On the Effects of Internal Nuclear Motion on the Hyperfine Structure of Deuterium

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The effects of internal nuclear motion on the hyperfine structure of deuterium are investigated, using Dirac theory for the electron and non-relativistic theory for the nucleus. Although the final result is in fair agreement with experiment, theoretical and experimental uncertainties are at present too large to allow any conclusions to be drawn concerning the possible deviation of nucleon magnetic fields from those of simple dipoles.

I. INTRODUCTION

THE accurate measurement of the hyperfine structure of hydrogen and deuterium by Nafe and Nelson[1] is not in complete agreement with Fermi's formula:[2]

$$h\nu = 8\pi/3 \cdot (2I+1)/I \cdot \mu_0 \mu \psi^2(0), \quad (1)$$

where I is the nuclear spin in units of $\hbar$, μ_0 the Bohr magneton, μ the nuclear magnetic moment and $\psi(0)$ the Schrödinger wave function evaluated at the origin. Although there are slight corrections to ν_D and ν_H arising from the intrinsic electromagnetic moment of the electron[3] and from the use of the exact relativistic wave functions for D and H, their ratio

$$\nu_D/\nu_H = \tfrac{3}{4}(m_D/m_H)^3 \mu_D/\mu_P \quad (2)$$

should be independent of these effects, as well as of the natural constants entering into (1), except for the ratios μ_D/μ_P and m_D/m_H, the former of which is known from the experiments of Bloch, Levinthal, and Packard,[4] of Bitter, Alpert, Nagle, and Poss[5] and of Siegbahn and Lindstrom.[6] Here m_D and m_H are the reduced masses of the deuterium and hydrogen atoms.

Using the value of μ_D/μ_P given by Bloch, Levinthal, and Packard, and that of ν_D/ν_H given by Nafe and Nelson, one finds:

$$\nu_D/\nu_H = \tfrac{3}{4}(m_D/m_H)^3 \mu_D/\mu_P [1+(1.7\pm 0.1)\times 10^{-4}]. \quad (3)$$

A. Bohr[7] has shown that most of this discrepancy can be accounted for by taking into consideration the structure of the deuteron. He points out that when the electron is close to the nucleus it moves rapidly compared to the nuclear motion and will therefore be bound to the apparently stationary proton rather than to the deuteron center of mass. This will be a good approximation inside a distance, ρ, which is large compared with the nuclear radius, $d=(\hbar^2/MW_0)^{\frac{1}{2}}$, but much smaller than the atomic radius a_0. Here W_0 is the binding energy of the deuteron. The order of magnitude of ρ may be estimated from the critical electron momentum, p_c, at which the electron energy, E, is equal to some mean nuclear excitation energy, $\bar{W}_N$, and hence at which the frequencies of the electronic and nuclear motions are equal; since p_c turns out to be greater than mc we may write

$$E \sim c p_c \sim \bar{W}_N, \quad p_c \sim \bar{W}_N/c.$$

The distance, ρ, corresponding to p_c is then given by

$$\rho \sim \hbar/p_c \sim \hbar c/\bar{W}_N = (\hbar/mc)mc^2/\bar{W}_N. \quad (4)$$

It is obvious, from (4), that $d \ll \rho \ll a_0$. The contribution to the h.f.s. from inside ρ must be calculated using a wave function with the electron centered on the proton; the contribution from outside will be relatively insensitive to where the electron is centered.

In first approximation, then, the proton h.f.s. will be unaffected by the deuteron structure; the neutron moment, however, will appear to the electron as a moment density distributed around the proton, and therefore its effect will nearly cancel when the electron is in the nucleus. Since the h.f.s. interaction is $\sim 1/r^2$, equal spherical shells in the atom contribute about equally up to the atomic radius, and one would expect a relative correction

$$\epsilon \sim \epsilon_0 = -(\mu_N/\mu_D) d/a_0 = +1.82\times 10^{-4} \quad (5)$$

which is in very good agreement with the experimental result (3). Bohr finds just this number by neglecting the range of the neutron-proton force compared with the deuteron radius, that is by taking for the nuclear wave function $\phi \approx (e^{-R/d}/R)$, and hence $d/2$ for the average distance between nucleons. He points out that since $R\phi$ must actually go to zero at $R=0$ the average distance between nucleons will be increased and therefore ϵ will be larger, $\epsilon = \epsilon_0 + \epsilon'$, where $\epsilon' \sim b\epsilon_0/d$ and b is the range of the force. For a square well potential one finds exactly $\epsilon' = b\epsilon_0/d$. Since $b/d \sim \frac{1}{3}$, this is an appreciable correction.

Bohr then suggests that this discrepancy might be compensated by the deviation of the proton and neutron magneti fields from simple dipole fields within distances comparable with the meson wave-length (or the range b) and shows that this might be expected to lead to a further correction $\epsilon'' \sim -b\epsilon_0/d$.

It appears, therefore, that the h.f.s. experiment might yield information on the structure of nucleons. In view

[1] J. E. Nafe and E. B. Nelson, Phys. Rev. **73**, 718 (1948).
[2] E. Fermi, Zeits. f. Physik **60**, 320 (1930).
[3] H. M. Foley and P. Kusch, Phys. Rev. **73**, 412 (1948).
[4] Bloch, Levinthal and Packard, Phys. Rev. **72**, 1125 (1947).
[5] Bitter, Alpert, Nagle, and Poss, Phys. Rev. **72**, 1273 (1947).
[6] K. Siegbahn and G. Lindstrom, Arkiv. f. Physik, Band 1 NR 6, 193 (1949).
[7] A. Bohr, Phys. Rev. **73**, 1109 (1948).

of this possibility it is of interest to evaluate all effects which do *not* depend on the nucleon structure as accurately as possible.

In the first place we would like to have a better estimate of the average distance between nucleons. In the second place, Bohr's model essentially ignores nuclear compared to electron excitation energies in the region where nuclear structure can influence h.f.s.; this is equivalent to the inequality $d \ll \rho$. Actually d is not very much smaller than ρ, and Bohr's assumption may not be sufficiently accurate for our purpose. It is necessary, then, to investigate in more detail the effect of the off-center Coulomb field on the deuterium wave function near the nucleus, and to compute the h.f.s. using this wave function. In order to carry out this program we will use ordinary first- and second-order perturbation theory. It will be convenient to start our calculation using an unperturbed electronic wave function which is centered on the proton; this wave function will give Bohr's result, and would be exact if ρ/d were sufficiently large. The relative correction to the neutron spin h.f.s. arising from the finiteness of ρ/d is found to be of the order of magnitude

$$\epsilon_N \sim -\epsilon_0(d/\rho)\log\rho/d. \tag{6}$$

That of the proton spin, in this order, is zero.

Furthermore, the effects of the deuteron D state on the h.f.s. correction must be considered. The spin moment correction will be smaller, since the neutron spin in the D state is more likely to be antiparallel than parallel to the spin in the S state. Also, since the electron will see no nuclear motion while it is inside ρ, that part of the normal orbital h.f.s. which comes from inside ρ will be missing, giving a relative correction to the h.f.s. of

$$\epsilon_L \sim -\rho/a_0 \sin^2\omega \sim -\epsilon_0(\rho/d)\sin^2\omega, \tag{7}$$

where $\sin^2\omega$ is the fraction of D state in the deuteron ground state. Although $\rho > d$, we shall see that ϵ_L is still small because the deuteron has so little orbital angular momentum.

