Nuclear-Mass and Anomalous-Moment Corrections to the Hamiltonian for an Atom in a Constant External Magnetic Field

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The Hamiltonian for a many-particle system in a homogeneous magnetic field is constructed by a straightforward extension of previous work on hydrogenic atoms by Grotch and Hegstrom. Relativistic-correction terms of order $\alpha^2\mu_B H$ are identical to those obtained many years ago by Abragam and Van Vleck and by Perl and Hughes. In addition, higher-order terms due to the anomalous moments and to nuclear motion are explicitly formulated in the present work. These terms are of orders $\alpha^3\mu_B H$ and $\alpha^2(m/M)\mu_B H$, respectively, and are coming to be within the range of present experimental measurements.

I. INTRODUCTION

Increasing precision in the measurement of the Zeeman effect in atoms[1] has led to a revived interest in the theory of the interaction of atomic systems with external electromagnetic fields. The theory of the interaction of hydrogenic atoms with a constant magnetic field has been discussed in detail recently by Grotch and Hegstrom.[2] The purpose of this paper is to extend the latter work to include many-electron systems, and thus to refine the earlier[3] theoretical treatments of the Zeeman effect for these systems. There is presently a need for such a refinement, since workers are now measuring atomic g factors with a precision of one part in 10^7 and higher.[1,4]

An atom is treated as a system of Dirac particles with anomalous magnetic moments. The system is governed by a generalized Breit equation (Sec. II). The anomalous moments, which arise owing to virtual radiative processes, are introduced via the Pauli interaction.[5] In Sec. III, the part of the wave function which depends on the usual center-of-mass (c.m.) coordinate is found explicitly for a neutral atom. This separation leads to a Hamiltonian which depends only on the internal coordinates and greatly simplifies the calculation of the higher-order corrections. A similar simplification occurs for ions, although the Hamiltonian for an ion must contain terms which depend on the c.m. coordinate. For both cases, the simplifield Hamiltonian is reduced to nonrelativistic form plus relativistic and magnetic terms (Sec. IV). Writing the Hamiltonian in this final form makes it suitable for perturbative calculation of the magnetic corrections employing the usual nonrelativistic wave functions.

II. EXTENDED BREIT FORMALISM

The desirable starting point for a treatment of higher-order corrections is, of course, the fully covariant quantum field theory. However, the corresponding calculations are much more difficult than those presented here. The starting point for the present work is the Breit equation[6] extended to include the anomalous-moment interactions. In the case of hydrogenic atoms, this simpler formalism has been shown[7] to lead to the same results for the magnetic-field-dependent energy as those obtained from the fully covariant theory, except for terms of order $\alpha^4(m/m_a)\mu_B H$, where α is the fine-structure constant, m is the electron mass, m_a is the nuclear mass, μ_B is the Bohr magneton, and H is the magnetic field strength. We expect that the Breit formalism also describes the Zeeman effect accurately for a many-electron atom [including corrections of orders $\alpha^3\mu_B H$ and $\alpha^2(m/m_a)\mu_B H$ considered here], but proof must await either comparison with a covariant field-theoretic treatment for the many-particle case, or (ultimately, in any case) comparison with precise experimental measurements.

Without further justification, then, I adopt as a starting point the extended Breit equation

$$\mathcal{H}\Psi(\vec{r}_1, \vec{r}_2, \ldots) = E\Psi(\vec{r}_1, \vec{r}_2, \ldots), \tag{1}$$

