^\Delta = \mathcal{L}_\Delta^{-1}[-(E_\Delta - H_1 - H_2 - H_3)\psi_n + \sum_i \varphi_i^{*(n)}], \quad (30)$$

where the  $\varphi_i^{*(n)}$  are the same as in Eq. (28). Note that  $\chi_n^\Delta \rightarrow \chi_n$  as  $E_\Delta \rightarrow E_n$ . Then

$$\mathcal{L}_\Delta \chi_n^\Delta = -(E_\Delta - E_n)\psi_n + \mathcal{G}\chi_n. \quad (31)$$

Direct evaluation shows that

$$\mathcal{G}\chi_n = \mathcal{G}\chi_n^\Delta - (E_\Delta - E_n)\Xi_n,$$

where  $\Xi$  is a function involving  $\epsilon_i$  and  $\psi_n$ . Then Eq. (31) is

$$(\mathcal{L}_\Delta - \mathcal{G})\chi_n^\Delta = -(E_\Delta - E_n)(\psi_n - \Xi). \quad (32)$$

Consider the complete three-body equation

$$\mathcal{L}\Omega_n = (\mathcal{G} + \mathcal{G}_\Delta)\Omega_n, \quad (33)$$

where  $\mathcal{G}_\Delta$  is the integral operator whose kernel is  $G_\Delta$ .  $\Omega_n$  is that eigenvector belonging to eigenvalue  $E_\Delta = E_n + \Delta E$  which goes over into  $\chi_n$  as  $\mathcal{G}_\Delta$  and  $\Delta E$  approach zero. We can therefore write

$$\Omega_n = \chi_n^\Delta + \chi_\Delta,$$

where  $\chi_\Delta$  is first-order small relative to  $\chi_n^\Delta$ . Equation (33) is then

$$(\mathcal{L}_\Delta - \mathcal{G})\chi_n^\Delta + (\mathcal{L}_\Delta - \mathcal{G})\chi_\Delta = \mathcal{G}_\Delta \chi_n^\Delta + \mathcal{G}_\Delta \chi_\Delta. \quad (34)$$

We multiply by  $\tilde{\chi}_n^\Delta$  on the left and integrate with respect to the  $\mathbf{p}_i$ . The fact that the center-of-mass motion has been separated out is indicated by a factor  $\delta(\mathbf{p}_1 + \mathbf{p}_2 + \mathbf{p}_3)\delta(E - \sum_i \epsilon_i)$ . The integrand is:

$$\begin{aligned} \Delta E(\psi_n^* + \Xi^*)\chi_n^\Delta + \Delta E(\psi_n^* + \Xi^*)\chi_\Delta \\ = -\tilde{\chi}_n^\Delta \mathcal{G}_\Delta \chi_n^\Delta - \tilde{\chi}_n^\Delta \mathcal{G}_\Delta \chi_\Delta. \end{aligned} \quad (35)$$

We seek the first-order energy shift  $\Delta E^{(1)}$ . The second terms on each side of the equation are at least second order small; the integrals involving  $\Xi$  give vanishing contributions; in the remaining terms,  $\chi_n^\Delta$  can be replaced by  $\chi_n$  to first order; and integration over the fourth coordinate of  $\psi_n^* \chi_n$  simply replaces  $\chi_n$  by  $(2\pi)^2 \psi_{n+++}$ . If we normalize our wave function according to the requirement

$$(2\pi)^2 \int \psi_{n+++}^* \psi_{n+++} d\mathbf{p}_1 d\mathbf{p}_2 d\mathbf{p}_3 \delta(\sum_i \mathbf{p}_i) = 1, \quad (36)$$

we obtain from Eq. (35) a first-order energy shift

$$\begin{aligned} \Delta E^{(1)} = & - \int d\mathbf{p}_1 d\mathbf{p}_2 d\mathbf{p}_3 \delta(\sum_i \mathbf{p}_i) \delta(E - \sum_i \epsilon_i) \tilde{\chi}_n \mathcal{G}_\Delta \chi_n \\ = & - \int d\mathbf{p}_1 d\mathbf{p}_2 d\mathbf{p}_3 \delta(\sum_i \mathbf{p}_i) \delta(E - \sum_i \epsilon_i) dk_{12} dk_{13} dk_{23} \\ & \times \tilde{\chi}_n(p_1 p_2 p_3) \mathcal{G}_\Delta(k_{12}, k_{13}, k_{23}) \\ & \times \chi_n(p_1 + k_{12} + k_{13}, p_2 - k_{12} + k_{23}, p_3 - k_{13} - k_{23}). \end{aligned} \quad (37)$$

We are now in a position to see why the covariant formalism which we have just outlined is unsuitable for the problem of deuterium, and what formalism can take its place. In deuterium, the basic interactions are the electron-proton Coulomb interaction and the neutron-proton interaction. There is, however, no known nuclear interaction which can be used in the *two-body* BS equation for the neutron-proton system.<sup>16</sup> One might expect that the recent proposed phenomenological potentials<sup>17</sup> could be incorporated into the formalism. These are, however, three dimensional, and only suitable for the noncovariant method which we shall adopt in the next section. Association of the phenomenological potential with the basic interaction kernel would lead, because of the strength of the interaction, to sizeable contributions from second- and high-order irreducible graphs, which would then destroy the agreement of the original zero-order equation with experiment. On the other hand, if one associated the phenomenological potential with the sum of all orders of irreducible diagrams, the basic interactions would remain undetermined. There seems to be no way of resolving this problem until the correct basic covariant interaction is discovered.

Equation (26), the end product of the reduction of the three-body equation, enables one to go over to a three-dimensional formalism, which is reducible and soluble. This is because the correct ground-state energy and wave function are well represented by a three-dimensional theory starting from Eq. (26). In a three-dimensional formalism we can incorporate the phenomenological potential, and expand the perturbation theory only in powers of  $\alpha$ . This procedure will yield all the logarithmic terms arising from retardation and recoil effects, and hence account for the exact covariant correction to within about ten percent.

### B. Three-Dimensional Method

We label the proton, neutron and electron by No. 1, No. 2, No. 3, respectively. The Hamiltonian in laboratory coordinates is the sum of a "large" part  $H_0$  consisting of the kinetic energies, nuclear interaction and the main Coulomb energy, and a "small" perturbation  $H_I$  consisting of the remaining electromagnetic interactions:

$$H_0 = (\alpha^1 \cdot \mathbf{p}_1 + \beta^1 M) + (\alpha^2 \cdot \mathbf{p}_2 + \beta^2 M) + (\alpha^3 \cdot \mathbf{p}_3 + \beta^3 m) + V_D(\mathbf{r}_2, \mathbf{r}_1) + V_c', \quad (38)$$

<sup>16</sup> H. A. Bethe and E. E. Salpeter, Phys. Rev. **84**, 1232 (1951); H. S. Green and S. N. Biswas, Progr. Theoret. Phys. (Kyoto) **18**, 121 (1957); S. N. Biswas, Progr. Theoret. Phys. (Kyoto) **19**, 725 (1958); J. S. Goldstein, Phys. Rev. **91**, 1516 (1953); G. C. Wick, Phys. Rev. **96**, 1124 (1954); R. E. Cutkosky, Phys. Rev. **96**, 1135 (1954).

<sup>17</sup> P. S. Signell and R. E. Marshak, Phys. Rev. **106**, 832 (1957); **109**, 1229 (1958), P. S. Signell, R. Zinn, and R. E. Marshak, Phys. Rev. Letters **1**, 416 (1958); J. L. Gammel, R. S. Christian, and R. M. Thaler, Phys. Rev. **105**, 311 (1957); J. L. Gammel and R. M. Thaler, Phys. Rev. **107**, 291 (1957); **107**, 1337 (1957).

$$\begin{aligned} H_I &= V - e\alpha^1 \cdot \mathbf{A} + e\alpha^3 \cdot \mathbf{A} - (ie\mu_{P'}/2M) \\ &\quad \times \sum_k \{ \beta^1 (\boldsymbol{\sigma}^1 \times \mathbf{k}) - ik\beta^1 \alpha^1 \} \cdot \mathbf{A}'(\mathbf{k}) \\ &\quad - (ie\mu_N/2M) \sum_k \{ \beta^2 (\boldsymbol{\sigma}^2 \times \mathbf{k}) - ik\beta^2 \alpha^2 \} \cdot \mathbf{A}'(\mathbf{k}) \\ &\quad + (ie^2\mu_{P'}/2M) \beta^1 \alpha^1 \cdot \nabla_1 (|\mathbf{r}_1 - \mathbf{r}_3|)^{-1} \\ &\quad + (ie^2\mu_N/2M) \beta^2 \alpha^2 \cdot \nabla_2 (|\mathbf{r}_2 - \mathbf{r}_3|)^{-1} \\ &\quad - (ie^2\mu_N/2M) \beta^2 \alpha^2 \cdot \nabla_2 (|\mathbf{r}_2 - \mathbf{r}_1|)^{-1} \\ &\equiv V + H_P + H_e + H_{P'} + H_{N'} + H_{P^Q} + H_{N^Q} + H_{NP}. \quad (39) \end{aligned}$$