II. THE HAMILTONIAN

We start from the Hamiltonian

$$H = H_e + H_c + H_D + H_N' + H_P' + H_L', \tag{1}$$

where H_e is the Dirac Hamiltonian of a free electron

$$H_e = c\mathbf{p}\cdot\boldsymbol{\alpha} + \beta mc^2. \tag{2}$$

H_c is the Coulomb proton-electron interaction

$$H_c = -e^2/|\mathbf{r}+\mathbf{R}/2|. \tag{3}$$

H_D is the deuteron Hamiltonian

$$H_D = P^2/M + V(\mathbf{R}, P_{ex}). \tag{4}$$

H_N', H_P' and H_L' are the neutron spin, proton spin and orbital h.f.s. interactions:

$$H_P' = e\boldsymbol{\alpha}\cdot\nabla_r \frac{1}{|\mathbf{r}+\mathbf{R}/2|} \times \boldsymbol{\mu}_P, \tag{5}$$

$$H_N' = e\boldsymbol{\alpha}\cdot\nabla_r \frac{1}{|\mathbf{r}-\mathbf{R}/2|} \times \boldsymbol{\mu}_N, \tag{6}$$

and

$$H_L' = -\frac{e^2}{c}\frac{\mathbf{v}\cdot\boldsymbol{\alpha}}{|\mathbf{r}+\mathbf{R}/2|} \tag{7}$$

and where $\mathbf{r}$ is the position vector of the electron relative to the deuteron center of mass, $\mathbf{p}$ is the momentum conjugate to $\mathbf{r}$, $\boldsymbol{\alpha}$, β are the Dirac sixteen component matrices

$$\boldsymbol{\alpha} = \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & 0 \end{pmatrix} \quad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

$$\beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$

$\mathbf{R}$ is the position vector of the neutron relative to the proton, $\mathbf{P}$ is the momentum conjugate to $\mathbf{R}$, M is the neutron-proton mass, or twice the reduced mass of the deuteron, P_{ex} is the coordinate exchange operator.

We will assume for convenience that the nuclear potential V may be written $V = [1 - t + tP_{ex}]V(\mathbf{R})$. Furthermore it can be shown that the use of the charge-exchange operator together with an identical particle formulation for the proton and neutron leads to the same results as our present simpler treatment.

We have left out the deuteron center-of-mass kinetic energy which has been shown by Breit and Meyerott[8] to necessitate the use of the reduced masses in $I(2)$ so long as internal nuclear motion is ignored. They have shown that the higher order corrections will be of order $m/M(e^2/\hbar c)^2 \log e^2/\hbar c$ which we may safely ignore. If, therefore, we imagine the problem solved in zero order without internal nuclear motion (as by Breit and Meyerott), it is evident that the wave function found may be split up into our wave function (with the true electron mass) plus a wave function which gives corrections of order m/M. The effect on our calculation of using both wave functions instead of the first will be of order $m/M(d/a_0)$ which is negligible. Finally, reduced mass corrections due specifically to the internal nuclear motion are included in the Hamiltonian (1) and can be shown to have very small effects.

The interaction of an electron with a vector potential $\mathbf{A}$ is

$$-c(-|e|/c)\boldsymbol{\alpha}\cdot\mathbf{A} = e\boldsymbol{\alpha}\cdot\mathbf{A}.$$

The vector potential of a fixed moment, $\boldsymbol{\mu}$, may be taken as

$$\mathbf{A}_\mu(\mathbf{r}) = \nabla_r(1/|\mathbf{r}-\mathbf{R}|)\times\boldsymbol{\mu}, \tag{8}$$

[8] G. Breit and E. R. Meyerott, Phys. Rev. **72**, 1023 (1947).

where $\mathbf{R}$ is the position of the moment, $\mathbf{r}$ that of the electron. At distances of the order $\hbar/Mc$ from the moment this potential must of course be modified because of the nucleon recoil. This modification would lead to a correction of order $\hbar/Mca_0$ where a_0 is the atomic radius. Since a calculation of effects taking place at a distance $\hbar/Mc$ from the nucleon would involve a relativistic theory of the nucleon, we shall not attempt to compute this correction.

We therefore take for the spin part of the h.f.s. interaction:

$$H_P'=e\boldsymbol{\alpha}\cdot\nabla_r\frac{1}{|\mathbf{r}+\mathbf{R}/2|}\times\boldsymbol{\mu}_P, \tag{5}$$

$$H_N'=e\boldsymbol{\alpha}\cdot\nabla_r\frac{1}{|\mathbf{r}-\mathbf{R}/2|}\times\boldsymbol{\mu}_N. \tag{6}$$

The vector potential of the nuclear current is taken to be

$$\mathbf{A}_L(\mathbf{r})=-(e/c)\mathbf{v}/|\mathbf{r}-\mathbf{R}|, \tag{9}$$

where $\mathbf{R}$ is the position vector of the source and $-\mathbf{v}$ its velocity.[9–11] In our case, $\mathbf{A}_L=-(e/c)\mathbf{v}/|\mathbf{r}+\mathbf{R}/2|$ and

$$\mathbf{v}=(i/2\hbar)(H_D\mathbf{R}-\mathbf{R}H_D)=\dot{\mathbf{R}}/2. \tag{10}$$

Naturally, $\mathbf{v}\neq\mathbf{P}/M$ if exchange forces are present. However, if the vector and scalar potentials are to satisfy the Lorentz condition, and therefore the field strengths Maxwell's equations, it is necessary to take $\mathbf{v}$ instead of $\mathbf{P}/M$ as the source of $\mathbf{A}$. We are thus led to

$$H_L'=-(e^2/2c)\left[\frac{\boldsymbol{\alpha}\cdot\mathbf{v}}{|\mathbf{r}+\mathbf{R}/2|}+\frac{\boldsymbol{\alpha}\cdot(\mathbf{r}+\mathbf{R}/2)\mathbf{v}\cdot(\mathbf{r}+\mathbf{R}/2)}{|\mathbf{r}+\mathbf{R}/2|^3}\right], \tag{11}$$

where the second term arises since we are dealing, not with an electron or a proton in a fixed field but with an electron-proton interaction; however, since it can easily be shown to differ from the first by $\boldsymbol{\alpha}$ dot a gradient, we may for our purposes simply take

$$H_L'=-(e^2/c)\boldsymbol{\alpha}\cdot\mathbf{v}/|\mathbf{r}+\mathbf{R}/2|. \tag{7}$$

Finally, since $\mathbf{v}$ and $\mathbf{R}$ do not commute, (7) must be symmetrized.

