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Relativistic Treatment of the Shielding of the Electron and Proton Magnetic Dipole Moments in Atomic Hydrogen†

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The Breit equation for two Dirac particles in an external magnetic field, with anomalous magnetic moments introduced phenomenologically as Pauli moments, is taken as the starting point for a Chraplyvy-Barker-Glover reduction. First-order perturbation theory employing the nonrelativistic wave function for the ^2S ground state is then used to derive expressions for the diagonal matrix elements of the Hamiltonian which depend linearly upon the field. These expressions are symmetric in the masses and anomalous moments of the particles and agree with previous results to relative order α^2. However, additional higher-order terms arise due to changes in the anomalous moments (in principle, obtainable from field theory), to reduced mass corrections, and to factorization of the moments as free-particle moments times shielding corrections. Contributions to the shielding expressions are interpreted as arising from (1) relativistic mass corrections, (2) spin-orbit coupling, and (3) spin-other-orbit coupling. In the case of atomic hydrogen the first two effects dominate the electron shielding and the latter dominates the proton shielding. Similar calculations and interpretations may be applied to magnetic shielding in larger atomic and molecular systems.

I. INTRODUCTION

Because of the relative ease of performing theoretical calculations as well as experimental measurements on the bound electron-proton system, the hydrogen atom has long provided a fruitful testing ground for physical theories. In addition, new concepts which have arisen from successful theoretical treatments of interactions in atomic hydrogen have found useful application in discussing similar interactions in larger atomic and molecular systems. New precision measurements[1,2] of the electron-proton g-factor ratio in atomic hydrogen in its ground electronic state have made it of interest to reinvestigate the theory behind these measurements, since the experimental precision will soon be beyond that of presently available theoretical calculations.[2]

Both the electron and the proton g factors are modified when the two particles become bound to form the hydrogen atom. Calculation of bound-state modifications to the electron g factor, based on the Dirac equation for the electron in a central Coulomb field and an external magnetic field, have been performed.[3] Similarly, the modification of the proton g factor to order α^2 (α is the fine-structure constant) is the well-known Lamb diamagnetic shielding correction.[4] The results of these calculations for the ^2S ground state are, to order α^2,

$$g_e(h) = 2(1 - \tfrac{1}{3}\alpha^2 Z^2),$$
$$g_p(h) = g_p(1 - \tfrac{1}{3}\alpha^2 Z), \tag{1}$$

where $g_e(h)$ and $g_p(h)$ are the electron and proton g factors for atomic hydrogen, g_p is the free proton g factor, and Z is the proton charge. These treatments may be extended[3,5] to higher order in α^2 (the next contributions, of order $\alpha^4 Z^4$ and $\alpha^4 Z^3$, are important for heavy atoms), but they then ignore important contributions discussed below. For example, it is commonly assumed that the Dirac result for the electron g factor $g_e = 2$ may be replaced in Eq. (1) by the more exact result obtained from quantum electrodynamics,[6]

$$g_e = 2[1 + \alpha/2\pi - 0.328\,\alpha^2/\pi^2 + O(\alpha^3)]. \tag{2}$$

This replacement is apparently a good approximation to order α^2, but not to order α^3, as is shown below. Furthermore, the above treatments neglect the effects of the motion of the proton, and they ignore the possibility of bound-state modifi-

cations to the "anomalous" magnetic moments obtained from quantum electrodynamics in the case of the electron and, in principle, from a more general field theoretic treatment in the case of the proton.