$V_D$  is the phenomenological  $n$ - $p$  potential, with modifications discussed below. This is part ordinary and part exchange:

$$V_D(\mathbf{r}_2, \mathbf{r}_1) = V_0(\mathbf{r}_2 - \mathbf{r}_1) + V_{\text{ex}}'(\mathbf{r}_2 - \mathbf{r}_1) \exp[i(\mathbf{r}_2 - \mathbf{r}_1) \cdot (\mathbf{p}_1 - \mathbf{p}_2)], \quad (40)$$

where  $V_{\text{ex}}'$  is a pure spacial function.  $V_c'$  and  $V$  are the low-momentum and high-momentum parts of the Coulomb interaction, defined by

$$V_c' = - (e^2/2\pi^2) \int_{q < q_0} \exp[i\mathbf{q} \cdot (\mathbf{r}_3 - \mathbf{r}_1)] q^{-2} dq, \quad (41)$$

$$V = - (e^2/2\pi^2) \int_{q > q_0} \exp[i\mathbf{q} \cdot (\mathbf{r}_3 - \mathbf{r}_1)] q^{-2} dq.$$

$V_c'$  is responsible for most of the ordinary Coulomb binding<sup>5</sup> if we choose the cutoff  $q_0$  appropriately in the range  $\alpha m < q_0 < m$ .  $\mu_{P'} = \mu_P - 1$  is the anomalous part of the proton moment, and

$$\begin{aligned} \mathbf{A}'(\mathbf{k}) &= (2\pi/k)^{1/2} \{ a_{k\lambda} \boldsymbol{\epsilon}_{k\lambda} \exp[i\mathbf{k} \cdot \mathbf{r}] \\ &\quad - a_{k\lambda}^* \boldsymbol{\epsilon}_{k\lambda} \exp[-i\mathbf{k} \cdot \mathbf{r}] \}. \quad (42) \end{aligned}$$

All interactions of  $\mu_{P'}$  and  $\mu_N$  are derived from the covariant Pauli interaction term.

The program is first to solve the zero-order equation

$$H_0\psi = E_0\psi \quad (43)$$

to obtain wave functions  $\psi$  whose accuracy is sufficient for the calculation of hfs perturbation energy to order  $(\alpha m/M)$  (hfs). The hyperfine splitting is then found by standard perturbation theory, with  $H_I$  as the perturbation. The hfs terms are those containing an interaction between the spin of the electron and the spin or orbital motion of the nucleus. All hfs expressions must of course, contain  $H_e$  at least once. Second- through fourth-order perturbations must be evaluated. If we denote the perturbation energy by the operators appearing in the matrix elements to be evaluated and denote terms by letters, following the convention of Newcomb and Salpeter<sup>5</sup> when possible, we see that we must consider the following perturbations:

(1) Second order:

$$(H_P, H_e) \equiv D, \quad (H_{P'}, H_e) \equiv P, \quad (H_{N'}, H_e) \equiv P'.$$

(2) Third order:

$$\begin{aligned} (H_P, H_e, V) &\equiv CD, & (H_{P'}, H_e, V) &\equiv CP, & (H_{N'}, H_e, V) &\equiv C:P, \\ (H_P, H_e, H_{P^Q}) &\equiv QD, & (H_{P'}, H_e, H_{P^Q}) &\equiv QP, & (H_{N'}, H_e, H_{P^Q}) &\equiv Q:P, \\ (H_P, H_e, H_{N^Q}) &\equiv Q:D, & (H_{P'}, H_e, H_{N^Q}) &\equiv Q:P', & (H_{N'}, H_e, H_{N^Q}) &\equiv QP'. \end{aligned}$$

(3) Fourth order:

$$\begin{aligned} (H_P, H_P, H_e, H_e) &\equiv DD, & (H_P, H_{P'}, H_e, H_e) &\equiv DP, \\ (H_{P'}, H_{P'}, H_e, H_e) &\equiv PP, & (H_P, H_{N'}, H_e, H_e) &\equiv D:P, \\ (H_{P'}, H_{N'}, H_e, H_e) &\equiv P:P, & (H_{N'}, H_{N'}, H_e, H_e) &\equiv PP'. \end{aligned}$$

To solve the zero-order equation, we transfer to a system of coordinates centered on the proton (adiabatic approximation):

$$\begin{aligned} \mathbf{r} &= \mathbf{r}_2 - \mathbf{r}_1, & \mathbf{r}_1 &= \mathbf{R}, \\ \boldsymbol{\rho} &= \mathbf{r}_3 - \mathbf{r}_1, & \mathbf{r}_2 &= \mathbf{r} + \mathbf{R}, \\ \mathbf{R} &= \mathbf{r}_1, & \mathbf{r}_3 &= \boldsymbol{\rho} + \mathbf{R}, \\ \mathbf{p} &= \mathbf{p}_2, & \mathbf{p}_1 &= -\mathbf{p} - \boldsymbol{\pi} - \mathbf{P}, \\ \boldsymbol{\pi} &= \mathbf{p}_3, & \mathbf{p}_2 &= \mathbf{p}, \\ \mathbf{P} &= \mathbf{p}_1 + \mathbf{p}_2 + \mathbf{p}_3, & \mathbf{p}_3 &= \boldsymbol{\pi}. \end{aligned} \quad (44)$$

In this system, Eq. (43) becomes

$$\begin{aligned} &\left\{ (-\boldsymbol{\alpha}^1 \cdot \mathbf{p} - \boldsymbol{\alpha}^1 \cdot \boldsymbol{\pi} + \beta^1 M) + (\boldsymbol{\alpha}^2 \cdot \mathbf{p} + \beta^2 M) \right. \\ &+ (\boldsymbol{\alpha}^3 \cdot \boldsymbol{\pi} + \beta^3 m) + V_0(\mathbf{r}) + V_{\text{ex}}'(\mathbf{r}) \exp[-2i\mathbf{r} \cdot (\mathbf{p} + \boldsymbol{\pi}/2)] \\ &\left. - (e^2/2\pi^2) \int_{q < q_0} \exp[i\mathbf{q} \cdot \boldsymbol{\rho}] q^{-2} d\mathbf{q} \right\} \psi(\mathbf{r}, \boldsymbol{\rho}) \\ &= E\psi(\mathbf{r}, \boldsymbol{\rho}). \end{aligned} \quad (45)$$

Now a phenomenological potential for the two-body problem is of the form

$$V_D(\mathbf{r}_2, \mathbf{r}_1) = V_0(\mathbf{r}) + V_{\text{ex}}'(\mathbf{r}) \exp[-2i\mathbf{r} \cdot \mathbf{p}].$$

If we expand  $\exp(-i\mathbf{r} \cdot \boldsymbol{\pi})$  in Eq. (45) to second order, we obtain

$$\begin{aligned} &\left\{ (-\boldsymbol{\alpha}^1 \cdot \mathbf{p} - \boldsymbol{\alpha}^1 \cdot \boldsymbol{\pi} + \beta^1 M) + (\boldsymbol{\alpha}^2 \cdot \mathbf{p} + \beta^2 M) + (\boldsymbol{\alpha}^3 \cdot \boldsymbol{\pi} + \beta^3 m) \right. \\ &+ V_D(\mathbf{r}) - i\boldsymbol{\pi} \cdot \mathbf{r} V_{\text{ex}} - (1/2)(\boldsymbol{\pi} \cdot \mathbf{r})^2 V_{\text{ex}} \\ &\left. - (e^2/2\pi^2) \int_{q < q_0} \exp[i\mathbf{q} \cdot \boldsymbol{\rho}] q^{-2} d\mathbf{q} \right\} \psi(\mathbf{r}, \boldsymbol{\rho}) \\ &= E\psi(\mathbf{r}, \boldsymbol{\rho}), \end{aligned} \quad (46)$$

where  $V_{\text{ex}} = V_D - V_0$ . Introduction of the Casimir pro-

jection operators for the three particles enables us to resolve any solution into components<sup>18</sup>:

$$\begin{aligned} \psi &= \psi^{(+++)} + \psi^{(++-)} + \psi^{(+-+)} + \dots \\ &= \begin{pmatrix} 1 \\ \Gamma_1(\mathbf{p}_1) \end{pmatrix} \begin{pmatrix} 1 \\ \Gamma_2(\mathbf{p}_2) \end{pmatrix} \begin{pmatrix} 1 \\ \Gamma_3(\mathbf{p}_3) \end{pmatrix} \psi_{+++} \\ &+ \begin{pmatrix} 1 \\ \Gamma_1(\mathbf{p}_1) \end{pmatrix} \begin{pmatrix} 1 \\ \Gamma_2(\mathbf{p}_2) \end{pmatrix} \begin{pmatrix} -\Gamma_3(\mathbf{p}_3) \\ 1 \end{pmatrix} \psi_{++-} + \dots, \end{aligned} \quad (47)$$

where

$$\Gamma_i(\mathbf{p}_i) = \boldsymbol{\sigma}^i \cdot \mathbf{p}_i / [E(\mathbf{p}_i) + m_i], \quad \sigma^i - \text{Pauli spinors.}$$

$\psi_{+++}, \psi_{++-}, \dots$  are eight component spinors, which we shall see can be taken to be products of constant spinors and scalar functions of the coordinates.