III. TRANSFORMATION TO A COORDINATE SYSTEM CENTERED ON THE PROTON

It is convenient, as has already been mentioned, to start from an unperturbed wave function which centers the electron on the proton. This can most easily be done by applying the transformation U, where

$$Uf(\mathbf{r},\mathbf{R})=f(\mathbf{r}+\mathbf{R}/2,\mathbf{R})$$

or

$$U=e^{i\mathbf{p}\cdot\mathbf{R}/2\hbar}. \tag{1}$$

U is obviously unitary in the space of $\mathbf{R}$ and $\mathbf{r}$. H will be modified as follows:

$$U^{-1}H_eU=H_e, \tag{2}$$

$$U^{-1}H_cU=-e^2/r, \tag{3}$$

$$U^{-1}H_P'U=e\boldsymbol{\alpha}\cdot\nabla(1/r)\times\boldsymbol{\mu}_P, \tag{4}$$

$$U^{-1}H_N'U=e\boldsymbol{\alpha}\cdot\nabla_r(1/|\mathbf{r}-\mathbf{R}|)\times\boldsymbol{\mu}_N, \tag{5}$$

$$U^{-1}H_L'U=-e^2/c(\mathbf{v}'_x\cdot\boldsymbol{\alpha}/r), \tag{6}$$

where

$$\begin{aligned}\mathbf{v}'&=U^{-1}\mathbf{v}U=U^{-1}[\mathbf{P}/M+i/2\hbar(V\mathbf{R}-\mathbf{R}V)]U\\&=\mathbf{P}/M+\mathbf{p}/2M+i/\hbar V_{ex}\mathbf{R}e^{i\mathbf{p}\cdot\mathbf{R}/\hbar}\\&=\mathbf{v}+\mathbf{p}/2M-1/\hbar^2V_{ex}\mathbf{R}\mathbf{p}\cdot\mathbf{R}+\cdots.\end{aligned} \tag{7}$$

The second term of (7) involves no nuclear coordinates, and hence will not contribute to the h.f.s. The third term of (7) may also be omitted; in first-order it does not contribute to the h.f.s., in second-order it is zero, and in third-order it is negligibly small.

This leaves $\mathbf{v}'=\mathbf{v}$ and

$$U^{-1}H_L'U=-(e^2/c)\mathbf{v}\cdot\boldsymbol{\alpha}/r. \tag{8}$$

Finally,

$$\begin{aligned}U^{-1}H_DU&=U^{-1}P^2/MU+U^{-1}VU,\\U^{-1}P^2/MU&=P^2/M+\mathbf{p}\cdot\mathbf{P}/M+p^2/4M,\\U^{-1}VU&=(V-V_{ex})+V_{ex}e^{i\mathbf{p}\cdot\mathbf{R}/\hbar}\\&=V+i/\hbar V_{ex}\mathbf{p}\cdot\mathbf{R}-1/2\hbar^2V_{ex}(\mathbf{p}\cdot\mathbf{R})^2+\cdots,\end{aligned}$$

or

$$U^{-1}H_DU=H_D+H'+H'',$$

where

$$H'=\mathbf{p}\cdot\mathbf{v},\quad H''=p^2/4M-1/2\hbar^2V_{ex}(\mathbf{p}\cdot\mathbf{R})^2. \tag{9}$$

Collecting our results (2)–(9), we may rewrite the transformed Hamiltonian:

$$H=H_e+H_c+H_D+H'+H''+H_P'+H_N'+H_L',$$

where

$$\left.\begin{aligned}&H_e=c\mathbf{p}\cdot\boldsymbol{\alpha}+\beta mc^2,\quad H_c=-e^2/r,\quad H_D=P^2/M+V,\\&H'=\mathbf{p}\cdot\mathbf{v},\quad H''=p^2/4M-1/2\hbar^2V_{ex}(\mathbf{p}\cdot\mathbf{R})^2,\\&H_P'=e\boldsymbol{\alpha}\cdot\nabla(1/r)\times\boldsymbol{\mu}_P,\ H_N'=e\boldsymbol{\alpha}\cdot\nabla(1/|\mathbf{r}-\mathbf{R}|)\times\boldsymbol{\mu}_N,\\&H_L'=-(e^2/c)(\boldsymbol{\alpha}\cdot\mathbf{v}/r).\end{aligned}\right\} \tag{10}$$

The significance of most of these terms is obvious. H'' is a reduced mass correction due to the centering of the electron on the proton rather than on the deuteron. The term of principal interest is H' which expresses the tendency of the nuclear motion to center the electron on the deuteron.

We note that the expectation of the orbital h.f.s. interaction is zero, i.e., $\langle H_L'\rangle=0$; this is not surprising, since in a coordinate system in which the proton is at rest there is no nuclear current and hence no magnetic moment due to the motion of charges.

Before proceeding to our calculation we note that since the h.f.s. coupling for an electron S state is of the

[9] A. J. F. Siegert, Phys. Rev. **52**, 787 (1937).
[10] W. E. Lamb, Jr. and L. I. Schiff, Phys. Rev. **54**, 651 (1938).
[11] R. G. Sachs, Phys. Rev. **74**, 433 (1948).

form

$$W=a\boldsymbol{\sigma}\cdot\mathbf{I}$$

one must have

$$\Delta W=W(F=I+\tfrac{1}{2})-W(F=I-\tfrac{1}{2})$$
$$=2I+1/I\cdot W(F=I+\tfrac{1}{2})$$

and hence it is only necessary to calculate the expectation of W for an eigenstate of $F=I+\frac{1}{2}$. The simplest such eigenstate is the one for which $m_I=+I$ and $m_J=+\frac{1}{2}$. Since we shall put our results in the form of relative corrections we may leave out the factor $2I+1/I$.

IV. EVALUATION OF THE PROTON SPIN H.F.S. FOR THE UNPERTURBED WAVE FUNCTIONS

We have, from III (10):

$$\langle H_P'\rangle=\langle e\boldsymbol{\alpha}\cdot\nabla(1/r)\times\boldsymbol{\mu}_P\rangle$$
$$=\mathbf{A}\cdot\boldsymbol{\mu}_P \tag{1}$$

where

$$\mathbf{A}=(\psi_0,\ e\boldsymbol{\alpha}\times\nabla(1/r)\psi_0).$$

Making use of the approximation

$$\psi_0=(1+\boldsymbol{\alpha}\cdot\mathbf{p}/2mc)u(0)\psi_s(r)$$
$$=\left(1+i\frac{\boldsymbol{\alpha}\cdot\mathbf{r}}{2r}\frac{\hbar/mc}{a_0}\right)u(0)\psi_s(r), \tag{2}$$

where

$$\psi_s(r)=\psi(0)e^{-r/a_0},$$

and $u(0)=\begin{bmatrix}1\\0\\0\\0\end{bmatrix}$ for spin up, $u(0)=\begin{bmatrix}0\\1\\0\\0\end{bmatrix}$ for spin down

we have

$$\mathbf{A}=e^3/\hbar c(u(0)\psi_s(r),\ (\boldsymbol{\sigma}\times\mathbf{r}/r)\times\nabla(1/r)u(0)\psi_s(r))$$
$$=8\pi/3\mu_0\psi^2(0)\boldsymbol{\sigma}, \tag{3}$$

and

$$\langle H_P'\rangle=8\pi/3\psi^2(0)\mu_0\langle\boldsymbol{\sigma}\cdot\boldsymbol{\mu}_P\rangle. \tag{4}$$

This is Fermi's formula for the h.f.s. of the proton moment in deuterium. $\langle\boldsymbol{\mu}_P\rangle$ includes the D state correction to the effective proton moment in the deuteron:

$$\langle\boldsymbol{\sigma}\cdot\boldsymbol{\mu}_P\rangle=\mu_P(1-\tfrac{3}{2}\sin^2\omega),$$

where $\sin^2\omega$ is the D state probability.

