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## ELECTRON $g$ FACTOR IN HYDROGENIC ATOMS

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The electron  $g$  factor is calculated to a high degree of accuracy for the ground state of hydrogenic atoms. In addition to binding corrections of order  $(Z\alpha)^2$ ,  $(Z\alpha)^2 m/M$ , and  $(Z\alpha)^2 (m/M)^2$ , radiative level shifts of order  $\alpha(Z\alpha)^2$  and  $\alpha(Z\alpha)^2 m/M$  are obtained.

These level shifts differ from those previously given in the literature. The origin of the discrepancies is discussed in some detail.

Experiments are currently being carried out by several groups to measure, with high precision, ratios of electron  $g$  factors for various hydrogenic atoms in the ground state.<sup>1</sup> It is therefore important to clarify the theoretical predictions and to take properly into account the radiative level shifts.

Hegstrom<sup>2</sup> has recently obtained an expression for the electron  $g$  factor through the use of a Chraplyvy-Barker-Glover expansion of a two-body Breit Hamiltonian, which contains an interaction of the system with a small constant magnetic field, and which also includes phenomenological Pauli interactions.<sup>3,4</sup> In the work reported here the  $g$  factor is calculated by a different method, using wave functions recently given by Brodsky and Primack.<sup>5</sup> The results of order  $(Z\alpha)^2$ ,  $(Z\alpha)^2 m/M$ , and  $(Z\alpha)^2 (m/M)^2$  agree with those of Hegstrom and also with experiment. However, the corrections of order  $\alpha(Z\alpha)^2$  and  $\alpha(Z\alpha)^2 m/M$ , which arise from radiative effects, differ from those given in Ref. 2 and also differ from some early work done by Lieb.<sup>6</sup> The origin of these discrepancies is discussed below.

The computational aspects of the work reported here are rather involved. Therefore only the essentials will be discussed and the details will be incorporated in a more extensive article on

the subject.

For simplicity we consider the hydrogen atom. Since nuclear spin considerations are unimportant in determining the electron  $g$  factor, the results obtained here are valid for all hydrogenic atoms. In the center-of-mass frame the Hamiltonian in the absence of a magnetic field is

$$H_0 = \vec{\alpha}_e \cdot \vec{p} + \beta_e m - \vec{\alpha}_p \cdot \vec{p} + \beta_p M - \frac{Z\alpha}{r} + \left( \frac{Z\alpha}{2r} \right) \left( \vec{\alpha}_e \cdot \vec{\alpha}_p + \frac{\vec{\alpha}_e \cdot \vec{r} \vec{\alpha}_p \cdot \vec{r}}{r^2} \right), \quad (1)$$

where subscripts  $e$  or  $p$  denote electron or proton variables. For hydrogen  $Z$  is unity, but since our results will be valid for  $Z \neq 1$  we keep  $Z$  arbitrary in Eq. (1). If a magnetic field is present, perturbations arise. Their effects may be calculated using ordinary perturbation theory. For this purpose, it is sufficient to use approximate eigenfunctions of  $H_0$ , suitably extended to a moving frame of reference.

Brodsky and Primack<sup>5</sup> have given such wave functions. It should be pointed out that they are solutions of a Hamiltonian which does not include the last term of Eq. (1) (the Breit interaction). However, for our purposes such wave functions are accurate enough. Ignoring the nuclear-spin

dependence of the wave function, we find that

$$\psi(\vec{r}, \vec{X}) = N \int \frac{d^3K}{(2\pi)^{3/2}} \left[ 1 + \frac{\vec{\alpha}_e \cdot \vec{K}}{2(m+M)} - \frac{\vec{K} \cdot \vec{p}}{4M^2} \right] \times \varphi(\vec{r}) f(\vec{K}) e^{i\vec{K} \cdot \vec{x}} \quad (2)$$

may be chosen as the unperturbed wave function, where  $f(\vec{K})$  is used to make an arbitrary packet.  $\varphi(\vec{r})$  is the center-of-mass wave function. The large components are  $\varphi_0(\vec{r})\chi_e$  and the small components are