We turn first to positive energy solutions in the energy range  $E \gtrsim 2M$  of which the ground state is the lowest. For these,  $\psi^{(+++)}$  is the main component, the others giving the effect of pair states on  $\psi$ .  $\psi_{++-}$  is at least  $\alpha^3$  smaller than  $\psi_{+++}$ ,<sup>19</sup> hence can be neglected;  $\psi_{+-+}$  and  $\psi_{-++}$  are  $(P/M)^3 \sim 10^{-4}$  smaller than  $\psi_{+++}$ ; while the other components are negligible. It appears that  $\psi_{-++}$  and  $\psi_{+-+}$  are not negligible. However, we can account for these as follows: the equations for these components express them in terms of  $\psi_{+++}$ ; if the expressions so obtained are then substituted back into the equation for  $\psi_{+++}$ , we get an equation for  $\psi_{+++}$  which involves only  $\psi_{+++}$  and includes the effect of  $\psi_{-++}$  and  $\psi_{+-+}$ . This equation for  $\psi_{+++}$  involves the nucleon potential plus correction terms. Furthermore, the nucleon part of the  $+++$  equation can be reduced to the Schrödinger equation for the nucleon system, plus relativistic corrections. Now the given phenomenological potential describes two-nucleon phenomena (in the momentum range of interest to us) when inserted into the Schrödinger equation. When using the phenomenological potential in the Schrödinger equation, the above corrections can therefore be ignored.

For negative-energy states, as in the two-body case,

<sup>18</sup> H. A. Bethe and E. E. Salpeter, *Handbuch der Physik*, edited by S. Flügge (Springer-Verlag, Berlin, 1957), Vol. 35, Part 1, p. 88.  
<sup>19</sup> E. E. Salpeter, *Phys. Rev.* **87**, 328 (1952); see also footnote 6.

we need only use hole theory to obtain the results that there exists a set of states having a pair present in addition to the particle, and that these differ from the corresponding positive-energy states by  $2m_i$  in energy.

To obtain positive-energy solutions in detail, we first transform Eq. (46) to momentum space:

$$\begin{aligned} & \{(-\alpha^1 \cdot \mathbf{p} - \alpha^1 \cdot \boldsymbol{\pi} + \beta^1 M) + (\alpha^2 \cdot \mathbf{p} + \beta^2 M) + (\alpha^3 \cdot \boldsymbol{\pi} + \beta^3 m)\} \\ & \times \psi(\mathbf{p}, \boldsymbol{\pi}) + \int V_D(-\mathbf{k}) \psi(\mathbf{p} + \mathbf{k}, \boldsymbol{\pi}) d\mathbf{k} \\ & - (e^2/2\pi^2) \int_{q < q_0} q^{-2} \psi(\mathbf{p}, \boldsymbol{\pi} + \mathbf{q}) d\mathbf{q} \\ & + \int S(-\mathbf{k}) \psi(\mathbf{p} + \mathbf{k}, \boldsymbol{\pi}) d\mathbf{k} = E\psi(\mathbf{p}, \boldsymbol{\pi}). \quad (48) \end{aligned}$$

The equation for the  $(+++)$  component is obtained using spinor identities.<sup>18</sup> The only wave function we need with great accuracy is the ground-state wave function, which we require correct to  $\alpha m/M$ . To obtain this, we use a perturbation procedure on the  $(+++)$  part of Eq. (48). The zero-order equation is

$$\begin{aligned} & E\tilde{\psi}_{+++}(\mathbf{p}, \boldsymbol{\pi}) \\ & = \{2M + m + p^2/2M + \pi^2/2m + \pi^2/4M\} \\ & \times \tilde{\psi}_{+++}(\mathbf{p}, \boldsymbol{\pi}) + \int V_D(-\mathbf{k}) \tilde{\psi}_{+++}(\mathbf{p} + \mathbf{k}, \boldsymbol{\pi}) d\mathbf{k} \\ & - (e^2/2\pi^2) \int_{q < q_0} q^{-2} \tilde{\psi}_{+++}(\mathbf{p}, \boldsymbol{\pi} + \mathbf{q}) d\mathbf{q}, \quad (49) \end{aligned}$$

and the remainder of the Hamiltonian Eq. (48) is treated as a perturbation. The solutions of this separable equation are of the form

$$\tilde{\psi}_{+++}(\mathbf{p}, \boldsymbol{\pi}) = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} w(\mathbf{p}) u(\boldsymbol{\pi}), \quad (50)$$

where  $w$  and  $u$  obey

$$Ww(\mathbf{p}) = (p^2/M)w(\mathbf{p}) + \int V_D(-\mathbf{k})w(\mathbf{p} + \mathbf{k})d\mathbf{k}, \quad (51)$$

$$\begin{aligned} \epsilon u(\boldsymbol{\pi}) & = (\pi^2/2m + \pi^2/4M)u(\boldsymbol{\pi}) \\ & - (e^2/2\pi^2) \int_{q < q_0} q^{-2} u(\boldsymbol{\pi} + \mathbf{q}) d\mathbf{q}, \quad (52) \end{aligned}$$

$$E = W + \epsilon + 2M + m.$$

Equation (51) is just the Schrödinger equation for the deuteron. Its solutions are the phenomenological wave functions. Equation (52) is the Schrödinger equation for the electron with its reduced mass in deuterium, moving in a Coulomb field which is cut off at  $q_0$ . Hereafter,  $m$  is taken to represent this reduced mass, unless otherwise stated. This gives the well-known reduced-mass correction to the hfs, which was the only term found by Breit and Meyerott.<sup>14</sup> The solutions of Eq. (52) are essentially hydrogenic wave functions, except

that they are cut off more rapidly at high momenta. We will return to this in Sec. C.

The perturbations to the solutions of Eq. (49) can be calculated in a straightforward manner to  $\alpha m/M$ . The result is that the zero-order solutions  $u_0(\boldsymbol{\rho})$  become centered on the center of mass, i.e.,

$$u_0(\boldsymbol{\rho}) \rightarrow u_0(\boldsymbol{\rho} - \mathbf{r}/2). \quad (53)$$

This result is expected, since the electron moving in a cut-off Coulomb potential "sees" only the average proton position, which is centered at the center of mass of the deuteron,  $\boldsymbol{\rho} - \mathbf{r}/2$ .

Finally, we must examine the positive-energy intermediate-state wave functions. There are two possible types of intermediate state: (1) excited state of deuterium (deuteron or electron or both); (2) excited (or ground) state of deuterium with a free photon of momentum  $\mathbf{k}$  in the field. In case (1), the wave functions are the same as those already found, with  $(mn)$  replacing  $(00)$ . In case (2), by conservation of momentum, we have  $\mathbf{P} = -\mathbf{k}$ . This means that we must examine  $+++$  states of the system in which we remove the restriction  $\mathbf{P} = 0$ . In this case, the intermediate state wave function is

$$\psi_{mn}' = \exp[i\mathbf{P} \cdot (\mathbf{R} + \mathbf{r}/2)] \psi_{mn}, \quad (54)$$

and the intermediate state will have, in addition to the deuterium excitation energy, the kinetic energy  $(\mathbf{P} - \boldsymbol{\pi})^2/4M$ .

### C. Hyperfine Energy

The principal hfs energy is given by second-order terms. The Dirac proton spin interaction is:

$$\begin{aligned} \Delta E^D & = -2 \sum_n \langle 0 | -e\boldsymbol{\alpha}^1 \cdot \mathbf{A} | n \rangle \\ & \times \langle n | e\boldsymbol{\alpha}^3 \cdot \mathbf{A} | 0 \rangle (E_n - E_0)^{-1}. \quad (55) \end{aligned}$$

Only positive energy states appear as intermediate states. All wave functions must appear to the maximum accuracy of Sec. B, since this term is  $\sigma$ (hfs). Thus, the shifted wave function of Eq. (53) must appear, or equivalently, the unshifted wave function and the slip correction. Thus,

$$\begin{aligned} \Delta E^D & = 2e^2 \sum_{n, \mathbf{k}, \lambda'} (E_n - E_0)^{-1} \\ & \times \langle \psi_0 | (2\pi/k)^{3/2} \alpha_{k\lambda}^1 \exp(i\mathbf{k} \cdot \mathbf{r}_1) | \psi_n^{(+++)} \rangle \\ & \times \langle \psi_n^{(+++)} | (2\pi/k)^{3/2} \alpha_{k\lambda}^3 \exp(-i\mathbf{k} \cdot \mathbf{r}_3) | \psi_0 \rangle \\ & = 4\pi e^2 \sum_{n, \mathbf{k}, \lambda'} (1/k) (E_n - E_0)^{-1} \\ & \times \{ \langle [\Gamma] w_0 u_0 | \alpha_{k\lambda}^1 \exp(i\mathbf{k} \cdot \mathbf{r}_1) | \psi_n^{(+++)} \rangle \\ & \times \langle \psi_n^{(+++)} | \alpha_{k\lambda}^3 \exp(-i\mathbf{k} \cdot \mathbf{r}_3) | [\Gamma] w_0 u_0 \rangle \\ & + \sum_{q, r} \langle [\Gamma] w_0 u_0 | \alpha_{k\lambda}^1 \exp(i\mathbf{k} \cdot \mathbf{r}_1) | \psi_n^{(+++)} \rangle \\ & \times \langle \psi_n^{(+++)} | \alpha_{k\lambda}^3 \exp(-i\mathbf{k} \cdot \mathbf{r}_3) | [\Gamma] w_q u_r \rangle \\ & \times \langle w_q u_r | \boldsymbol{\pi} \cdot \mathbf{v} | w_0 u_0 \rangle (E_0 - E_{qr})^{-1} \\ & + \sum_{q, r} (E_0 - E_{qr})^{-1} \langle w_0 u_0 | \boldsymbol{\pi} \cdot \mathbf{v} | w_q u_r \rangle \\ & \times \langle [\Gamma] w_q u_r | \alpha_{k\lambda}^1 \exp(i\mathbf{k} \cdot \mathbf{r}_1) | \psi_n^{(+++)} \rangle \\ & \times \langle \psi_n^{(+++)} | \alpha_{k\lambda}^3 \exp(-i\mathbf{k} \cdot \mathbf{r}_3) | [\Gamma] w_0 u_0 \rangle \\ & \equiv \Delta_1 + \Delta_2 + \Delta_3. \quad (56) \end{aligned}$$