It is understood that there are corrections of order $(e^2/\hbar c)^2$ to (4) which arise from the approximation (2); however they will cancel in the deuterium-hydrogen ratio and be negligible in all higher order terms. The reduced mass corrections to (4) we have already discussed in II.

V. EVALUATION OF THE NEUTRON SPIN H.F.S. FOR THE UNPERTURBED WAVE FUNCTIONS

We have, again from III (10):

$$\langle H_N'\rangle=\langle e\boldsymbol{\alpha}\cdot\nabla_r(1/|\mathbf{r}-\mathbf{R}|)\times\boldsymbol{\mu}_N\rangle. \tag{1}$$

The nuclear wave function consists of an S and a D term:

$$\Phi_0=\Phi_S+\Phi_D.$$

$\langle H_N'\rangle$ may then be divided into three parts: an S term, a D term and a cross term. We will consider first the S term.

$$\Phi_S=\cos\omega/(4\pi)^{\frac{1}{2}}[\phi_S(R)/R]\chi,$$

where χ is a spin function and

$$\int_0^\infty\phi_s^2(R)dR=1.$$

If we call

$$\mathbf{B}=(\Phi_s,\ \nabla_r(1/|\mathbf{r}-\mathbf{R}|)\times\boldsymbol{\mu}_N\Phi_s)$$
$$=\cos^2\omega/4\pi\nabla_r\int dR\phi_s^2(R)\int d\Omega_R/|\mathbf{r}-\mathbf{R}|\times\boldsymbol{\mu}_N \tag{2}$$

and make use of the formulas

$$\left.\begin{aligned}1/|\mathbf{r}-\mathbf{R}|&=\sum_{l=0}^{\infty}R^l/r^{l+1}P_l(\cos\gamma)\quad R<r\\&=\sum_{l=0}^{\infty}r^l/R^{l+1}P_l(\cos\gamma)\quad R>r\end{aligned}\right\} \tag{3}$$

$$P_l(\cos\gamma)=4\pi/2l+1\sum_{m=-l}^{l}Y_{lm}^*(\theta,\phi)Y_{lm}(\Theta,\Phi), \tag{4}$$

where $\cos\gamma=\mathbf{r}\cdot\mathbf{R}/rR$, and the Y_{lm} are normalized spherical harmonics, then

$$\left.\begin{aligned}\int\frac{d\Omega_R}{|\mathbf{r}-\mathbf{R}|}=\int\frac{d\Theta\sin\Theta d\Phi}{|\mathbf{r}-\mathbf{R}|}&=4\pi/r\quad R<r\\&=4\pi/R\quad R>r\end{aligned}\right\} \tag{5}$$

and

$$\mathbf{B}=\cos^2\omega\nabla\left[\frac{1}{r}\int_0^r\phi_s^2dR+\int_r^\infty\phi_s^2/R^{dR}\right]\times\boldsymbol{\mu}_N$$
$$=\cos^2\omega\nabla\frac{1}{r}\int_0^r\phi_s^2(R)dR\times\boldsymbol{\mu}_N, \tag{6}$$

which is of the same form as $\mathbf{A}$ in IV except that $\nabla(1/r)$ is replaced by

$$\left(\nabla\frac{1}{r}\right)\int_0^r\phi_s^2(R)dR;$$

we may therefore write, using IV (3):

$$\langle H_N'\rangle_s=8\pi/3\cos^2\omega\mu_0\langle\boldsymbol{\sigma}\cdot\boldsymbol{\mu}_N\rangle_s\psi^2(0)2/a_0$$
$$\times\int_0^\infty e^{-2/a_0}dr\int_0^r\phi_s^2(R)dR \tag{7}$$

$$=8\pi/3\cos^2\omega\psi^2(0)\mu_0\langle\boldsymbol{\sigma}\cdot\boldsymbol{\mu}_N\rangle_s$$
$$\times\left[1-2/a_0\int_0^\infty R\phi_s^2(R)dR\right]. \tag{8}$$

The first term in the bracket evidently gives the Fermi formula for the neutron spin h.f.s. without the D state correction to the effective neutron moment. The second term, to which we shall return later, is Bohr's correction. All higher terms are negligible.

We consider next the D state expectation

$$\langle H_N'\rangle_D=\langle e\boldsymbol{\alpha}\cdot\nabla_r(\Phi_D,\ 1/|\mathbf{r}-\mathbf{R}|\times\boldsymbol{\mu}_N\Phi_D)\rangle, \tag{9}$$

$$\Phi_D=\sin\omega\phi_D(R)/RY_D(\Omega_R),\quad \int_0^\infty \phi_D^2(R)dR=1,$$

where

$$Y_D=\bar{S}_{12}\chi_1=[(2/20)^{\frac{1}{2}}\chi_1Y_{20}+(6/20)^{\frac{1}{2}}\chi_0Y_{21}+(12/20)^{\frac{1}{2}}\chi_{-1}Y_{22}],$$

$$\bar{S}_{12}=1/(32\pi)^{\frac{1}{2}}\left(\frac{3\boldsymbol{\sigma}_P\cdot\mathbf{R}\boldsymbol{\sigma}_N\cdot\mathbf{R}}{R^2}-1\right).$$

In the expansion (3) the only terms which do not integrate to zero over nuclear angles are the harmonics of order 0, 2 and 4. Those of order 4 need not be considered since their gradient will consist of harmonics of order 3 and 5 which will in turn integrate to zero over electron angles.

The zeroth-order term in (3) evidently gives an analogous result to the S state expectation:

$$\langle H_N'\rangle_D{}^{L=0}=8\pi/3\ \sin^2\omega\psi^2(0)\mu_0\langle\boldsymbol{\sigma}\cdot\boldsymbol{\mu}_N\rangle_D\times\left[1-2/a_0\int_0^\infty R\phi_D^2(R)dR\right], \tag{10}$$

$$\langle\boldsymbol{\sigma}\cdot\boldsymbol{\mu}_N\rangle_D=(Y_D,\ (\mu_N)_zY_D)=-\tfrac{1}{2}\mu_N.$$

The first term in (10) is the D state correction to the effective neutron moment that was missing from (8). The second term is a further correction of the Bohr type, which, as we have already mentioned, will decrease the entire correction because the D state spin is effectively pointing against the S state spin.

An elementary calculation based on the expansions (3) and (4) and on the approximation IV (2) shows that the terms of order two in (3) add

$$\langle H_N'\rangle_D{}^{L=2}=8\pi/3\ \sin^2\omega\mu_0\mu_N\psi^2(0)\times\int_0^\infty R/4a_0\phi_D^2(R)dR \tag{11}$$

and that the cross term

$$\langle H_N'\rangle_{DS}=2R\langle e\boldsymbol{\alpha}\cdot(\Phi_S\nabla_r(1/|\mathbf{r}-\mathbf{R}|)\times\boldsymbol{\mu}_N\Phi_D)\rangle \tag{12}$$

(where R indicates that only the real part is to be taken) adds

$$\langle H_N'\rangle_{DS}=(8\pi/3)\ \sin\omega\cos\omega\psi^2(0)\mu_0\mu_N\times\int_0^\infty(2)^{\frac{1}{2}}/4(R/a_0)\phi_D\phi_SdR \tag{13}$$

to (8) and (10).