where, in natural units ($\hbar = c = 1$),

$$\begin{aligned}
&\mathcal{H} = \sum_i \mathcal{H}(i) + \sum_{i<j} U(i,j),\\
&\mathcal{H}(i) = \vec{\alpha}_i \cdot \vec{\pi}_i + \beta_i m_i - \kappa_i(\beta_i \vec{\sigma}_i \cdot \vec{\mathrm{H}}_i - i\beta_i \vec{\alpha}_i \cdot \vec{\mathrm{E}}_i),\\
&U(i,j) = e_i e_j r_{ij}^{-1}\left(1 - \frac{\vec{\alpha}_i \cdot \vec{\alpha}_j}{2} - \frac{\vec{\alpha}_i \cdot \vec{r}_{ij}\,\vec{\alpha}_j \cdot \vec{r}_{ij}}{2r_{ij}^2}\right)\\
&\qquad + \beta_i \beta_j \kappa_i \kappa_j\left(\frac{\vec{\sigma}_i \cdot \vec{\sigma}_j}{r_{ij}^3} - \frac{3\vec{\sigma}_i \cdot \vec{r}_{ij}\,\vec{\sigma}_j \cdot \vec{r}_{ij}}{r_{ij}^5}\right.\\
&\qquad\qquad \left. - (\tfrac{8}{3}\pi)\vec{\sigma}_i \cdot \vec{\sigma}_j \delta^3(\vec{r}_{ij})\right),
\end{aligned} \tag{2}$$

$$\vec{\pi}_i = \vec{\mathrm{p}}_i - e_i \vec{\mathrm{A}}_i,$$

$$\vec{\mathrm{A}} = \vec{\mathrm{H}} \times \tfrac{1}{2}\vec{r}_i,$$

$$\vec{\mathrm{H}}_i = \vec{\mathrm{H}} + \sum_{j\neq i} e_j \vec{\alpha}_j \times \vec{r}_{ij}/r_{ij}^3,$$

$$\vec{E}_i = \sum_{j\neq i} e_j \vec{r}_{ij}/r_{ij}^3 .$$

In the above equations $\vec{\pi}_i$ is the mechanical momentum for the ith particle, $\vec{A}_i$ is the magnetic vector potential at position $\vec{r}_i$ in the laboratory frame, $\vec{H}$ is the constant external magnetic field, $\vec{H}_i$ and $\vec{E}_i$ are the magnetic and electric fields experienced by particle i, and other symbols have their usual definitions. The anomalous magnetic moments κ_i, which arise from virtual radiative processes, are

$$\kappa_e = -(e/2m_e)(\alpha/2\pi - 0.328\alpha^2/\pi^2 + \cdots) ,$$

$$\kappa_p = 1.793\,(e/2m_p) ,$$

$$\kappa_n = -1.913\,(e/2m_p)$$

for the electron, proton, and neutron, where α is the fine-structure constant.

Not included in the above Hamiltonian are additional perturbations which also arise from virtual radiative processes and, for example, provide contributions to the Lamb shift in atomic hydrogen[8,9] and helium[10] and to the helium fine structure.[10] These additional radiative effects also give rise to magnetic-field-dependent terms[9] of order $\alpha^3\mu_B H$. Except for S states, for which they vanish,[11] these terms must be evaluated for each particular atomic state and added to the results from the Breit equation in order to obtain final results complete to order $\alpha^3\mu_B H$. These corrections appear to be quite difficult to calculate and are discussed further in Appendix A. We now proceed to a simplification of the extended Breit equation.

III. SEPARATION OF c.m. COORDINATE

The first simplification is the elimination of the dependence on the c.m. coordinate, as was done for the two-particle case.[2] The method was apparently first used by Lamb[12]; here I present a slightly different formulation of Lamb's method. I use conventional definitions[13] of the c.m. coordinate $\vec{R}$ and the internal coordinates $\vec{r}_{ia}$:

$$\vec{R} = \sum_i (m_i/M)\vec{r}_i ,$$
$$\vec{r}_{ia} = \vec{r}_i - \vec{r}_a \qquad (i\neq a) . \tag{3}$$

The corresponding conjugate momenta are

$$\vec{P} = \sum_i \vec{p}_i ,$$
$$\vec{p}_{ia} = \vec{p}_i - (m_i/M)\sum_j \vec{p}_j \qquad (i\neq a) . \tag{4}$$

Here $M = \sum m_i$ is the sum of the rest masses of the particles. The subscript a refers to any specific particle, but the most natural choice is the nucleus. The inverse relations to Eqs. (3) and (4) are

$$\begin{aligned}
\vec{r}_a &= \vec{R} - \sum_{j\neq a} (m_j/M)\vec{r}_{ja} ,\\
\vec{r}_i &= \vec{R} + \vec{r}_{ia} - \sum_{j\neq a} (m_j/M)\vec{r}_{ja} \qquad (i\neq a) ,\\
\vec{p}_a &= (m_a/M)\vec{P} - \sum_{j\neq a} \vec{p}_{ja} ,\\
\vec{p}_i &= (m_i/M)\vec{P} + \vec{p}_{ia} \qquad (i\neq a) .
\end{aligned} \tag{5}$$