$$\{2m - [M/(m+M)](V - \epsilon)\}^{-1} \vec{\sigma}_e \cdot \vec{p} \varphi_0(\vec{r}) \chi_e,$$

where  $\chi_e$  is a two-component electron spinor and  $\varphi_0(\vec{r})$  is a normalized solution of

$$(\vec{p}^2/2m_r + V)\varphi_0(\vec{r}) = \epsilon \varphi_0(\vec{r}), \quad (3)$$

where  $m_r$  is the reduced mass.  $N$  is a normalization constant given by

$$N = 1 - \frac{1}{4}(Z\alpha)^2 [M/(m+M)]^2.$$

If the atom is placed in a small constant magnetic field, perturbations arise which contribute to the Zeeman interaction of the electron. We have interactions

$$V_1 = -\frac{1}{2}e \vec{\alpha}_e \cdot \vec{H} \times \vec{x}_e,$$

and

$$V_2 = \frac{Z^2\alpha e}{4M\mathcal{r}} \left[ \vec{\alpha}_e \cdot \vec{H} \times \vec{x}_p + \frac{\vec{\alpha}_e \cdot \vec{r}(\vec{r} \cdot \vec{H} \times \vec{x}_p)}{r^2} \right], \quad (4)$$

where

$$\vec{x}_e = \vec{X} + [M/(m+M)]\vec{r}$$

and

$$\vec{x}_p = \vec{X} - [m/(m+M)]\vec{r}.$$

The contributions of both of these terms to the energy are obtained through first-order perturbation theory, using Eq. (2) as the unperturbed wave function. The results are expressed in terms of powers of  $Z\alpha$  and  $m/M$ .

We obtain (retaining only spin-dependent terms)

$$\Delta E_1 = \langle V_1 \rangle = -\frac{e}{2m} \langle \vec{\sigma}_e \cdot \vec{H} \rangle \times \left[ 1 - \frac{1}{3}(Z\alpha)^2 \left( 1 - \frac{2m}{M} + \frac{3m^2}{M^2} \right) \right],$$

and

$$\Delta E_2 = \langle V_2 \rangle = -\frac{e}{2m} \langle \vec{\sigma}_e \cdot \vec{H} \rangle \left[ -\frac{1}{3}Z(Z\alpha)^2 \frac{2m^2}{M^2} \right]. \quad (5)$$

Corrections to Eq. (5) are of order  $(Z\alpha)^4$  and higher.

In addition to  $\Delta E_1$  and  $\Delta E_2$  there are corrections which arise from radiative processes. The lowest-order radiative corrections are of two types: (a) self-energy corrections which arise from modifications of the bound-electron propagator; (b) vacuum-polarization corrections which stem from modifications of the proton propagator. A general formalism for handling such radiative level shifts has been developed by Brodsky and Erickson.<sup>7</sup> For the case of a constant magnetic field, we obtain a contribution of zero (to the desired accuracy) from the vacuum-polarization term. This differs from the result obtained by Lieb<sup>6</sup> many years ago.<sup>8</sup>

As discussed in Ref. 7 the contributions to (A) above are numerous. However, to order  $\alpha(Z\alpha)^2m/M$  we only need to consider

$$\Delta E(M) = \frac{\alpha}{2\pi} \left( -\frac{e}{2m} \right) \langle \beta_e \vec{\sigma}_e \cdot \vec{H} - i\vec{\gamma}_e \cdot \vec{E} \rangle. \quad (6)$$

In other words, only the expectation value of the Pauli interaction is needed.