From the second terms in (8) and (10) and from (11) and (13) we find a relative correction to the h.f.s. of

$$\epsilon=-\mu_N/\mu_D\Big[2/a_0\cos^2\omega\int_0^\infty R\phi_S^2dR-5/4a_0\sin^2\omega\int_0^\infty R\phi_D^2dR-(\sqrt{2}/4a_0\cos\omega\sin\omega\int_0^\infty R\phi_D\phi_SdR\Big] \tag{14}$$

or

$$\epsilon=-\mu_N/\mu_D\cdot d/a_0[\cos^2\omega\langle2\alpha R\rangle_S-5/4\ \sin^2\omega\langle\alpha R\rangle_D-\sqrt{2}/4\ \cos\omega\ \sin\omega\langle\alpha R\rangle_{DS}], \tag{15}$$

where

$$\alpha=1/d=(MW_0/\hbar^2)^{\frac{1}{2}}$$

and W_0 is the binding energy of the deuteron.

VI. EVALUATION OF ϵ

We have available for the determination of the nuclear ground state wave functions the deuteron binding energy, which determines their asymptotic form through the constant $\alpha=1/d$, low energy scattering data which determines the "effective range," $r_0=1.59\times10^{-13}$ cm,[12] the deuteron magnetic moment which determines (non-relativistically) the D state probability and the deuteron quadrupole moment which essentially determines a cut-off for the D state radial wave function.

Our main task is to find a good number for $\langle2\alpha R\rangle_S$ since the second and third terms of V (15) are quite small.

The asymptotic form of the S state wave function is:

$$\phi_s(R)\rightarrow Ce^{-\alpha R}. \tag{1}$$

Let us define two functions, u and v, such that $v=e^{-\alpha R}$ and

$$u=[\phi_s(R)]/C; \tag{2}$$

then

$$\frac{r_0}{2}=\int_0^\infty(v^2-u^2)dR. \tag{3}$$

The constant C is determined by (3):

$$C=(2\alpha/1-r_0\alpha)^{\frac{1}{2}}. \tag{4}$$

If, then, following (3), we put for convenience

$$\int_0^\infty R(v^2-u^2)dR=(r_0/2)^2\lambda, \tag{5}$$

where we expect $\lambda\sim1$, we have

$$\langle2\alpha R\rangle_S=\int_0^\infty\phi_S^2\cdot2\alpha RdR=1+\alpha r_0+(1-\lambda)(\alpha r_0)^2/(1-r_{0\alpha})=1+\alpha r_0+\delta. \tag{6}$$

[12] H. A. Bethe, Phys. Rev. **76**, 38 (1949).

The unknown λ should be fairly close to one, so that the correction term δ in (6) may be expected to be smaller than $(\alpha r_0)^2$. We shall find that this is in fact the case. Unfortunately, (6) is not as accurate as we might wish. As a check, we have calculated $\langle 2\alpha R\rangle_S$ for an exponential, square well and Hulthen potential, the latter having properties closely resembling those of the Yukawa potential.

One finds, for the square well:

$$\langle 2\alpha R\rangle_S = 1+\alpha r_0+0.07, \tag{7}$$

for the exponential well:

$$\langle 2\alpha R\rangle_S = 1+\alpha r_0-0.08, \tag{8}$$

and for the Hulthen well:

$$\langle 2\alpha R\rangle_S = 1+\alpha r_0+0.03. \tag{9}$$

In calculating (7)–(9) the two parameters available for each potential were of course chosen so that α and r_0 remained fixed.

We have in all, then,

$$\langle 2\alpha R\rangle_S = 1+\alpha r_0 \pm 0.07 = 1.37 \pm 0.07. \tag{10}$$

The remaining two terms in V (15) are so small that an accuracy of 25 percent in their calculation is sufficient. This may be obtained simply by using the asymptotic D state wave function

$$\left.\begin{aligned} &\phi_D = (A(2\alpha)^{\frac{1}{2}}/\alpha^2R^2)e^{-\alpha R}(1+\alpha R+\tfrac{1}{3}\alpha^2R^2) \text{ for } R>b \\ &\text{and} \\ &\phi_D = 0 \text{ for } R<b. \end{aligned}\right\} \tag{11}$$

A and b are to be found by simultaneously normalizing and matching the deuteron quadrupole moment. This procedure yields

$$A = 0.47, \quad \alpha b = \tfrac{1}{2}, \tag{12}$$

and an elementary integration shows that

$$\langle \alpha R\rangle_{DS} = 0.55 \pm 0.15, \quad \langle \alpha R\rangle_D = 0.66 \pm 0.15. \tag{13}$$

Choosing $\sin^2\omega$ so that it will give, in a non-relativistic calculation, the measured magnetic moment of the deuteron, we have:

$$\sin^2\omega = 0.04, \quad \cos^2\omega = 0.96. \tag{14}$$

Finally, inserting the results (10), (13) and (14) into V (15) gives

$$\epsilon = -\mu_N d/\mu_D a_0 (1.24 \pm 0.08). \tag{15}$$

VII. EFFECT OF H' ON THE NEUTRON SPIN H.F.S.

We note first that $H' = \mathbf{p}\cdot\mathbf{v}$ has transitions between nuclear states of opposite parity whereas $H_P' = e\boldsymbol{\alpha}\cdot\nabla(1/r)\times\boldsymbol{\mu}_P$ has transitions only between nuclear states of the same parity. Therefore, in this order, the effect of H' on the proton spin h.f.s. is zero.

The neutron term is:

$$E_N = -2\sum_m \left[\sum_{n+} \frac{(H_N')_{0n,\,0m}H_{n0,\,m0}'}{E_n - E_0 + W_m - W_0} - \sum_{n-} \frac{(H_N')_{n0,\,0m}H_{0n,\,m0}'}{E_0 - E_n + W_m - W_0}\right], \tag{1}$$

where $E_{n\pm}$ refer to electron energies and W_m to nuclear energies. Summation over the indices m and n will be understood, although frequently the indices will be left out for convenience of notation.

E_N arises from a distortion of the electronic wave function inside the distance ρ, which is smaller than the electron Compton wave-length. It is therefore reasonable to suppose that most of E_N comes from electron energies corresponding to momenta that are greater than mc, and that the continuum states of the Coulomb field may be replaced by plane waves.