Therefore any treatment which hopes to obtain all the higher-order corrections to a given order beyond α^2 must employ a theory which considers all the corrections mentioned above. Although a rigorous treatment of the proton anomalous moment is difficult, it is possible to incorporate the experimental value of the free proton moment as a parameter in the theory, thus treating only bound-state corrections to this quantity. A reasonable starting point for a theoretical discussion of this problem is the Bethe-Salpeter equation.[7] The author is currently investigating a treatment of the problem employing this equation. However, the more approximate but simpler Breit equation[8] is chosen for an initial treatment presented here, since it is much less difficult to work with. Furthermore, since the Breit equation can be derived,[9-11] with certain approximations, from the Bethe-Salpeter equation, it is expected that the results of more refined future treatments can be presented in a form similar to that of the results obtained here. In fact, since Brodsky and Primack have shown[10] that, except for terms of relative order $(Z\alpha)^4 m_e/M_p$, the Breit equation gives the same results for the hydrogen Zeeman effect as does the Bethe-Salpeter equation, we can expect the results of our present treatment for any given order less than $(Z\alpha)^4 m_e/M_p$ to be correct if we introduce correct expressions (which will include bound-state modifications) for the anomalous moments into the Breit equation.

A word on terminology may be appropriate. Results obtained for the magnetic moment of a particle in a modifying environment are commonly factored into a free-particle value times a correction as in Eq. (1). In the case of the proton and other nuclei in atoms this is commonly called a "shielding" correction[12] implying that the nuclear moment is shielded in some sense by its environment, usually resulting in a decrease in magnitude of interaction with the applied field. This term is seldom used in the case of the electron. In this work the term shielding is used in the general sense of an environmental correction factor for both the electron and proton. Indeed, the results obtained here show clearly that when all contributing terms are included, the expressions for the electron and proton g factors are completely symmetrical and that therefore the correction factors may be given the same physical interpretation.

II. THEORY

Our starting point is the Breit equation[8] for two Dirac particles, with electric charges e_1 and e_2 and coordinates $\vec{r}_1$ and $\vec{r}_2$ in a uniform external magnetic field $\vec{H}$

$$[\mathcal{H}(1)+\mathcal{H}(2)+U(1,2)]\Psi(1,2)=E\Psi(1,2)\,, \tag{3}$$

where $\mathcal{H}(1)=c\vec{\alpha}_1\cdot\vec{\pi}_1+\beta_1 m_1c^2-a_1(h)(e_1\hbar/2m_1c)(\beta_1\vec{\sigma}_1\cdot\vec{H}_1-i\beta_1\vec{\alpha}_1\cdot\vec{E}_1)\,,$

$$\begin{aligned}\vec{\pi}_1&=\vec{p}_1-(e_1/c)\vec{A}_1,\\ \vec{A}_1&=\tfrac{1}{2}\vec{H}\times\vec{r}_1,\end{aligned} \tag{4}$$

(with similar terms for particle 2), and $a_1(h)$ is the anomalous part of the g factor for particle 1 in the bound system. For a free particle $g=2(1+a)$ as in Eq. (2); an h in parentheses distinguishes quantities which depend on the bound-state environment (hydrogen atom) from corresponding ones for the free particles. We have thus introduced the anomalous magnetic moments into the Breit equation phenomenologically as Pauli moments[13]; the validity of this procedure in the two-body case has been discussed by Breit and Meyerott.[14] The other terms appearing in Eqs. (3) and (4) are defined as follows: $U(1,2)$ is the Breit operator

$$U(1,2)=(e_1e_2/r)[1-(\vec{\alpha}_1\cdot\vec{\alpha}_2/2)-(\vec{\alpha}_1\cdot\vec{r}\,\vec{\alpha}_2\cdot\vec{r}/2r^2)]\,. \tag{5}$$

$\vec{H}_1$, $\vec{E}_1$, and $\vec{H}_2$, $\vec{E}_2$ are the magnetic and electric fields experienced by particles 1 and 2, respectively, which may be written[14]

$$\begin{aligned}\vec{H}_1&=\vec{H}+e_2\vec{\alpha}_2\times\vec{r}/r^3, \quad \vec{E}_1=e_2\vec{r}/r^3\,,\\ \vec{H}_2&=\vec{H}-e_1\vec{\alpha}_1\times\vec{r}/r^3, \quad \vec{E}_2=-e_1\vec{r}/r^3\,,\end{aligned} \tag{6}$$

$\vec{r}=\vec{r}_1-\vec{r}_2$, and the other quantities have their usual meanings.