The  $\beta_e \vec{\sigma}_e \cdot \vec{H}$  term in  $\Delta E(M)$  receives contributions from coupling large-large and small-small components of the wave function. Evaluating this term to order  $\alpha(Z\alpha)^2m/M$  we obtain

$$\frac{\alpha}{2\pi} \left( -\frac{e}{2m} \right) \langle \vec{\sigma}_e \cdot \vec{H} \rangle \left[ 1 - \frac{1}{8}(Z\alpha)^2 \left( 1 - \frac{2m}{M} \right) \right]. \quad (7)$$

The  $\vec{\gamma}_e \cdot \vec{E}$  term in  $\Delta E(M)$  also gives a contribution since it couples large and small components of the wave function. The small components are modified by the introduction of a magnetic field, and this modification is needed in calculating the effect of radiative corrections.<sup>9</sup> For this term we obtain a correction

$$\frac{\alpha}{2\pi} \left( -\frac{e}{2m} \right) \langle \vec{\sigma}_e \cdot \vec{H} \rangle \left[ \frac{1}{3}(Z\alpha)^2 \left( 1 - \frac{2m}{M} \right) \right]. \quad (8)$$

Adding Eqs. (7) and (8) we obtain

$$\Delta E(M) = \frac{\alpha}{2\pi} \left( -\frac{e}{2m} \right) \langle \vec{\sigma}_e \cdot \vec{H} \rangle \times \left[ 1 + \frac{1}{8}(Z\alpha)^2 \left( 1 - \frac{2m}{M} \right) \right]. \quad (9)$$

If we now combine Eqs. (5) and (9) and factor

out  $1 + \alpha/2\pi$  we obtain

$$\Delta E = -\frac{e}{2m} \left(1 + \frac{\alpha}{2\pi}\right) \langle \vec{\sigma}_e \cdot \vec{H} \rangle \left[ 1 - \frac{1}{3}(Z\alpha)^2 \left(1 - \frac{2m}{M} + \frac{3m^2}{M^2}\right) - \frac{1}{3}Z(Z\alpha)^2 \frac{m^2}{M^2} + \frac{\alpha}{4\pi}(Z\alpha)^2 \left(1 - \frac{2m}{M}\right) \right]. \quad (10)$$

Extraneous terms, all of which are of higher order than the expressions considered in this paper, have been introduced in Eq. (10) in order to conveniently factor the free-electron  $g$  factor.

The free-electron  $g$  factor is known to order  $\alpha^2$ . There are, of course, binding corrections to higher-order radiative corrections. However, we expect that these binding corrections will bring in additional powers of  $(Z\alpha)^2$ . Therefore inclusion of higher-order radiative corrections may be accomplished by replacing the  $1 + \alpha/2\pi$  in Eq. (10) by  $g_e/2$  where  $g_e$  denotes the free-electron  $g$  factor. The electron  $g$  factor in the ground state (1S) is therefore

$$g(1S) = g_e \left[ 1 - \frac{1}{3}(Z\alpha)^2 \left(1 - \frac{2m}{M} + \frac{3m^2}{M^2}\right) - \frac{1}{3}Z(Z\alpha)^2 \frac{m^2}{M^2} + \frac{\alpha}{4\pi}(Z\alpha)^2 \left(1 - \frac{2m}{M}\right) \right]. \quad (11)$$

Equation (11) is not in agreement with Eq. (14) of Ref. 2. Instead of the term  $(\alpha/4\pi)(Z\alpha)^2(1-2m/M)$ , Hegstrom has  $(\alpha/12\pi)(Z\alpha)^2(1-2m/M) + \delta_e$ , where  $\delta_e = -(26/15\pi)\alpha(Z\alpha)^2$  is the result of Ref. 6.<sup>10</sup>

The first difference between our results is clearly algebraic. To check this we have done a Foldy-Wouthuysen expansion<sup>4</sup> of Hegstrom's Hamiltonian in the limit as  $M$  tends to infinity. For S states we find

$$\mathcal{K}_1 = -\frac{e}{2m} \vec{\sigma}_e \cdot \vec{H} \left(1 - \frac{\vec{p}^2}{2m^2}\right) - \frac{e}{2m} a_1(h) \vec{\sigma}_e \cdot \vec{H} + \frac{e}{2m} a_1(h) \frac{1}{2m^2} \vec{\sigma}_e \cdot \vec{p} \vec{p} \cdot \vec{H}, \quad (12)$$

as opposed to that given in Ref. 2 [Eq. (7)]. We may replace  $\vec{\sigma}_e \cdot \vec{p} \vec{p} \cdot \vec{H}$  by  $\frac{1}{3}\vec{p}^2 \vec{\sigma}_e \cdot \vec{H}$  to obtain

$$\mathcal{K}_1 = -\frac{e}{2m} \vec{\sigma}_e \cdot \vec{H} \left(1 - \frac{\vec{p}^2}{2m^2}\right) - \frac{e}{2m} a_1(h) \vec{\sigma}_e \cdot \vec{H} \left(1 - \frac{p^2}{6m^2}\right). \quad (13)$$