Note also that $\vec{r}_{ij}$ depends only on internal coordinates:

$$\vec{r}_{ij} = \vec{r}_i - \vec{r}_j = \vec{r}_{ia} - \vec{r}_{ja} . \tag{6}$$

I next define

$$\vec{q} \equiv \sum_i \vec{q}_i \equiv \sum_i (\vec{p}_i + e_i\vec{A}_i) = \vec{P} + \sum_i e_i\vec{A}_i , \tag{7}$$

where q is the $\vec{\pi}$ used in Ref. 2. In classical mechanics the variable corresponding to $\vec{q}$ is a constant of the motion.[2] One expects that $\vec{q}$ may also be a constant of the motion in the quantum-mechanical case. That this is indeed so is shown by computing

$$[\mathcal{H}, \vec{q}] = \sum_i [\mathcal{H}(i), \vec{q}] + \sum_{i<j} [U(i,j), \vec{q}] . \tag{8}$$

The first summation in Eq. (8) is zero, since it reduces to

$$\sum_i \sum_j [\vec{\alpha}_i\cdot\vec{\pi}_i, \vec{q}_j] = \sum_i \sum_j \{e_j[\vec{\alpha}_i\cdot\vec{p}_i, \vec{A}_j] - e_i[\vec{\alpha}_i\cdot\vec{A}_i, \vec{p}_j]\} = 0 . \tag{9}$$

Each term in the second summation is also zero, since $U(i,j)$ depends only on the internal coordinates. Thus $\vec{q}$ commutes with the Hamiltonian and is a constant of the motion.

We next evaluate the commutators

$$[q_r, q_s] = \sum_i \sum_j [q_{ir}, q_{js}] = -i\epsilon_{rst} H_t \sum_i e_i . \tag{10}$$

If the total charge of the system $\sum_i e_i$ is zero, the components of $\vec{q}$ commute. In that case $\mathcal{H}$ and the components of $\vec{q}$ form a set of mutually commuting operators, and the wave function can be chosen to be a simultaneous eigenfunction of these operators:

$$\begin{aligned}
\mathcal{H}\Psi &= E\Psi ,\\
\vec{q}\Psi &= \vec{K}\Psi ,
\end{aligned} \tag{11}$$

where the eigenvalue $\vec{K}$ is a constant vector. The latter equation may be rewritten

$$-i\nabla_{\vec{R}}\Psi = \left(\vec{K} - \sum_i e_i\vec{A}_i\right)\Psi \equiv \vec{\Pi}\Psi . \tag{12}$$

It can be easily shown (see Appendix B) that, for a neutral system, $\sum_i e_i\vec{A}_i$ is independent of $\vec{R}$. Thus, Eq. (12) may be easily solved for Ψ:

$$\Psi(\vec{R}, \vec{r}_{1a}, \vec{r}_{2a}\cdots) = \psi(\vec{r}_{1a}, \vec{r}_{2a}\cdots)\, e^{i\vec{\Pi}\cdot\vec{R}} . \tag{13}$$

By allowing $\mathcal{H}$ [Eq. (2)] to operate on Eq. (13), a corresponding equation for ψ is obtained. It has the form

$$\mathcal{H}'\psi = E\psi \,, \tag{14}$$

where $\mathcal{H}'$ has exactly the same form as $\mathcal{H}$, but with the mechanical momentum $\vec{\pi}_a$ of a particle a replaced by

$$\vec{p}_a - \sum_{i\neq a} e_i \vec{A}_{ia} \,, \tag{15}$$

and with the mechanical momenta $\vec{\pi}_i$ of the other particles ($i \neq a$) replaced by

$$\vec{p}_i - e_i \vec{A}_{ia} \,, \tag{16}$$

where

$$\begin{aligned} \vec{p}_a &= (m_a/M)\vec{K} - \sum_{j\neq a} \vec{p}_{ja} \,, \\ \vec{p}_i &= (m_i/M)\vec{K} + \vec{p}_{ia} \,, \\ \vec{A}_{ia} &= \vec{H}\times\tfrac{1}{2}\vec{r}_{ia} \,. \end{aligned} \tag{17}$$

The transformed Breit equation, Eq. (14), thus depends only on internal coordinates.