A simple calculation shows that the slip corrections to the intermediate states cancel. Detailed consideration of the matrix elements and the use of spin identities yields

$$\Delta_1 = (2\pi/3)(e^2/Mm)\langle\boldsymbol{\sigma}^1 \cdot \boldsymbol{\sigma}^3\rangle |u_0(0)|^2. \quad (57)$$

Thus,  $\Delta_1$  is just the Fermi hyperfine energy associated with the Dirac part of the proton moment, with the reduced mass correction. Actually  $u_0$  is not the hydrogenic wave function, but rather the solution with the truncated potential. However, the third-order perturbation returns the high-momentum part of the wave function via  $V$ , so that Eq. (57) with this correction in fact does involve the hydrogenic wave function at the origin.  $\Delta_2 + \Delta_3$  gives rise to the usual  $D$ -state orbital hfs terms. This term is missing without the slip correction, due to our particular choice of proton-centered coordinates for our zero-order problem. The slip term brings back the orbital contribution by recentering the electron wave function on the center of mass. If we take

$$\mathbf{u}_L = (1/2)(e/2M)\mathbf{L} = (e/4M)\mathbf{L} \quad (58)$$

(the factor of  $\frac{1}{2}$  appears because only one particle in the deuteron is charged) we find

$$\Delta_2 + \Delta_3 = (8\pi/3)\mu_0 |u_0(0)|^2 \langle\boldsymbol{\sigma}^3 \cdot \mathbf{u}_L\rangle. \quad (59)$$

$\Delta E^P$ , which involves the anomalous moment of the proton, adds the contribution of  $\mu_{P'}$  to Eq. (57):

$$\Delta E^P = (2\pi/3)(\mu_{P'} e^2/mM)\langle\boldsymbol{\sigma}^1 \cdot \boldsymbol{\sigma}^3\rangle |u_0(0)|^2. \quad (60)$$

The slip terms vanish, there being no anomaly associated with the orbital motion.

The final second-order term is  $\Delta E^{P'}$ , the neutron-electron interaction. This again splits into two parts  $\Delta_1 + \Delta_2$ :

$$\begin{aligned} \Delta_1 &= (2\pi/3)(e^2\mu_N/Mm)\langle\boldsymbol{\sigma}^2 \cdot \boldsymbol{\sigma}^3\rangle \int d\mathbf{r}d\boldsymbol{\rho} |w_0(\mathbf{r})|^2 \\ &\quad \times [u_0(\boldsymbol{\rho}) - (1/2)\mathbf{r} \cdot \nabla_{\boldsymbol{\rho}} u_0(\boldsymbol{\rho})] \delta^3(\mathbf{r} - \boldsymbol{\rho}) \\ &\quad \times [u_0(\boldsymbol{\rho}) - (1/2)\mathbf{r} \cdot \nabla_{\boldsymbol{\rho}} u_0(\boldsymbol{\rho})] \\ &= (2\pi/3)(e^2\mu_N/Mm)\langle\boldsymbol{\sigma}^2 \cdot \boldsymbol{\sigma}^3\rangle \left\{ \int d\mathbf{r}d\boldsymbol{\rho} |w_0(\mathbf{r})|^2 \right. \\ &\quad \times |u_0(\boldsymbol{\rho})|^2 \delta^3(\mathbf{r} - \boldsymbol{\rho}) - \int d\mathbf{r}d\boldsymbol{\rho} |w_0(\mathbf{r})|^2 \\ &\quad \left. \times [\mathbf{r} \cdot \nabla_{\boldsymbol{\rho}} u_0(\boldsymbol{\rho})] u_0(\boldsymbol{\rho}) \delta^3(\mathbf{r} - \boldsymbol{\rho}) \right\}. \end{aligned} \quad (61)$$

If we choose the Coulomb cutoff to be about  $20\alpha m$ , we find that for  $r \sim d \ll r_0 \sim a_0/5$  [where  $d$  is "deuteron radius,"  $d = (MW_0)^{-\frac{1}{2}}$ ] the electronic wave function to a few percent is  $\psi = (4\pi)^{-\frac{1}{2}} u_0(0) \sin kr/kr$ , where  $u_0(0)$  is the hydrogenic wave function at the origin, and  $k \sim \alpha m$ . The second integrand of Eq. (61) becomes  $o(d/\alpha_0)^2$  and hence negligible. The first integrand has the hydrogenic

wave-function tail returned to it by the third-order perturbation, and so contributes  $\int d\mathbf{r} |w_0(\mathbf{r})|^2 |u_0(0)|^2 \times (1 - 2r/a_0)$ , which is the neutron Fermi energy and the Bohr-Low  $S$ -state  $d/a_0$  correction.<sup>20</sup>  $\Delta_2$ , which vanishes for the  $S$ -state components of  $w_0$ , is the  $L=2$  Low correction, so that

$$\begin{aligned} \Delta E^{P'} &= (2\pi/3)(e^2\mu_N/Mm)\langle\boldsymbol{\sigma}^2 \cdot \boldsymbol{\sigma}^3\rangle |u_0(0)|^2 \\ &\quad \times \left\{ 1 - (2/a_0) \int r |w_S(\mathbf{r})|^2 d\mathbf{r} + \sqrt{2}/(4a_0) \right. \\ &\quad \left. \times \int r w_S(\mathbf{r}) w_D(\mathbf{r}) d\mathbf{r} + 5/(4a_0) \int r |w_D(\mathbf{r})|^2 d\mathbf{r} \right\}. \end{aligned} \quad (62)$$

This completes the second-order terms.

The third-order terms, as well as the fourth-order terms are of order  $(\alpha m/M) \ln(M/m)$  and hence require the use only of product wave functions, without the  $d/a_0$  slip correction. Furthermore, the region of integration of  $k$  is now  $k > m$ , so that the energy denominators involve nuclear and electronic excitations, and the matrix elements require careful consideration in the absence of closure.<sup>21</sup>

Consider, for example,  $\Delta E^{CD}$ , with the following order of operators:

$$\Delta E_1^{CD} = \sum_{nn'} \langle 0 | H_e | n \rangle \langle n | H_P | n' \rangle \langle n' | V | 0 \rangle \times (E_n - E_0)^{-1} (E_{n'} - E_0)^{-1}. \quad (63)$$

$H_P$  involves only emission,  $H_e$ , absorption. Written in detail, this is

$$\begin{aligned} \Delta E_1^{CD} &= \sum_{nn'} (E_n - E_0)^{-1} (E_{n'} - E_0)^{-1} \\ &\quad \times \langle 0 | e\boldsymbol{\alpha}^3 \cdot \sum_{\lambda k} (2\pi/k)^{\frac{1}{2}} a_{k\lambda} \boldsymbol{\epsilon}_{k\lambda} \exp(i\mathbf{k} \cdot \mathbf{r}_3) | n \rangle \\ &\quad \times \langle n | -e\boldsymbol{\alpha}^1 \cdot (2\pi/k)^{\frac{1}{2}} a_{k\lambda}^* \boldsymbol{\epsilon}_{k\lambda} \exp(-i\mathbf{k} \cdot \mathbf{r}_1) | n' \rangle \\ &\quad \times \left\langle n' \left| - (e^2/2\pi^2) \int_{q>q_0} \exp[i\mathbf{q} \cdot (\mathbf{r}_3 - \mathbf{r}_1)] q^{-2} d\mathbf{q} \right| 0 \right\rangle \\ &= \sum_{nn'\lambda} (E_n - E_0)^{-1} (E_{n'} - E_0)^{-1} (2\pi)^{-3} (e^4/\pi) \\ &\quad \times \int d\mathbf{k} \int_{q<q_0} d\mathbf{q} (1/k) q^{-2} \langle 0 | \alpha_{k\lambda}^3 \exp(i\mathbf{k} \cdot \mathbf{r}_3) | n \rangle \\ &\quad \times \langle n | \alpha_{k\lambda}^1 \exp(-i\mathbf{k} \cdot \mathbf{r}_1) | n' \rangle \langle n' | \exp[i\mathbf{q} \cdot (\mathbf{r}_3 - \mathbf{r}_1)] | 0 \rangle. \end{aligned} \quad (64)$$

For positive energy intermediate states,  $|n'\rangle$  has an electron of momentum  $\mathbf{q}$  (if we neglect the spread of ground-state momenta relative to  $\mathbf{q}$ , in what follows) and a proton of momentum  $-\mathbf{p} - \mathbf{q}$ ;  $|n\rangle$  has an electron

<sup>20</sup> A. Bohr, Phys. Rev. **73**, 1109 (1948); F. E. Low, Phys. Rev. **77**, 361 (1950); F. E. Low and E. E. Salpeter, Phys. Rev. **83**, 478 (1951).