The difference between  $\mathcal{K}_1$  as given by Eq. (13) and  $\mathcal{K}_1$  of Eq. (7) in Hegstrom's article is

$$\Delta \mathcal{K}_1 = -(e/2m) a_1(h) \vec{\sigma}_e \cdot \vec{H} (\vec{p}^2/3m^2).$$

Hence

$$\langle \Delta \mathcal{K}_1 \rangle = -(e/2m) \langle \vec{\sigma}_e \cdot \vec{H} \rangle [\alpha(Z\alpha)^2/6\pi]. \quad (14)$$

If this correction term is added to the  $\alpha(Z\alpha)^2/12\pi$  term of Hegstrom, the number  $\alpha(Z\alpha)^2/4\pi$  emerges, as already obtained in Eq. (11) through the present approach.

The second difference concerns the addition of  $\delta_e$ . It would appear that adding  $-(26/15\pi)\alpha(Z\alpha)^2$  to the anomalous moment  $\alpha/2\pi$  leads to double counting. The reason is that this correction term is supposedly the complete  $\alpha(Z\alpha)^2$  correction due to radiative shifts [i.e., the sum of terms of type (A) and (B) as discussed above]. However, introduction into the formalism of the Pauli interaction [as contained in Eq. (3) of Ref. 2] with the  $\alpha/2\pi$  coefficient already includes all significant contributions of the type (A) previously referred to. Therefore electron self-energy corrections should not be counted again. Vacuum-polarization contributions should be included and may be incorporated in  $\delta_e$ . However, as discussed in footnote 8, these should be zero. Therefore the complete result, including lowest-

order radiative corrections, is given by Eq. (11) above.

The conclusions of this paper [e.g., Eq. (11)] are presently in agreement with Hegstrom's most recent results.<sup>11</sup> Experiments done so far are in agreement with Eq. (11). Hughes and Robinson have measured the ratio of the  $g$  factor in hydrogen to that in deuterium. They obtain

$$g(\text{H})/g(\text{D}) = 1 + (7.2 \pm 3.0) \times 10^{-9}.$$

Larson, Valberg, and Ramsey have also measured the same ratio and have obtained

$$g(\text{H})/g(\text{D}) = 1 + (9.4 \pm 1.4) \times 10^{-9}.$$

From Eq. (11) we find the theoretical value to be

$$g(\text{H})/g(\text{D}) = 1 + 9.7 \times 10^{-9} - 1.6 \times 10^{-11} - 1.7 \times 10^{-11}. \quad (15)$$

The second, third, and fourth numbers in this expression are, respectively, the terms of order  $\alpha^2 m/M$ ,  $\alpha^2 (m/M)^2$ , and  $\alpha^3 m/M$ .

The experiments mentioned above are not precise enough to measure the smallest terms of Eq. (15) and therefore they do not check the radiative corrections given in this paper. One way of measuring the coefficient of the  $\alpha(Z\alpha)^2$  term

in Eq. (11) would be to measure the ratio of  $g$  factors for two atoms with different  $Z$ . For example a measurement of the hydrogen-to-helium (singly ionized) ratio to one part in  $10^8$  would determine the coefficient to about 10%.

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<sup>1</sup>W. M. Hughes and H. G. Robinson, Phys. Rev. Letters **23**, 1209 (1969); D. J. Larson, P. A. Valberg, and N. F. Ramsey, Phys. Rev. Letters **23**, 1369 (1969).

<sup>2</sup>R. A. Hegstrom, Phys. Rev. **184**, 17 (1969).

<sup>3</sup>Z. V. Chraplyvy, Phys. Rev. **91**, 388 (1953), and **92**, 1310 (1953); W. A. Barker and F. N. Glover, Phys. Rev. **99**, 317 (1955).