Using the approximation

$$\phi(p) = \psi(0)(e^2/r)_{P0}(u(p),\, u(0))/E(p) - E_0, \tag{2}$$

where

$$\phi(p) = (u(p)e^{i\mathbf{p}\cdot\mathbf{r}/\hbar},\, \psi_0(r)),$$

$u(p)$ is a Dirac spinor amplitude and

$$(e^2/r)_{p0} = 4\pi\hbar^2/p^2,$$

we have:

$$H_N' = e\boldsymbol{\alpha}\cdot\nabla_r(1/|\mathbf{r}-\mathbf{R}|)\times\boldsymbol{\mu}_N,$$

$$(H_N')_{0n} = -i/\hbar e^{i\mathbf{p}\cdot\mathbf{R}/\hbar}\psi(0)(1/r)_{p0} \times (u(0),\, e\boldsymbol{\alpha}\times\mathbf{p}\cdot\boldsymbol{\mu}_N u(p)) + O(e^2/\hbar c), \tag{3}$$

$$H_{n0,\,m0}' \cong \mathbf{v}_{m0}\cdot\mathbf{p}\phi(\mathbf{p}) = \mathbf{p}\cdot\mathbf{v}_{m0}\psi(0)(e^2/r)_{p0} \times (u(p),\, u(0))/E(p) - E_0, \tag{4}$$

$$E_N(+) = 2\psi^2(0)ie^2/h\sum_{P+}(1/r)_{p0}{}^2 e^{i\mathbf{p}\cdot\mathbf{R}/\hbar}\frac{\mathbf{p}\cdot\mathbf{v}_{m0}}{E(p)-E_0} \times \frac{(u(0),\, e\boldsymbol{\alpha}\times\mathbf{p}\cdot\boldsymbol{\mu}_N u(p))(u(p),\, u(0))}{E(p)-E_0+W_m-W_0}$$

$$= 2\psi^2(0)ie^2/h\sum_{P}(1/r)_{p0}{}^2 e^{i\mathbf{p}\cdot\mathbf{R}/\hbar}\frac{\mathbf{p}\cdot\mathbf{v}_{m0}}{E(p)-E_0} \times \frac{(u(0),\, e\boldsymbol{\alpha}\times\mathbf{p}\cdot\boldsymbol{\mu}_N\Lambda^+(\mathbf{p})u(0))}{E(p)-E_0+W_m-W_0}, \tag{5}$$

where

$$\Lambda^+(\mathbf{p}) = (c\mathbf{p}\cdot\boldsymbol{\alpha}+\beta mc^2+|E(p)|)/2|E(p)| = 1 \text{ for } E>0 = 0 \text{ for } E<0,$$

and where it is understood that the unlabeled nuclear operators in (5) go from the state 0 to m. Since the term we are calculating is only a small correction, we may for simplicity assume that the nuclear ground state is

spherically symmetric. In that case, on the average,

$$(u(0), \boldsymbol{\alpha}\times\mathbf{p}\cdot\boldsymbol{\mu}_N\Lambda^+(\mathbf{p})u(0))=icp^2\boldsymbol{\sigma}\cdot\boldsymbol{\mu}_N/3E(p)$$

(where from now on $E(p)$ is always to mean a positive number) and (5) becomes:

$$E_N(+)=-(2/3)e^3c/\hbar\psi^2(0)\boldsymbol{\sigma}\cdot\boldsymbol{\mu}_N\int\frac{d\mathbf{p}}{(2\pi\hbar)^3}(1/r)^2{}_{p0}\times\frac{p^2\mathbf{p}\cdot\mathbf{v}_{m0}e^{i\mathbf{p}\cdot\mathbf{R}/\hbar}}{E(p)[E(p)-E_0][E(p)-E_0+W_m-W_0]}.$$

Carrying through the same procedure for the negative energy sums one finds in all:

$$E_N=-4/3\pi\psi^2(0)e^3c\boldsymbol{\sigma}\cdot\boldsymbol{\mu}_N\int\frac{d\Omega_p dp\mathbf{p}\cdot\mathbf{v}_{m0}}{E(p)}\times\left[\frac{e^{i\mathbf{p}\cdot\mathbf{R}/\hbar}}{D+}-\frac{e^{-i\mathbf{p}\cdot\mathbf{R}/\hbar}}{D-}\right] \quad (6)$$

where

$$D\pm=(E(p)\mp E_0)(E(p)\mp E_0+W_m-W_0).$$

Integrating over angles,

$$E_N=\frac{16i}{3}\psi^2(0)e^3c\boldsymbol{\sigma}\cdot\boldsymbol{\mu}_N\mathbf{v}_{m0}\cdot\frac{\mathbf{R}}{R}\int_0^\infty\frac{pdp}{E(p)}\times\left[\frac{1}{D+}+\frac{1}{D-}\right]\frac{(pR/\hbar)\cos(pR/\hbar)-\sin(pR/\hbar)}{(pR/\hbar)^2}. \quad (7)$$

The integrand is seen to behave as a constant for small p, as $1/p$ for p greater than mc but less than h/R, and as $1/p^3$ for still greater momenta. Relativistic momenta, therefore, contribute most strongly, as was assumed. In fact, compared to the energies involved in (7), the rest energy of the electron is negligible, and we may set:

$$\frac{1}{D+}+\frac{1}{D-}\cong\frac{2E(p)}{c^2p^2}\cdot\frac{1}{cp+W_m-W_0}$$

so that

$$E_N=32i\psi^2(0)(e^3/3\hbar c^2)\boldsymbol{\sigma}\cdot\boldsymbol{\mu}_N\mathbf{v}_{m0}\cdot\mathbf{R}J(a_m), \quad (8)$$

where

$$J(a)=\int_0^\infty\frac{dx}{x+a}\cdot\frac{x\cos x-\sin x}{x^3}$$

and

$$x=pR/h,\quad a_m=\frac{(W_m-W_0)}{hc}R\sim R/\rho\ll 1.$$

Since the parameter a is small, the integral may be expanded in powers of a; one finds:

$$J(a)=-\tfrac{1}{3}[\log(1/\gamma a)+4/3-(3\pi/16)a+\cdots], \quad (9)$$

$\gamma=1.78$ is Euler's constant.

The last term in (9) is negligible. Dropping it, we have, from (8):

$$E_N=-\frac{16i}{3}\psi^2(0)(e^3/\hbar c^2)\cdot\frac{2}{3}\sum_m\left\{\boldsymbol{\sigma}\cdot\boldsymbol{\mu}_N\left[\log\frac{1}{\gamma a_m}+\frac{4}{3}\right]\mathbf{R}\right\}_{0m}\cdot\mathbf{v}_{m0} \quad (10)$$

and dividing the logarithm into more manageable parts,

$$E_N=-\frac{16i}{3}\psi^2(0)(e^3/\hbar c^2)\mu_N\cdot\frac{2}{3}\left[\left(\log\frac{mc^2}{|W_0|}\frac{\hbar/mc}{\gamma\cdot d/2}+\frac{4}{3}\right)\langle\mathbf{R}\cdot\mathbf{v}\rangle-\langle\log(2\alpha R)\mathbf{R}\cdot\mathbf{v}\rangle-\sum_m\mathbf{R}_{0m}\cdot\mathbf{v}_{m0}\log\frac{W_m-W_0}{|W_0|}\right]. \quad (11)$$

The first two expectations are easily evaluated:

$$\langle\mathbf{R}\cdot\mathbf{v}\rangle=\langle\mathbf{R}\cdot[\mathbf{P}/M-i/2\hbar(\mathbf{R}V-V\mathbf{R})]\rangle=(3/2)i\hbar/M(1+\eta t), \quad (12)$$

where

$$\eta=-2M/3\hbar^2\langle R^2V(R)\rangle.$$

If the exchange potential is binding, then $\eta>0$. Although η depends on the well shape of V, it will be of the order of magnitude of force range divided by nuclear radius, and since t is probably smaller than one, their product will not vary sufficiently (corresponding to different assumptions as to well shape) to affect our results significantly. We recall that t was defined as the fraction of exchange force in the deuteron.