<sup>21</sup> The calculation of the third- and fourth-order  $S$ -state log terms closely parallels that of C. Greiffinger, Ph.D. thesis, Cornell University, 1954 (unpublished).



of momentum  $\mathbf{q}$ , center-of-mass of momentum  $-\mathbf{k}$  {hence c.m. energy  $[(\mathbf{q}+\mathbf{k})^2/4M]$ }, and proton of momentum  $-\mathbf{p}-\mathbf{q}-\mathbf{k}$ ; and the left-hand matrix element yields  $\mathbf{k}=-\mathbf{q}$ .

When Eq. (64) is evaluated in detail for the  $S$  state, one obtains

$$\Delta E_1^{CD} = (\text{hfs})(\alpha/\pi)(m/M)(1/4\pi)S_1^{CD}, \quad (65)$$

where

$$(\text{hfs}) = (2\pi/3)(e^2/Mm)\langle\boldsymbol{\sigma}^1 \cdot \boldsymbol{\sigma}^3\rangle |u_0(0)|^2,$$

and

$$S_1^{CD} = M \int dk k [E_3(k)]^{-1} d\Omega_k (k+E_3(k)-m)^{-1} \\ \times \sum_q \langle w_0 | \exp(\frac{1}{2}i\mathbf{k} \cdot \mathbf{r}) | w_q \rangle \langle w_q | \exp(-\frac{1}{2}i\mathbf{k} \cdot \mathbf{r}) | w_0 \rangle \\ \times [k^2/4M + E_3(k) + W_q - W_0 - m]. \quad (66)$$

The results for other orderings of the operators in Eq. (63) for positive energy intermediate states are best expressed in terms of auxiliary quantities:

$$a = k + E_3(k) - m, \\ b_q = E_3(k) - m + k^2/4M + W_q - W_0, \quad (67) \\ c_q = k + k^2/4M + W_q - W_0.$$

Then

$$S_{+++}^{CD} = 2M \int_{k>k_0} dk d\Omega k [E_3(k)]^{-1} \\ \times \sum_q \{ (ab_q)^{-1} + (ac_q)^{-1} + (b_q c_q)^{-1} \} \\ \times \langle w_0 | \exp(-\frac{1}{2}i\mathbf{k} \cdot \mathbf{r}) | w_q \rangle \\ \times \langle w_q | \exp(\frac{1}{2}i\mathbf{k} \cdot \mathbf{r}) | w_0 \rangle. \quad (68)$$

For negative energy intermediate states, we associate with each positive energy process a negative energy (pair) process having the same temporal order of emission and absorption. Consider first electron pair states.

$$I_2 = -2M \int dk d\Omega k [E_3(k)]^{-1} [k+E_3(k)-m]^{-1} [E_3(k)-m]^{-1} \\ \times \{ \sum_q \langle w_0 | \exp(-\frac{1}{2}i\mathbf{k} \cdot \mathbf{r}) | w_q \rangle \langle w_q | \exp(\frac{1}{2}i\mathbf{k} \cdot \mathbf{r}) k^2/2M | w_0 \rangle [E_3(k)-m+W_q-W_0]^{-1} \\ + (1/M) \sum_q \langle w_0 | \exp(-\frac{1}{2}i\mathbf{k} \cdot \mathbf{r}) | w_q \rangle \langle w_q | \exp(\frac{1}{2}i\mathbf{k} \cdot \mathbf{r}) \mathbf{k} \cdot \mathbf{p} | w_0 \rangle [E_3(k)-m+W_q-W_0]^{-1} \\ + \sum_q \langle w_0 | \exp(-\frac{1}{2}i\mathbf{k} \cdot \mathbf{r}) | w_q \rangle \langle w_q | -2i \sin(\frac{1}{2}\mathbf{k} \cdot \mathbf{r}) V_{\text{ex}} | w_0 \rangle [E_3(k)-m+W_q-W_0]^{-1} \}. \quad (71)$$

This is evaluated term by term. It is convenient to write the denominator in the form

$$[E_3(k)-m+W_q-W_0]^{-1} = [E_3(k)-m]^{-1} \\ + [E_3(k)-m]^{-1} [E_3(k)-m+W_q-W_0]^{-1}.$$

Each term of  $I_2$  then becomes the sum of two terms, one allowing closure, the other not. For the latter, we separate the region of integration into two regions,  $k < B$  and  $k > B$ , where  $B \sim 20$  Mev. In the region  $k < B$  we can expand the exponents in the matrix elements, and in the region  $k > B$  we use the fact that  $(W_q - W_0) \sim k^2/M$  for those matrix elements giving sizable con-

tributions. We can also neglect  $m$  with respect to  $k$  for the logarithmic terms. The term by term evaluation gives

$$S_1^{CD} = \frac{1}{2} \int dk d\Omega k [E_3(k)]^{-1} (k+E_3(k)-m)^{-1}. \quad (69)$$

The negative energy proton and electron intermediate states yield a result which differs from Eq. (69) by the presence of an additional  $+2m$  in the denominator.

To evaluate the first term of Eq. (68), designated  $I$ , we separate off the logarithmic contribution by writing

$$[E_3(k)-m+k^2/4M+W_q-W_0]^{-1} \\ = [E_3(k)-m]^{-1} - (k^2/4M+W_q-W_0) \\ \times [E_3(k)-m+W_q-W_0]^{-1} [E_3(k)-m]^{-1}. \quad (70)$$

This separates  $I$  into two terms  $I_1 + I_2$ .  $I_1$  is not of logarithmic order; in evaluating it, closure can be used, and the net result is to return to the zero-order hydrogenic wave function the high-momentum tail. Evaluation of  $I_2$  is aided by

$$\langle w_q | \exp(\frac{1}{2}i\mathbf{k} \cdot \mathbf{r}) | w_0 \rangle (W_q - W_0) \\ = \langle w_q | [H_D, \exp(\frac{1}{2}i\mathbf{k} \cdot \mathbf{r})] | w_0 \rangle,$$

where  $H_D = -\nabla^2/M + V_0 + V_{\text{ex}}$ . Upon evaluating the commutator, we obtain

tributions. We can also neglect  $m$  with respect to  $k$  for the logarithmic terms. The term by term evaluation gives

$$I \equiv S_1^{CD} = -2\pi \ln(M/m) - (2\pi/3)iM \sum_q \langle w_0 | \mathbf{r} | w_q \rangle \\ \cdot \langle w_q | \mathbf{v} | w_0 \rangle \ln[(W_q - W_0)/m] \\ + (4\pi M/6) \langle w_0 | (1 - \ln \gamma m r) r^2 V_{\text{ex}} | w_0 \rangle, \quad (72)$$

where  $\mathbf{v} = (i/2)(H_D \mathbf{r} - \mathbf{r} H_D) = \mathbf{p}/M - i\mathbf{r} V_{\text{ex}}$ . The remaining terms of Eq. (68) can be calculated in the same fashion, with extra care taken for the third term. Similarly, the negative energy state contributions are obtained from the above discussion:  $S_{+-}^{CD} = S_{+++}^{CD}$

(since  $m$  is neglected with respect to  $k$  in the denominators) and  $S_{\rightarrow\rightarrow}^{CD}$  and  $S_{\rightarrow-}^{CD}$  are obtained directly from Eq. (69). Thus the net  $CD$  contribution is

$$S^{CD}/4\pi = -4 \ln(M/m) - 2iM \sum_q \ln[(W_q - W_0)/m] \times \langle w_0 | \mathbf{r} | w_q \rangle \cdot \langle w_q | \mathbf{v} | w_0 \rangle + 2M \langle w_0 | (2/3 - C - \ln mr) r^2 V_{ex} | w_0 \rangle + 1. \quad (73)$$

The remaining third-order terms are calculated in the same way. The calculation is simplified by introducing  $f$  factors, as done by Newcomb and Salpeter,<sup>5</sup> which relate the Pauli integrands to the  $CD$  integrands. With this aid, all integrals are reduced to the general type of  $I$  above. The  $QP$ ,  $Q'P$ ,  $Q:D$ ,  $Q:P'$ , and  $QP'$  terms all give vanishing contributions to our order. The final result can be expressed in terms of one  $S$  integral, if we use the relation  $\langle \sigma^1 \rangle = \langle \sigma^2 \rangle = \frac{1}{2} \langle \sigma^D \rangle$  valid for the deuteron ground state. Then

$$S^S/4\pi = -2(\mu_P + 1) \ln(M/m) - 2i(\mu_P - \mu_N)M \sum_q \mathbf{r}_{0q} \cdot \mathbf{v}_{q0} \ln[(W_q - W_0)/m] + (\mu_P - \mu_N)[1 + 2M \langle w_0 | (2/3 - C - \ln mr) \times r^2 V_{ex} | w_0 \rangle] \quad (74)$$

is the net third order energy, arising from the exchange of a single transverse photon, and considering the  $S$ -state component of the deuteron ground state.