In order to solve Eq. (3) for the wave function $\Psi(1,2)$ and energy E for the ^2S ground state, we first employ a Chraplyvy-Barker-Glover reduction,[15,16] which is essentially a Foldy-Wouthuysen transformation for two particles. Once this transformation has been performed, the lowest-order terms of the Hamiltonian matrix elements which define the g factors may be obtained quite simply from ordinary first-order

perturbation theory using the well-known Schrödinger solution for the unperturbed wave function. In addition, since the transformation is unitary, each term in the transformed Hamiltonian is Hermitian, and thus may be given a simple physical interpretation. Barker and Glover[16] have applied this transformation to the Breit equation for the case $\vec{H}=0$, and have obtained terms in the Hamiltonian corresponding to the rest masses, the Schrödinger Hamiltonian, relativistic mass corrections, spin-orbit, spin-other-orbit, orbit-orbit, Darwin, and spin-spin terms, plus higher-order terms. With $\vec{H}\neq 0$, additional terms are introduced corresponding to the electronic and nuclear Zeeman interactions. The terms of interest in the present case are those linear in H:

$$\mathcal{H}_1 = -\frac{e_1\hbar}{2m_1c}\{[1+a_1(h)]\vec{\sigma}_1\cdot\vec{H}+\vec{L}_1\cdot\vec{H}\}\left(1-\frac{p_1^2}{2m_1^2c^2}\right)-\frac{e_2\hbar}{2m_2c}\{[1+a_2(h)]\vec{\sigma}_2\cdot\vec{H}+\vec{L}_2\cdot\vec{H}\}\left(1-\frac{p_2^2}{2m_2^2c^2}\right),$$

$$\mathcal{H}_2 = -\frac{e_1e_2\hbar}{4m_1^2c^2}[1+2a_1(h)]\vec{\sigma}_1\cdot\frac{\vec{r}\times\vec{\pi}_1}{r^3}+\frac{e_1e_2\hbar}{4m_2^2c^2}[1+2a_2(h)]\vec{\sigma}_2\cdot\frac{\vec{r}\times\vec{\pi}_2}{r^3}, \tag{7}$$

$$\mathcal{H}_3 = \frac{e_1e_2\hbar}{2m_1m_2c^2}[1+a_1(h)]\vec{\sigma}_1\cdot\frac{\vec{r}\times\vec{\pi}_2}{r^3}-\frac{e_1e_2\hbar}{2m_1m_2c^2}[1+a_2(h)]\vec{\sigma}_2\cdot\frac{\vec{r}\times\vec{\pi}_1}{r^3}.$$

These terms are familiar and have the following interpretation.[17] The term $\mathcal{H}_1$ represents the direct interaction of the particle spins with the field times a factor which has the appearance of a relativistic mass correction. The second term $\mathcal{H}_2$ represents the spin-orbit interactions for each particle,[18] but with the canonical momentum $\vec{p}$ replaced by the mechanical momentum $\vec{\pi}$. Likewise, $\mathcal{H}_3$ clearly represents the spin-other-orbit interactions. These are the lowest-order terms contributing to the g factors,[19] and the only ones that will be considered here. Additional terms are of order α^4 or higher. Also, it is apparent that similar terms will appear in the treatment of larger atomic and molecular systems, and thus similar interpretations will apply to these systems.

III. CALCULATION, RESULTS, AND DISCUSSION

In order to calculate the g factors, we transform the total relativistic Hamiltonian to relative and center-of-mass coordinates, choosing the center of mass to be stationary. We then choose the leading term

$$\mathcal{H}_0 = [(m_1+m_2)/2m_1m_2]p^2+e_1e_2/r, \tag{8}$$

as the zero-order Hamiltonian for a perturbation treatment. In the case of the hydrogen atom, the familiar ground-state solution to this Schrödinger Hamiltonian (8) may be written

$$\Psi_0(1,2) = (\pi)^{-\frac{1}{2}}(Z/a_0')^{\frac{3}{2}}\exp[-(Z/a_0')r]\chi^{m_S}(1)\chi^{m_I}(2) \tag{9}$$

for charges $e_1=-e$, $e_2=Ze$, and masses $m_1=m$, $m_2=M$. The scaled Bohr radius is

$$a_0' = [(M+m)/Mm]\hbar^2/e^2, \tag{10}$$

and χ^{m_S} and χ^{m_I} are spin functions satisfying the equations

$$\sigma_z^e\chi^{m_S} = 2m_S\chi^{m_S},$$
$$\sigma_z^p\chi^{m_I} = 2m_I\chi^{m_I}. \tag{11}$$