One finds for η, by direct calculation:

$\eta=\frac{1}{3}$ for a Hulthen well,
$\eta=\frac{2}{5}$ for a square well.

The second term in (11) contributes

$$\langle\log(2\alpha R)\mathbf{R}\cdot\mathbf{v}\rangle=3hi/2M\left[\frac{1}{3}+\int_0^\infty\phi_s{}^2\log 2\alpha R dR-2t/3\int_0^\infty\phi_s{}^2\log 2\alpha R(MV/\hbar^2)R^2dR\right] \quad (13)$$

of which the last two terms are negligible.

Finally, the summation

$$K=\sum_m\mathbf{R}_{0m}\cdot\mathbf{v}_{m0}\log\frac{W_m-W_0}{|W_0|}$$

contributes about one-half of E_N. Therefore a 10 percent error in K will be cut to 5 percent in E_N. It turns out that to within 10 percent one can approximate K by

the simple formula

$$K\cong 3i\hbar/2M(1+\eta t)\left[\log\frac{3(1+\eta t)}{\langle\alpha^2R^2\rangle}+\frac{1}{3}\right]. \quad (14)$$

Note also that $\langle\alpha^2R^2\rangle$ is practically independent of assumptions about well shape:

$$\langle\alpha^2R^2\rangle=1/2(1-r_0\alpha). \quad (15)$$

From (11)–(14) we find a relative correction to the h.f.s. of

$$\epsilon_N=(4/\pi)(e^2/\hbar c)(m/M)\mu_N/\mu_D$$
$$\times\left\{(1+\eta t)\left[1+\log\frac{mc^2 2\alpha(\hbar/mc)\langle\alpha^2R^2\rangle}{|W_0|3\gamma(1+\eta t)}\right]-\frac{1}{3}\right\} \quad (16)$$

which, it is of interest to note, is of order of magnitude

$$\epsilon_N\sim-\epsilon_0 d/\rho[1+\log\rho/d], \quad (17)$$

where ρ is the critical distance defined in I (4).

Numerically,

$$\epsilon_N=(\mu_N/\mu_D)(d/a_0)[0.155(1+\xi t)\pm 10 \text{ percent}], \quad (18)$$

where $\xi=\frac{1}{4}$ for a Hulthen well, $\xi=\frac{3}{10}$ for a square well.

VIII. ORBITAL H.F.S.

We have seen in III that our unperturbed wave function gave zero orbital h.f.s. Therefore the effect of the perturbation H' on the wave function must give us both the normal orbital h.f.s. and the correction to it which was discussed in I.

The orbital h.f.s. is therefore given by

$$E_L=-2\sum_m\left[\sum_{n+}\frac{H_{0n,0m'}(H_L')_{n0,m0}}{E_n-E_0+W_m-W_0}-\sum_{n-}\frac{H_{n0,0m'}(H_L')_{0n,m0}}{E_0-E_n+W_m-W_0}\right] \quad (1)$$

where

$$H'=\mathbf{p}\cdot\mathbf{v},\quad H_L'=-(e^2/c)\frac{\boldsymbol{\alpha}\cdot\mathbf{v}}{r}.$$

The neglect of electron energies in (1) leads simply to the expectation of the normal h.f.s. which until now has been missing. To see this, we add and subtract

$$E_F=-2\sum_m\sum_{n\pm}H_{0n,0m'}(H_L')_{n0,m0}/W_m-W_0 \quad (2)$$
$$=2ie^2/2c\hbar\langle\mathbf{p}\cdot\mathbf{v}\mathbf{R}\cdot\boldsymbol{\alpha}/r\rangle \quad (3)$$
$$=-2e^2/4\hbar Mc\langle(\mathbf{L}/2)\cdot\hbar\nabla\times\boldsymbol{\alpha}/r\rangle \quad \mathbf{L}=\mathbf{R}\times\mathbf{P}$$

plus terms which do not contribute to the h.f.s.

$$E_F=\tfrac{1}{2}\langle e\boldsymbol{\alpha}\cdot\nabla(1/r)\times e\mathbf{L}/2Mc\rangle, \quad (4)$$
$$E_F=\langle e\boldsymbol{\alpha}\cdot\nabla(1/r)\times\boldsymbol{\mu}_L\rangle, \quad (4')$$

since we are interested only in the real part of the expression. The factor $\frac{1}{2}$ in (4) appears because only one of the nuclear particles is charged. It is easily seen that, as stated, (4) is precisely the normal orbital h.f.s. interaction.

We are left with the difference of (1) and (4), which is a high energy term, and where we may again use the plane wave approximation. Notice that in deriving (4) no such approximation was made, or may be made, since the h.f.s. comes equally from all radii up to a_0.

Using the plane wave approximation for intermediate electron states, a straightforward calculation of the same type as the one in VII leads to

$$E_L'=E_L-E_F=4/3\cdot e^4/mc^3\cdot\psi^2(0)\sum_m\boldsymbol{\sigma}\cdot\mathbf{v}_{0m}\times\mathbf{R}_{m0}H(m), \quad (5)$$

$$H(m)=\int_0^\infty\frac{dx}{(1+x^2)^{\frac{1}{2}}}\left[\frac{1}{(1+x^2)^{\frac{1}{2}}+1+\delta_m}+\frac{1}{(1+x^2)^{\frac{1}{2}}-1+\delta_m}\right],$$

where

$$\delta_m=(W_m-W_0)/mc^2\gg 1,\quad x=p/mc$$
$$H(m)=2/\delta_m[\log 2\delta_m+0(1/\delta_m^2)]$$

so that

$$E_L'=\frac{8}{3}\frac{e^4}{c}\psi^2(0)\sum_m\frac{\boldsymbol{\sigma}\cdot\mathbf{v}_{0m}\times\mathbf{R}_{m0}}{W_m-W_0}\times\log\left[\frac{2|W_0|}{mc^2}\frac{(W_m-W_0)}{|W_0|}\right] \quad (6)$$

and since for a constant logarithm the sum would vanish

$$E_L'=\frac{8}{3}\frac{e^4}{c}\psi^2(0)\sum_m\boldsymbol{\sigma}\cdot\frac{\mathbf{v}_{0m}\times\mathbf{R}_{m0}}{W_m-W_0}\log\frac{W_m-W_0}{|W_0|} \quad (7)$$

which is a relative correction to the h.f.s. of

$$\epsilon_L=(4/\pi)(\mu_L/\mu_D)(e^2/\hbar c)mc^2/|W_0|\cdot L, \quad (8)$$

where

$$\mu_L=e\hbar/2Mc$$

and

$$L=\frac{1}{\hbar}\sum_m\boldsymbol{\sigma}\cdot M\mathbf{v}_{0m}\times\mathbf{R}_{m0}\frac{\log(W_m-W_0/|W_0|)}{(W_m-W_0)/|W_0|}. \quad (9)$$

ϵ_L is easily seen to be a correction of order

$$\epsilon_L\sim-\rho/a_0\sin^2\omega$$

since

$$(e^2/\hbar c)mc^2/|W_0|\sim\rho/a_0$$

and L is of order $\sin^2 w$.