The third-order energy also contains a non-negligible  $D$ -state term, arising from the nuclear  $CD$  matrix element. For  $\Delta E_1^{CD}$ , this is:

$$\begin{aligned} \Delta E_1^{CD} &= (\pi e^2 / Mm) |u_0(0)|^2 \\ &\times (e^2 / 4\pi^2) (m/M) \sum_q M \int dk d\Omega \\ &\times k [E_3(k)]^{-1} [k + E_3(k) - m]^{-1} \\ &\times [E_3(k) - m + W_q - W_0 + k^2 / 4M]^{-1} \\ &\times \langle w_0 | 2i\sigma^3 \cdot \mathbf{p} \times \mathbf{k} \exp(\frac{1}{2}i\mathbf{k} \cdot \mathbf{r}) | w_q \rangle \\ &\times \langle w_q | \exp(-\frac{1}{2}i\mathbf{k} \cdot \mathbf{r}) | w_0 \rangle. \quad (75) \end{aligned}$$

The small amount of  $D$  state makes the entire term small enough, so that only the lead term need be retained. The integrals vary as  $1/k^3$  for large  $k$ . We can thus restrict ourselves to the region  $k < B$  and expand the exponentials. This yields

$$\Delta E^{CD} = - (8\pi/3) (e^2 / 4Mm) |u_0(0)|^2 (2e^2 m / \pi) \times \sigma^3 \cdot \sum_q \mathbf{r}_{0q} \times \mathbf{p}_{q0} (W_q - W_0)^{-1} \ln[(W_q - W_0)/m]. \quad (76)$$

The constant logarithmic term vanishes, since

$$\sum_q \mathbf{r}_{0q} \times \mathbf{p}_{q0} / (W_q - W_0) = 0,$$

a relation easily derived by expressing  $\mathbf{p}$  as a commutator of  $\mathbf{r}$  and  $H_D$  and using closure. Then

$$\begin{aligned} \Delta E^{CD} &= - (8\pi/3) (e^2 / 4Mm) |u_0(0)|^2 (2e^2 / \pi) \\ &\times (m / |W_0|) \sigma^3 \cdot \sum_q \mathbf{r}_{0q} \times \mathbf{p}_{q0} \ln[(W_q - W_0) / |W_0|] \\ &\times [(W_q - W_0) / |W_0|]^{-1} \quad (77) \end{aligned}$$

is the  $D$ -state correction.

The fourth-order energy is calculated in the same manner, the only complication arising from the multiplicity of terms to be considered. The Pauli terms are again gotten from the corresponding  $DD$  terms by use of appropriate  $f$  factors. Since two transverse photons are exchanged, the intermediate state can be a "spin-flipped" singlet  $n-p$  state, and such states must be included. The final result is

$$\begin{aligned} S^d/4\pi &= [(3/4)\mu_N^2 + (1/4)(\mu_P + 1)(3\mu_P - 1)] \ln(M/m) \\ &- (\mu_N - \mu_P)^2 \{ (3/8) \sum_q |\langle w_0 | w_q^s \rangle|^2 \\ &\times \ln[(W_q - W_0)/m] + \frac{1}{2} \}, \quad (78) \end{aligned}$$

where  $|w_q^s\rangle$  signifies eigenstates of the singlet  $n-p$  system.

As in hydrogen, there is a nucleon structure correction to the hyperfine energy. This has been calculated by Sessler and Mills<sup>7</sup> using the three-dimensional method, which is expected to represent the correct covariant value (which cannot be calculated directly in deuterium) as well here as in  $H^1$ . Their numerical results will be employed in Sec. D.

There is another possible correction, which would arise in the event that a spin-orbit potential is present in the nuclear two-body interaction. Feshbach<sup>22</sup> has pointed out the electromagnetic interaction introduced by gauge invariance due to the presence of a potential of the form  $V_{LS} = V(\mathbf{r})\mathbf{L} \cdot \mathbf{S}$  and Sessler and Foley<sup>23</sup> have calculated the effect of this added interaction term on the hfs. They find an additional hyperfine energy of magnitude

$$\Delta E_{LS}/E^F = -0.004(\Delta\mu)_{LS}, \quad (79)$$

where

$$\begin{aligned} (\Delta\mu)_{LS} &= - (e/16) \langle 0 | V(\mathbf{r}) [(\mathbf{S} \cdot \mathbf{r})^2 - r^2(\mathbf{S} \cdot \mathbf{J})] | 0 \rangle \\ &= (e/12) [\langle S | r^2 V | S \rangle - (1/\sqrt{2}) \langle S | r^2 V | D \rangle \\ &\quad + \frac{1}{2} \langle D | r^2 V | D \rangle]. \end{aligned}$$

We return to this effect in Sec. D.

### D. Numerical Results and Discussion

If we take the ground-state wave function of the deuteron to be of the form

$$\begin{aligned} \omega_0 &= (4\pi)^{-\frac{1}{2}} \cos\omega \{ [\varphi_S(\mathbf{r})/r] \chi_1 + \sin\omega \{ [\varphi_D(\mathbf{r})/r] \\ &\times \{ (2/20)^{\frac{1}{2}} \chi_1 Y_{20} + (6/20)^{\frac{1}{2}} \chi_0 Y_{21} \\ &\quad + (12/20)^{\frac{1}{2}} \chi_{-1} Y_{22} \}, \quad (80) \end{aligned}$$

we can collect all of our corrections into the formula

<sup>22</sup> H. Feshbach, Phys. Rev. **107**, 1626 (1957).  
<sup>23</sup> A. M. Sessler, Ph.D. thesis, Columbia University, 1953 (unpublished). A. M. Sessler and H. M. Foley, Phys. Rev. **98**, 6 (1955); **110**, 995 (1958).



Note that the extremely low (1-2%)  $D$  state suggested by Newton<sup>27</sup> seems to be excluded.

The spin-orbit term remains to be discussed. When first introduced the L-S potential was taken to be independent of isotopic spin and attractive. This was objected to by Feshbach<sup>22</sup> and Sessler and Foley,<sup>23</sup> on grounds discussed above. In reply, Signell, Marshak, and de Swart<sup>28</sup> pointed out that Feshbach's value for  $(\Delta\mu)_{SL}$  was too large, and that a phenomenological wave function gave

$$(\Delta\mu)_{SL} = -0.024 \text{ nm.} \quad (94)$$

Since this value was still too large, in that it still precluded the presence of  $D$  state in the ground-state wave function, these authors suggested that the  $\mathbf{L}\cdot\mathbf{S}$  potential may be isotopic-spin dependent, having the given value in the  $I=1$  state, and either vanishing or having a "wiggly tail" in the  $I=0$  state (the latter being insensitive to the presence of the  $\mathbf{L}\cdot\mathbf{S}$  force in the scattering). They would then set  $(\Delta\mu)_{SL}=0$ , and with this, the hyperfine correction would vanish as well. The status of this entire question must await a final determination of the presence of a spin-orbit potential (and its isotopic spin dependence if present) in the  $n$ - $p$  system.

Although the SM wave function gives better agreement with  $\delta_{\text{exp}}$  (omitting the  $\mathbf{L}\cdot\mathbf{S}$  term) there is one important feature in which this wave function is deficient. The high percentage of  $D$  state gives a magnetic moment which is 0.024 nm smaller than the observed moment. This discrepancy is of the same magnitude as, and opposite in sign to, the discrepancy which led to the first suggestion of 4%  $D$  state. If the SM percent  $D$  state is accepted, we must then look for another source of magnetic interaction which would contribute a term to the hyperfine anomaly, which would have to be taken into account in Eq. (93) when comparing  $\delta_{\text{theor}}$  and  $\delta_{\text{exp}}$ .

Finally, we must recall the discrepancy in the H<sup>1</sup> hfs discussed in Sec. I. If an error in the value of  $\alpha$  is its cause, this would have no effect on the deuterium anomaly. But if there existed nucleon polarization terms, or a singular charge distribution, which would cancel the existent structure correction, we would expect the same cancellation to occur in deuterium, since the deuteron is loosely bound, and the effect of the binding on such intrinsic nucleon characteristics is expected to be negligible. In this event, the second and fourth terms in Eq. (93) would vanish, leading to a result

$$\begin{aligned} \delta_{\text{theor}}' &= (267 \pm 22) \times 10^{-6} - 0.004(\Delta\mu)_{SL}, \\ &\quad 7\% D \text{ state} \quad (95) \\ &= (290 \pm 27) \times 10^{-6} - 0.004[\Delta\mu]_{SL}, \\ &\quad 4\% D \text{ state.} \end{aligned}$$

<sup>27</sup> R. G. Newton and T. Fulton, Phys. Rev. **107**, 1103 (1957); R. G. Newton and J. H. Scofield, Phys. Rev. **110**, 785 (1958).

<sup>28</sup> J. J. de Swart, R. E. Marshak, and P. S. Signell, Nuovo cimento **6**, 1189 (1957); Progr. Theoret. Phys. (Kyoto) **20**, 171, 181 (1958).

Both cases diverge considerably from the experimental value.<sup>29, 30</sup>

It is thus of prime importance to redetermine  $\alpha$  accurately, and to obtain more information both on the nucleon structure and the possible spin-orbit potentials. Until such questions are settled, the theoretical value for the H<sup>2</sup> hyperfine anomaly remains in doubt. On the other hand, the theoretical expressions for this anomaly can help provide a check on suggested values for these quantities.