<sup>4</sup>The expansion referred to is essentially a two-body generalization of the Foldy-Wouthuysen expansion for a single particle. See L. L. Foldy and S. A. Wouthuysen, Phys. Rev. **78**, 29 (1950).

<sup>5</sup>S. J. Brodsky and J. R. Primack, Ann. Phys. (N.Y.) **52**, 315 (1969).

<sup>6</sup>E. H. Lieb, Phil. Mag. **46**, 311 (1955).

<sup>7</sup>S. J. Brodsky and G. W. Erickson, Phys. Rev. **148**, 26 (1966).

<sup>8</sup>According to Brodsky and Erickson (Ref. 7) [Eqs.

(C1) and (C2)] and earlier work on p. 882 of N. M. Kroll and F. Pollock, Phys. Rev. **86**, 876 (1952), the vacuum-polarization contribution is

$$\frac{\alpha}{2\pi} \left\langle \beta \vec{q}^2 \int_0^1 dv \frac{2v^2(1-v^2/3)}{4m^2 + \vec{q}^2(1-v^2)} \vec{\gamma} \cdot \vec{A}(\vec{q}) \right\rangle.$$

For a constant magnetic field,  $\vec{A}(\vec{q}) \sim \vec{H} \times \nabla_q \delta^3(\vec{q})$ . Because of the presence of  $\vec{q}^2$  in the numerator, terms involving  $\vec{A}(\vec{q})$  give zero. The magnetic field dependence arising from the  $A_0(\vec{q})$  term turns out to contribute to order  $\alpha(Z\alpha)^4$ . Lieb has used a different Coulomb gauge in which  $A_i(\vec{q}) \sim H\delta(q_x)\delta'(q_y)\delta(q_z)\delta_{i1}$ . However, it is readily seen that the above result will also be zero for this choice as well. We believe that Lieb obtained a nonzero result [(4/15 $\pi$ ) $\alpha(Z\alpha)^2$ ] by using Eq. (40) of Kroll and Pollock instead of the above expression. Equation (40) of the aforementioned work is an approximation which is valid for the purpose of calculating  $\alpha(Z\alpha)$  corrections to the hyperfine splitting, but is not accurate enough for obtaining  $\alpha(Z\alpha)^2$  corrections to the Zeeman effect.

<sup>9</sup>The large components are essentially unaffected. There is, however, a normalization correction linear in the magnetic field, but it does not affect the calculations done here.

<sup>10</sup>The  $-(26/15\pi)\alpha(Z\alpha)^2$  term gives the binding correction from lowest-order radiative corrections, as calculated by Lieb. It is clear that there is a discrepancy between this number and the result of our Eq. (9), which represents the complete radiative correction as calculated here. We have discussed the origin of part of this discrepancy in footnote 8. Our results also disagree with those of Lieb for terms of type (A) discussed above (i.e., vertex corrections).

<sup>11</sup>R. A. Hegstrom, Phys. Rev. (Erratum, to be published).

## ENERGY SPECTRA OF ELECTRONS FROM AUTOIONIZATION STATES IN HELIUM BY ELECTRON IMPACT

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Energy spectra of electrons ejected from autoionization states in helium excited by electron impact have been measured at bombarding energies from 65 to 250 eV as a function of the angle to the primary electron beam.

The height of peaks of the energy spectra due to optically forbidden transitions from the ground state compared with those due to optically allowed transitions increases as the impact energy is reduced; this trend was most marked for the triplet-state ( $2s2p$ )<sup>3P</sup> excitation.

Certain autoionizing states of helium have been observed by optical absorption,<sup>1</sup> by electron energy-loss measurements of forward-scattered electrons,<sup>2-4</sup> and by energy-spectra measurements of ejected electrons from states excited by ion impact.<sup>5,6</sup> In this paper we show part of

the observations on these states by the measurements of the energy spectra of electrons ejected after bombardment with electrons as a function of the impact energy as well as of the ejected angle.<sup>7</sup> Mehlhorn<sup>8</sup> has previously observed autoionization of helium by this electron-impact