Using first-order perturbation theory, we find for the diagonal Hamiltonian matrix elements linear in the magnetic field H

$$\Delta E_e = 2[1+a_e(h)]\mu_0Hm_S\left[1-\tfrac{1}{2}\alpha^2Z^2\left(\frac{M}{M+m}\right)^2+\tfrac{1}{6}\alpha^2Z^2\left(\frac{M}{M+m}\right)^2\frac{1+2a_e(h)}{1+a_e(h)}-\tfrac{1}{3}\alpha^2Z^3\left(\frac{m}{M+m}\right)^2\right],$$
$$-\Delta E_p = 2[1+a_p(h)]Z\mu_nHm_I\left[1-\tfrac{1}{2}\alpha^2Z^2\left(\frac{m}{M+m}\right)^2+\tfrac{1}{6}\alpha^2Z^2\left(\frac{m}{M+m}\right)^2\frac{1+2a_p(h)}{1+a_p(h)}-\tfrac{1}{3}\alpha^2Z\left(\frac{M}{M+m}\right)^2\right], \tag{12}$$

where $\mu_0=e\hbar/2mc$, $\mu_n=e\hbar/2Mc$ are the Bohr and nuclear magnetons, respectively. It should be noted that these expressions, which define the g factors, are completely symmetrical in the masses and anom-

alous moments of the two particles. Each expression consists of four contributing terms arising from Eqs. (7). The first term corresponds to the usual lowest-order Zeeman effect, the second to a relativistic mass correction, the third to a spin-orbit correction, and the fourth to a spin-other-orbit correction. Also, the relative magnitudes of m and M determine which terms are most important. For example, if we set $a_e(h) = a_e = \alpha/2\pi - 0.328\,\alpha^2/\pi^2$, $a_p(h) = a_p$, and retain only terms up to order α^2, we recover Eqs. (1) for the g factors with the Dirac result $g_e = 2$ replaced by the quantum electrodynamic result [Eq. (2)] for the free electron. Whereas the relativistic mass correction and the spin-orbit coupling term combine to give the correction in the case of the electron, the spin-other-orbit term is the only contributor to this order in the case of the proton. It is interesting to note that the two corrections turn out to be equal.

The above expressions (12), which apply to the ^2S ground state of atomic hydrogen, are correct to (at least) relative order α^2. It can be easily shown that no off-diagonal contributions occur to this order, and that the next contributions are of relative order α^4. However, Eqs. (12) also contain three types of contributions of higher order than α^2 (but lower than α^4). The first of these involves reduced mass corrections, primarily of order $\alpha^2 m/M$. A second type of contribution arises because the spin-orbit terms have factors involving the anomalous moments. This introduces a correction of order $\alpha^3 Z^2$ for the electron, for example. A third type is due to changes of the anomalous moments from their free-particle values. Such a correction has been calculated for the electron[20] to be $-(26/15\pi)\alpha^3 Z^2$. Additional corrections[21] to the transformed Hamiltonian, due to the motion of the center of mass, appear when an external electric field is present but do not contribute in the present case. Nuclear polarization effects[22] are expected to be of order $\alpha^4(m/M)^3$ here, and therefore they are ignored.