### III. hfs OF TRITIUM

The ground state of the triton has spin  $\frac{1}{2}$ , and magnetic moment nearly equal to that of the proton. The wave function can be taken to consist almost entirely of an  $S$ -state spatial function symmetric in all nucleon coordinates, and a spin function with the two neutrons in a relative singlet state and with the proton's spin pointing in the direction of the triton's spin. The entire hyperfine energy is then due to the proton. In the absence of Bohr-Low terms we start from a nonadiabatic approximation which centers the electron on the c.m. The third-order perturbation containing  $V$  will then restore the high-momentum part of the electron wave function to its adiabatic motion around the proton. We label the proton, neutron, and electron by Nos. 1-4, respectively, and use the coordinate system of Morita *et al.*<sup>31</sup> These authors have obtained the best triton (and He<sup>3</sup>) wave functions to date. Hard-core interaction potentials were employed and excellent agreement with the experimental data were obtained. We also introduce an electron-c.m. relative coordinate,  $\varrho_4$ .

The second-order hfs terms give the Fermi energy.

<sup>29</sup> The two problems outlined may be related, as it is possible that the same magnetic term which accounts for the discrepancy in the deuteron moment, also gives rise to a hfs contribution which restores agreement between Eq. (95) and Eq. (92). This has led us to the following conjecture: If we take as a spin-orbit potential

$$V_{\mathbf{L}\cdot\mathbf{S}} = \frac{1}{2}(1 + \tau^1 \cdot \tau^2)V \text{ (Signell-Marshak),}$$

the  $I=0$  potential would be repulsive, of opposite sign and equal magnitude to the triplet value. The insensitivity of the  $I=0$  scattering to the presence of an  $\mathbf{L}\cdot\mathbf{S}$  term of suggested magnitude, makes the verification of this hypothesis via  $n$ - $p$  scattering data unlikely at present. A careful study of its effect on other electromagnetic phenomena, such as photodisintegration of the deuteron or electron-deuteron scattering, may yield more decisive results. See footnote 30 for references.

Such a repulsive potential would contribute +0.024 nm to the deuteron magnetic moment, by Eq. (94), and this would just account for the remaining magnetic interaction needed to bring  $\mu_D$  into agreement with  $\mu_{\text{SM}}$ . By Eq. (95), a contribution  $-0.004 \times 0.024 = -96 \times 10^{-6}$ , would be made to the hfs anomaly, yielding a value  $\delta_{\text{theor}}' = (171 \pm 22) \times 10^{-6}$ , which agrees excellently with Eq. (92).

If the hydrogen discrepancy is due to an error in  $\alpha$ , the entire agreement would of course break down, and the virtual absence of  $\mathbf{L}\cdot\mathbf{S}$  forces in the  $I=0$  state would be indicated.

<sup>30</sup> E. Butkov, Nuovo cimento **13**, 809 (1959); J. J. de Swart and R. E. Marshak, Phys. Rev. **111**, 272 (1958).

<sup>31</sup> M. Marita, T. Ohmura, and M. Yamada, Progr. Theoret. Phys. (Kyoto) **15**, 223 (1956); Progr. Theoret. Phys. (Kyoto) **17**, 326 (1956); Phys. Rev. **101**, 508 (1956). J. M. Blatt and G. Derrick, Nuclear Phys. **8**, 310 (1958).

Consider the first third-order term  $\Delta E_1^{CD}$ :

$$\begin{aligned} \Delta E_1^{CD} &= \sum_{nn'} (E_n - E_0)^{-1} (E_{n'} - E_0)^{-1} \\ &\quad \times \langle 0 | e\alpha^4 \cdot \sum_{\mathbf{k}} (2\pi/k)^{3/2} a_{\mathbf{k}\lambda} \mathbf{e}_{\mathbf{k}\lambda} \exp(i\mathbf{k} \cdot \mathbf{r}_4) | n \rangle \times \cdots \\ &= \sum_{nn'} (E_n - E_0)^{-1} (E_{n'} - E_0)^{-1} (2\pi)^{-3} \\ &\quad \times (e^4/\pi) \int d\mathbf{k} \int_{q>q_0} d\mathbf{q} (1/k) (1/q^2) \\ &\quad \times \langle 0 | \alpha_{\mathbf{k}\lambda}^4 e^{S_P}(i\mathbf{k} \cdot \mathbf{r}_4) | n \rangle \langle n | \alpha_{\mathbf{k}\lambda}^4 \exp(-i\mathbf{k} \cdot \mathbf{r}_1) | n' \rangle \\ &\quad \times \langle n' | \exp[i\mathbf{q} \cdot (\mathbf{r}_4 - \mathbf{r}_1)] | 0 \rangle. \quad (96) \end{aligned}$$

The nuclear matrix elements are

$$\begin{aligned} \langle 0 | w_m \rangle \langle w_m | \alpha_{\mathbf{k}\lambda}^4 \exp[-i\mathbf{k} \cdot (1/3)(\boldsymbol{\rho}_3 - \boldsymbol{\rho}_1)] | w_q \rangle \\ \times \langle w_q | \exp[i\mathbf{k} \cdot (1/3)(\boldsymbol{\rho}_3 - \boldsymbol{\rho}_2)] | w_0 \rangle. \quad (97) \end{aligned}$$

The spin part is seen to be the same as in the deuteron. Evaluating the remaining expressions in Eq. (96), we have

$$\begin{aligned} \Delta E_1^{CD} &= (2\pi/3) (e^2/Mm) \langle \boldsymbol{\sigma}^1 \cdot \boldsymbol{\sigma}^4 | u_0(0) |^2 \\ &\quad \times (e^2/4\pi^2) (m/M) S, \quad (98) \end{aligned}$$

$$S_1^{CD+++} = M \sum_q \int dkd\Omega k [E_4(k)]^{-1} (k + E_4(k) - m)^{-1}$$

$$\begin{aligned} &\times (k^2/6M + E_4(k) - m + W_q - W_0)^{-1} \\ &\times \langle w_0 | \exp[-(1/3)i\mathbf{k} \cdot (\boldsymbol{\rho}_3 - \boldsymbol{\rho}_2)] | w_q \rangle \\ &\times \langle w_q | \exp[(1/3)i\mathbf{k} \cdot (\boldsymbol{\rho}_3 - \boldsymbol{\rho}_2)] | w_0 \rangle. \quad (99) \end{aligned}$$

Comparing with deuterium, we see that if we replace the deuterium nuclear elements by Eq. (97) and the denominators Eq. (67) by

$$\begin{aligned} a &= k + E_4(k) - m, \\ b_q &= E_4(k) - m + k^2/6M + W_k - W_0, \\ c_q &= k + W_q - W_0 + k^2/6M, \end{aligned} \quad (100)$$

we get the same result as Eq. (68) for  $S_{+++}^{CD}$ . This similarity to deuterium terms holds for all third-order terms, when they are considered in detail.

In the fourth-order terms as well, the expressions for  $S$  are similar to those of deuterium, except that one replaces the deuterium nuclear matrix elements throughout by

$$\begin{aligned} \langle w_0 | \exp[(1/3)i\mathbf{k} \cdot (\boldsymbol{\rho}_3 - \boldsymbol{\rho}_2)] \boldsymbol{\sigma}_1^1 | w_q \rangle \\ \times \langle w_q | \exp[-(1/3)i\mathbf{k} \cdot (\boldsymbol{\rho}_3 - \boldsymbol{\rho}_2)] \boldsymbol{\sigma}_1^1 | w_0 \rangle. \quad (101) \end{aligned}$$

To evaluate  $I$ , given by

$$\begin{aligned} I &= 2M \int_{k>k_0} dkd\Omega (1/2k) \\ &\times \sum_q \langle w_0 | \exp[(1/3)i\mathbf{k} \cdot (\boldsymbol{\rho}_3 - \boldsymbol{\rho}_2)] | w_q \rangle \\ &\times \langle w_q | \exp[-(1/3)i\mathbf{k} \cdot (\boldsymbol{\rho}_3 - \boldsymbol{\rho}_2)] | w_0 \rangle \\ &\times [k + W_q - W_0 + k^2/6M]^{-1}, \quad (102) \end{aligned}$$

we again write

$$\begin{aligned} [k + W_q - W_0 + k^2/6M]^{-1} \\ = k^{-1} - (k^2/6M + W_k - W_0)(k + W_k - W_0)^{-1} k^{-1}, \end{aligned}$$

and set  $I = I_1 + I_2$ , where  $I_1$  contains no log correction, and  $I_2$  is:

$$\begin{aligned} I_2 &= -M \int dkd\Omega (1/k^2) \\ &\times \sum_q \langle w_0 | \exp[(1/3)i\mathbf{k} \cdot (\boldsymbol{\rho}_3 - \boldsymbol{\rho}_2)] | w_q \rangle \\ &\times \langle w_q | \exp[-(1/3)i\mathbf{k} \cdot (\boldsymbol{\rho}_3 - \boldsymbol{\rho}_2)] | w_0 \rangle \\ &\times (k^2/6M + W_q - W_0)(k + W_q - W_0)^{-1}. \quad (103) \end{aligned}$$