Since L is small, we do not require high accuracy in its calculation, which would in any case be difficult to obtain, the effective uncertainty in the ground state being much greater here than in VII. We will therefore

calculate L using free intermediate nuclear states. Some justification for this procedure may be found from scattering experiments which appear to indicate very small phase shifts for odd states. Most of the error will thus come from inside the force range, and may be estimated by comparing the results for two different ground states, both of which are chosen to match the known deuteron magnetic moment and quadrupole moment, and both of which have the same asymptotic form.

We have seen in V that the D state wave function is

$$\Phi_D=\sin\omega(\phi_D(R)/R)[(2/20)^{\frac{1}{2}}\chi_1 Y_{20} +(6/20)^{\frac{1}{2}}\chi_0 Y_{21}+(12/20)^{\frac{1}{2}}\chi_{-1}Y_{22}]. \quad (10)$$

If we take

$$\left.\begin{aligned}\phi_D&=A(2\alpha)^{\frac{1}{2}}/\alpha^2R^2(1+\alpha R+\alpha^2R^2/3) \quad R>b\\ &=(2\alpha)^{\frac{1}{2}}(B\alpha^2R^2+C\alpha^3R^3) \quad R<b\end{aligned}\right\} \quad (11)$$

then a simple numerical integration leads to

$$L=-0.10\sin^2\omega. \quad (12)$$

If we take

$$\phi_D=(2\alpha)^{\frac{1}{2}}A\left[\frac{e^{-\alpha R}}{\alpha^2R^2}(1+\alpha R+\tfrac{1}{3}\alpha^2R^2) -\frac{e^{-\beta R}}{\alpha^2R^2}(1+\beta R+\tfrac{1}{3}\beta^2R^2)-\frac{1}{6}\frac{\beta^2-\alpha^2}{\alpha^2}e^{-\beta R}(1+\beta R)\right] \quad (13)$$

then we find

$$L=-0.08\sin^2\omega. \quad (14)$$

Choosing L to be the mean of (12) and (14), and allowing an extra 20 percent error for the intermediate states, we have:

$$L=-(0.09\pm0.03)\sin^2\omega \quad (15)$$

and

$$\epsilon_L=(4/\pi)(\mu_L/\mu_D)(e^2/\hbar c)(mc^2/|W_0|)L \quad (16)$$
$$=(\mu_N d/\mu_D a_0)(0.05\pm0.02).$$

IX. HIGHER ORDER TERMS

There remain terms of three types which must still be investigated:

(a) Second-order h.f.s. terms of the form

$$\delta_a\sim-\sum_n(H_p')_{0n}(H_p')_{n0}/E_n-E_0$$

which are of order $(e^2/\hbar c)^2m/M\log(e^2/\hbar c)m/M$ and hence negligible.

(b) Higher order corrections of H' on the h.f.s. of the form

$$\delta_b\sim\sum_{n,m}H_{0n}'H_{nm}'(H_p')_{m0}/(E_n-E_0)(E_m-E_0)$$

which are of order m/M, and

(c) Corrections of H'' on the h.f.s. of the form

$$\delta_c\sim-\sum H_{0m}''(H_P')_{m0}/E_p-E_0$$

which are also of order m/M. However, when the terms (b) and (c) are taken together they practically cancel, and the high energy difference which remains is of order $\hbar c/e^2(d/a_0)^2$ which is small enough to neglect.

X. RESULTS

We have found, in all, the following effects of the internal nuclear motion on the deuterium h.f.s.:

From the unperturbed wave function which Bohr chose as his starting point, the relative correction

$$\epsilon=-\mu_N d/\mu_D a_0(1.24\pm0.08) \quad (1)$$

and, due to a modification of this wave function, the relative correction

$$\epsilon_N=\mu_N d/\mu_D a_0[0.155(1+\xi t)\pm0.015],$$

where t is the fraction of exchange force and

$\xi=\frac{1}{4}$ for a Hulthen well,
$\xi=\frac{3}{10}$ for a square well.

One would expect t to be about $\frac{1}{2}$ (Serber) or $\frac{2}{3}$ (symmetric), and ξ to be about $\frac{1}{4}$ or $\frac{1}{3}$. We will choose ξt to be 0.16 for the purpose of assigning a number to our calculation; actually the difference between 0.16 and either of the two extremes that can be constructed using the above numbers is about 0.04 and negligible.

This gives

$$\epsilon_N=\mu_N d/\mu_D a_0(0.18\pm0.02). \quad (2)$$

From the absence of an orbital interaction inside the distance ρ the relative correction

$$\epsilon_L=\mu_N d/\mu_D a_0(0.05\pm0.02) \quad (3)$$

so that our final correction is

$$\epsilon+\epsilon_N+\epsilon_L=-\mu_N d/\mu_D a_0[1.01\pm0.12] =+(1.83\pm0.22)\times10^{-4}. \quad (4)$$

It is worth remarking that over 60 percent of the final uncertainty comes from the calculation of $\langle 2\alpha R\rangle_S$ in VI, so that an improved knowledge of the S state wave function alone would make a much more accurate theoretical determination of the deuterium h.f.s. possible.

It must also be emphasized that we were forced to choose $\sin^2\omega=0.04$ in order for our non-relativistic calculation to be self-consistent, although this number is in considerable doubt, and of course adds to our uncertainty.

Although our result is in fair agreement with the experimental effect, $(1.7\pm0.1)\times10^{-4}$, the present accuracy of theory and experiment is not sufficient to exclude some deviation of the nucleons themselves from simple dipoles. An effect of order

$$[1.83+0.22-(1.7-0.1)]\times10^{-4}=0.45\times10^{-4}$$

is in fact large enough to allow corrections due to a nucleon structure extending over distances of the order of the range of the nuclear forces.

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

$$K=\mu_D/\mu_P=0.3070126\pm0.0000021. \quad (5)$$

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

$$K=0.3070210\pm0.0000050 \quad (6)$$

and

$$K=0.3070183\pm0.0000015. \quad (7)$$

The result (7) is larger than (5) by about two parts in one hundred thousand, and would make the discrepancy (using Nafe and Nelson's determination of the h.f.s.) 1.5×10^{-4}, which would be hard to account for on the basis of this calculation alone.

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

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Numerical Value of the Lamb Shift

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

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

I

The formula for the Lamb shift of a hydrogen level n_0, l has been derived by many authors[2] and is for s states

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

and for states with $l\neq0$

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

where

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

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

This average energy is defined by[3]

$$\ln\frac{k_0(n_0,l)}{\mathrm{Ry}}\sum_n|(n_0 0|p_x|n)|^2(E_n-E_0) =\sum_n|(n_0 l|p_x|n)|^2(E_n-E_0)\ln\frac{E_n-E_0}{\mathrm{Ry}}, \quad (3)$$

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

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

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