Now, if we write the bound-state corrections to the anomalous magnetic moments in the form of a small additive correction to each free-particle moment

$$a(h) = a + \delta\,, \tag{13}$$

then Eqs. (12) give the following expressions for the two g factors:

$$g_e(h) = g_e\left[1 - \tfrac{1}{3}\alpha^2 Z^2\left(\frac{M}{M+m}\right)^2 + \frac{1}{12\pi}\alpha^3 Z^2\left(\frac{M}{M+m}\right)^2 + \delta_e\right],$$

$$g_p(h) = g_p\left[1 - \tfrac{1}{3}\alpha^2 Z\left(\frac{M}{M+m}\right)^2 + \delta_p\right], \tag{14}$$

which are good to orders α^3 and $\alpha^2 m/M$ if δ_e and δ_p are of order α^2 or higher. The g-factor ratio for $Z = 1$ is then given by the expression

$$\frac{g_e(h)}{g_p(h)} = \frac{g_e}{g_p}\left[1 + \frac{1}{12\pi}\alpha^3\left(\frac{M}{M+m}\right)^2 + \delta_e\right](1 - \delta_p)\,. \tag{15}$$

If we can now find values δ_e and δ_p for the bound-state corrections to the anomalous moments of the electron and proton which are correct to order α^3, we can then calculate a numerical correction to the above g-factor ratio to that order. Since there is no way of calculating δ_e and δ_p within the formalism of the Breit equation, one must employ a field theoretic treatment of the hydrogen atom in an external magnetic field. Fortunately, such a treatment has been performed by Lieb,[20] who finds for the electron $\delta_e = -(26/15\pi)\alpha^3 Z^2$. However, since Lieb's result is obtained by approximating the proton as a fixed Coulomb source, possible additional reduced mass and nuclear recoil corrections to δ_e should also be investigated. Thus, as a first approximation, we recalculate δ_e from Lieb's Eq. (11),[20] after replacing the electron mass m by the reduced mass $mM/(m+M)$ in the nonrelativistic hydrogenic wave function. We find, in addition to the original α^3 term, corrections of order $\alpha^3 m/M$ clearly negligible. Also, it is difficult to imagine additional Feynman diagrams which would contribute corrections of order $\alpha m/M$ to δ_e, although contributions of order $\alpha^2 m/M$, which are of somewhat higher order than α^3, may be possible. Thus Lieb's result appears to be correct to order α^3. Similarly, applying the Lieb treatment to the proton in hydrogen, we find bound-state corrections to the proton anomalous moment of order $\alpha^3 Z^2 m/M$ and higher. Although this treatment neglects the strong interactions, it seems unlikely that strong interactions are responsible for *changes* in the proton anomalous moment to the order we are considering. Thus, it appears that $\delta_p = 0$ to order α^3.

If we substitute the values $\delta_e = -(26/15\pi)\alpha^3$, $\delta_p = 0$ in Eq. (15), we obtain, to order α^3,

$$g_e(h)/g_p(h) = (g_e/g_p)[1 - (99/60\pi)\alpha^3] = (g_e/g_p)(1 - 2.04\times10^{-7})\,. \tag{16}$$

For reasons discussed above, it appears likely that Eq. (16) is correct to order α^3. Even so, the author is currently reinvestigating corrections to orders α^3 and higher by means of a full field theoretic treat-

ment of the two-body problem.

The ratio $g_e(h)/g_p(h)$ has been measured with a fractional uncertainty of 3×10^{-7}, and experiments are being performed to even greater precision.[1,2] Thus, correction terms of orders α^3 and $\alpha^2 m/M$ will be important. On the other hand, if experiments on the free proton g factor reach a precision comparable to that of the free electron experiments,[23] a direct experimental test of these theoretical results may be possible.

IV. SUMMARY

It has been shown that shielding corrections to the electron and proton magnetic dipole moments for the ground state of atomic hydrogen may be obtained in a very straight forward and simple manner from the Breit equation. These corrections agree with previous theoretical results to order α^2, and give higher-order terms which are within the range of present experiments. In addition, a utilization of the Chraplyvy-Barker-Glover transformation has made it possible to give each of these correction terms a simple physical interpretation, according to which the shielding of both electron and proton arise from the same three effects: relativistic variation of mass, spin-orbit coupling, and spin-other-orbit coupling. To lowest order, the first two effects are unimportant for the proton, the latter effect is unimportant for the electron. However, for particles of equal or nearly equal masses, all three effects are important for each particle. The theory may be extended, in principle, to excited states and to larger atomic and molecular systems, where similar results and physical interpretations apply. In particular, the usual diamagnetic shielding of nuclei in atoms and molecules emerges naturally from the term in the transformed Hamiltonian which describes the coupling of the spin of the nucleus with the orbital motion of the electrons in the presence of a magnetic field.