Setting, as before,  $(k + W_q - W_0)^{-1} = k^{-1} - (W_q - W_0) \times [k(k + W_q - W_0)]^{-1}$  we find that each term in  $I_2$  involves one part in which closure can be used, and another in which only the region  $k < B$  contributes, where the exponentials can be expanded. The result is

$$\begin{aligned} I &= -(4\pi/2) \ln(M/m) + (4\pi M/6)(8/9) \\ &\times \langle w_0 | (1 - \ln[(2\gamma m \rho_3)/3]) \rho_3^2 V_{12}^{\text{ex}}(\rho_3) | w_0 \rangle \\ &- (2/3)i(4\pi/3) \sum_q \langle w_0 | \boldsymbol{\rho}_3 | w_q \rangle \cdot \langle w_q | M \mathbf{v}_3 | w_0 \rangle \\ &\quad \times \ln[(W_q - W_0)/m]. \quad (104) \end{aligned}$$

Proceeding in the same fashion with all third-order terms, we obtain:

$$\begin{aligned} S^S/4\pi &= -2(\mu_P + 1) \ln(M/m) + (16/9)M\mu_P \\ &\times \langle w_0 | (5/6 - \ln[(2\gamma m \rho_3)/3]) \rho_3^2 V_{12}^{\text{ex}}(\rho_3) | w_0 \rangle \\ &+ (4/3)\mu_P - (8/3)\mu_P i \sum_q \langle w_0 | \boldsymbol{\rho}_3 | w_q \rangle \\ &\quad \cdot \langle w_q | M \mathbf{v}_3 | w_0 \rangle \ln[(W_k - W_0)/m]. \quad (105) \end{aligned}$$

In evaluating the fourth-order terms, we need not distinguish between the various intermediate spin states, there being no difference in the interaction between the proton and the two singlet neutrons in the spin-up or spin-down state. The net fourth-order term is

$$S^d/4\pi = (1/4)(\mu_P + 1)(3\mu_P - 1) \ln(M/m). \quad (106)$$

The hyperfine anomaly is defined as in Eq. (91). If we write out the correction terms of hydrogen explicitly,<sup>5</sup> we have

$$\begin{aligned} \delta &= (\alpha/\pi\mu_T)(m/M) \{ -2(\mu_P + 1) \ln(M/m) \\ &+ (1/4)(\mu_P + 1)(3\mu_P - 1) \ln(M/m) \\ &- (8/3)\mu_P i \sum_q \langle w_0 | \boldsymbol{\rho}_3 | w_q \rangle \\ &\cdot \langle w_q | M \mathbf{v}_3 | w_0 \rangle \ln[(W_q - W_0)/m] \\ &+ (16M/9)\mu_P \langle w_0 | (5/6 - \ln[(2\gamma m \rho_3)/3]) \\ &\times \rho_3^2 V_{12}^{\text{ex}}(\rho_3) | w_0 \rangle + (4/3)\mu_P \} \\ &- (\alpha/\pi\mu_P)(m/M) \{ -2(\mu_P + 1) \ln(M/m) \\ &+ (1/4)(\mu_P + 1)(3\mu_P - 1) \ln(M/m) + (1/8)(\mu_P - 1)^2 \\ &+ (\mu_P/\mu_T)\delta(\text{proton structure}) - \delta(\text{proton structure}) \\ &\quad + \delta(\text{other}). \quad (107) \end{aligned}$$

Since  $\mu_T = 1.0664\mu_P$ , terms which are the same except for factors of  $1/\mu_T$  and  $1/\mu_P$ , cancel to the required order. Evaluation of Eq. (107) with the Morita wave function gives

$$\delta_{\text{theor}} = +(17 \pm 2) \times 10^{-6} + \delta(\text{other}) \quad (108)$$

to be compared with<sup>32</sup>

$$\delta_{\text{exp}} = (-5.7 \pm 0.2) \times 10^{-6}. \quad (109)$$

The origin of  $\delta_{\text{other}}$  is perhaps the following: There are many possible states which could combine to give the observed  $J = \frac{1}{2}$  triton ground state. The near equality of  $\mu_P$  and  $\mu_T$ , together with energy considerations, leads one to choose the completely symmetric  $S$  state with singlet neutrons as the predominant state. Nevertheless, the residual magnetism in the triton must be accounted for, as well as that of He<sup>3</sup>, and, by charge independence, the sum of the moments of the mirror nuclei H<sup>3</sup> and He<sup>3</sup> must obey a further relation. Mixing in  $\sim 4\%$   $D$  state into the ground-state wave function matches the sum of the mirror moments, but leaves a discrepancy of  $\pm 0.27$  nm in H<sup>3</sup> and He<sup>3</sup>, respectively, between calculated and observed moments. This residual magnetism is then ascribed to (unknown) exchange currents. The 4%  $D$  state in tritium leads to a negligible orbital hfs correction.

In order to bring Eq. (108) into agreement with the experimental value Eq. (109),<sup>33</sup> we must have

$$\delta(\text{other}) \sim -23 \times 10^{-6}. \quad (110)$$

#### IV. hfs OF He<sup>3+</sup>

Sessler and Foley,<sup>23</sup> Sessler and Mills,<sup>7</sup> and Novick and Commins<sup>34</sup> have calculated all of the known hfs correction terms, with the exception of the mass correction, which we now discuss. Here the protons do not contribute to the hfs, and the only terms which are involved are the single photon  $C:P$  term and the double photon  $PP'$  term. These are calculated as in deu-

<sup>32</sup> A. G. Prodell and P. Kusch, Phys. Rev. **106**, 87 (1957); Wm. Duffy, private communication from P. Kusch.

<sup>33</sup> Our conjectured  $\mathbf{L} \cdot \mathbf{S}$  contribution contributes  $+0.021$  nm to the magnetic moment of H<sup>3</sup> and He<sup>3</sup> (both the same sign); this is far too small to account for the residual magnetism. A hfs correction term  $\delta_{\text{hfs}}^{LS} = \mp 6 \times 10^{-6}$  is added to H<sup>3</sup> and He<sup>3</sup>, respectively. The net effect is small, and does not alter the picture significantly in any direction. The same may be said for an isotopic spin independent  $\mathbf{L} \cdot \mathbf{S}$  potential, or one of the SM form (vanishing in the  $I=0$  state).

<sup>34</sup> R. Novick and E. D. Commins, Phys. Rev. **111**, 822 (1958).

terium and tritium, and yield

$$S^S/4\pi = 2\mu_N \{ (4/3)iM \sum_a \langle w_0 | \mathbf{g}_3 | w_a \rangle \cdot \langle w_a | \mathbf{v}_3 | w_0 \rangle \ln[(W_a - W_0)/m] - (8/9) \langle w_0 | (5/6 - \ln[(2\gamma m \rho_3)/3]) \times \rho_3^2 V_{12}^{\text{ex}}(\rho_3) | w_0 \rangle - 2/3 \} \quad (111)$$

$$S^d/4\pi = \mu_N^2 (3/4) \ln(M/m). \quad (112)$$

The net correction is then

$$\Delta = (\alpha/\pi\mu_{\text{He}^3})(m/M)2\mu_N \{ (4/3)iM \sum_a \langle w_0 | \mathbf{g}_3 | \omega_a \rangle \cdot \langle w_a | \mathbf{v}_3 | w_0 \rangle \ln[(W_a - W_0)/m] - (8/9) \langle w_0 | (5/6 - \ln[(2\gamma m \rho_3)/3]) \rho_3^2 \times V_{12}^{\text{ex}}(\rho_3) | w_0 \rangle - 2/3 + (3/8)\mu_N \ln(M/m) \}. \quad (113)$$

Evaluation of this gives

$$\Delta = (-29 \pm 3) \times 10^{-6}. \quad (114)$$

The anomaly is defined as in Eq. (2). Its experimental value is<sup>32</sup>

$$\delta_{\text{exp}} = (-186 \pm 9) \times 10^{-6}. \quad (115)$$

The theoretical value, excluding mass and exchange corrections, is<sup>34</sup>

$$\begin{aligned} \delta_{\text{theor}}' &= -173 \times 10^{-6}, & r_{0S} &= 2.7 \text{ f} \\ &= -159 \times 10^{-6}, & r_{0S} &= 2.4 \text{ f}. \end{aligned} \quad (116)$$

Inclusion of the latter effects yields

$$\begin{aligned} \delta_{\text{theor}} &= -(202 \pm 3) \times 10^{-6} + \delta_{\text{exch}}, & r_{0S} &= 2.7 \text{ f} \\ &= -(188 \pm 3) \times 10^{-6} + \delta_{\text{exch}}, & r_{0S} &= 2.4 \text{ f}, \end{aligned} \quad (117)$$

so that, by comparing Eq. (115) and Eq. (117), we find

$$\begin{aligned} \delta_{\text{exch}} &= (+16 \pm 12) \times 10^{-6}, & r_{0S} &= 2.7 \text{ f} \\ &= (+2 \pm 12) \times 10^{-6}, & r_{0S} &= 2.4 \text{ f}. \end{aligned} \quad (118)$$

The value for  $r_{0S} = 2.7$  f compares well with Eq. (110), whereas the other does not. It should be noted that a redetermination of  $\alpha$ , which could have a sizeable effect here, as well as a more accurate determination of  $r_{0S}$  (and a consequent recalculation of the other theoretical terms of He<sup>3+</sup> in reference 33) are necessary before any final conclusions can be drawn.

In general, the corrections given by Eq. (108) and Eq. (114) are of a magnitude which seems compatible with the experimental results. It seems, then, that the difficulties associated with the deuterium hfs are due to uncertainties in the value of  $\alpha$  and the properties of the  $n-p$  system, rather than to some large intrinsic error in the method of calculation of the correction terms.