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[18]This includes the Thomas precession factor. It is interesting to note that the Dirac part of the moment is modified by the $\frac{1}{2}$ factor, whereas the Pauli part is not. There is a good reason why this is true, which can be seen by considering the classical expression for the energy including the kinematic Thomas precession $\mathcal{H}=-\gamma_1\vec{S}_1\cdot(\vec{H}-\vec{v}_1\times\vec{E}_1/c)-\vec{S}_1\cdot\vec{\omega}_T$, where γ is the gyromagnetic ratio and ω_T is the Thomas precession frequency. If we write $\gamma_1=\gamma_{1,\mathrm{Dirac}}+\gamma_{1,\mathrm{Pauli}}=e_1/m_1c+a_1e_1/m_1c$ and substitute this into the above expression, we find that since $\vec{\omega}_T=(\vec{v}_1\times\vec{a}_1)/2c^2=(e_1/2m_1c^2)\vec{v}_1\times\vec{E}_1$,

the Thomas precession term cancels exactly half of the Dirac moment term in the $\vec{v}_1 \times \vec{E}_1$ expression while leaving alone the Pauli term, resulting in the expression for $\mathcal{H}_2$ in Eq. (7).

[19]Of course, the terms involving the canonical momentum $\vec{p}$ do not contribute here to the field-dependent energy, but are included in $\mathcal{H}_2$ and $\mathcal{H}_3$ to emphasize the interpretation of these terms as spin-orbit and spin-orbit interactions. In the case of molecules, however, terms involving $\vec{p}$ contribute due to the departure from spherical symmetry (see Ref. 12).

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X-Ray Yields in the K and L Series of Low-Z Muonic Atoms

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Experiments are reported which remove the discrepancies between the earlier observed K and L x-ray yields from low-Z muonic atoms and those calculated from theory. We have made direct measurements of the K/L yield ratios for targets of $4 \leq Z \leq 8$ and a determination of the absolute K x-ray yield for $Z=3$. They agree excellently with the calculated values.

I. INTRODUCTION

A long standing discrepancy in the field of muonic x rays was the anomalously low yield of x rays with energies below approximately 100 keV.[1,2] In muonic atoms, this corresponds to $Z < 8$ for μ-K x rays and $Z < 15$ for μ-L x rays. Because of the low energies of these x rays, the pulses produced in the sodium-iodide detectors used in the experiments would necessarily be small, and could give rise to electronic inefficiencies in the coincidence circuits which might produce such effects. Realizing this, the investigators took many precautions to greatly amplify the low-energy pulses and tested for experimental inefficiencies by using low-energy γ rays from radioactive sources. These tests indicated that no apparent inefficiencies were introduced which might cause coincidence losses due to time jitters resulting from clipping the sodium-iodide pulses or inappropriate discriminator settings. However, the yields given in Ref. 2 were somewhat higher than those given in Ref. 1, although both were considerably lower than the calculated yields.

When a new type of fast discriminator was developed which used the crossover point of an amplifier pulse rather than the front end of the pulse to generate a coincidence pulse, we decided to repeat the yield measurements for low Z materials.[3] Using this new apparatus we found *no* discrepancy between theory[4] and experiment. Furthermore, the experimental ratios of the higher transition yields (i.e., K_β to K_∞) can be compared to theory and they favor an initial capture distribution which is more strongly peaked than the $2l+1$ distribution.

EXPERIMENTAL PROCEDURE

The experiment was performed with the muon beam from the Chicago cyclotron. The experimental arrangement is essentially the same as in Refs. 1 and 2 except for the coincidence instrumentation and the refinement of the detection apparatus. The pulse from the sodium-iodide crystal was amplified by a Model-101 nonoverload linear amplifier and sent into a Model-501 fast discriminator which generated a fast coincidence