This procedure of finding the simultaneous eigenfunctions of $\mathcal{H}$ and $\vec{q}$ is similar to a gauge transformation, and is equivalent to a unitary transformation of the original Breit equation, Eq. (1). In fact, a system with nonvanishing total electric charge may be treated similarly by making the unitary transformation[2]

$$\begin{aligned} \Psi &= U\Psi' \,, \\ \mathcal{H}' &= U^{-1}\mathcal{H}U \,, \\ U &= \exp\left(-i\sum e_i \vec{A}_i \cdot \vec{R}\right). \end{aligned} \tag{18}$$

Then the mechanical momentum of each particle transforms into

$$\begin{aligned} &\vec{\pi}_i' \equiv U^{-1}\vec{\pi}_i U = \vec{p}_i - e_i[\vec{A}_i - \vec{A}(\vec{R})] - (m_i/M)\sum_j e_j \vec{A}_j \,, \\ &\vec{A}(\vec{R}) = \vec{H}\times\tfrac{1}{2}\vec{R} \,, \end{aligned} \tag{19}$$

where $\vec{p}_i$ is given by Eq. (5). In Ref. 2 it is shown that, even though the unitary transformation does not eliminate the c. m. coordinate from the Hamiltonian of a system with nonzero total charge, it does greatly reduce the contribution of $\vec{R}$ to the energy. Also note that Eq. (19) reduces to Eqs. (15) and (16) for a neutral system.

The importance of a careful treatment of the c.m. coordinate has been discussed previously.[2] In particular, setting $\vec{R}$ and $\vec{P}$ equal to zero (unless the unitary transformation is first performed) leads to the omission of contributions to the Zeeman energy of order $\alpha^2(m_e/M)\mu_B H$.

IV. REDUCTION TO NONRELATIVISTIC FORM

The second simplification of the extended Breit equation, Eq. (1), is its reduction to a nonrelativistic form (the Schrödinger equation) plus relativistic and magnetic terms. In one way this is not really a simplification, since numerous terms are generated in the reduced Hamiltonian. For practical computations, however, the reduced form is desirable, since nonrelativistic atomic wave functions [approximate eigenfunctions of $\mathcal{H}_0$ in Eq. (21) below] are relatively easy to obtain. Furthermore, the magnetic and relativistic terms in the reduced Hamiltonian are usually quite small compared to $\mathcal{H}_0$ and thus can be treated perturbatively using nonrelativistic zero-order wave functions.

The Hamiltonian of Eq. (14) is transformed to nonrelativistic form using the methods of Chraplyvy[14] and Barker and Glover[14] as was done for the two-particle case.[2] Dropping the prime in Eq. (19) so that in Eqs. (21) below

$$\vec{\pi}_i \equiv \vec{p}_i - e_i[\vec{A}_i - \vec{A}(\vec{R})] - (m_i/M)\sum_j e_j \vec{A}_j \,, \tag{20}$$

one obtains for the reduced Hamiltonian

$$\begin{aligned} \mathcal{H} &= \sum_i m_i + \sum_{n=0}^{7} \mathcal{H}_n \,, \\ \mathcal{H}_0 &= \sum_i (\pi_i^2/2m_i) + \sum_{i<j} (e_i e_j/r_{ij}) \,, \\ \mathcal{H}_1 &= -\sum_i (\pi_i^4/8m_i^3) \,, \\ \mathcal{H}_2 &= -\sum_i \sum_{j\neq i} (\pi e_j/m_i)(g_i\mu_{0i} - e_i/2m_i)\delta^3(\vec{r}_{ij}) \,, \\ \mathcal{H}_3 &= -\sum_i \sum_{j\neq i} (e_j/m_i)(g_i\mu_{0i} - e_i/2m_i) r_{ij}^{-3} \vec{S}_i \cdot \vec{r}_{ij}\times\vec{\pi}_i \,, \\ \mathcal{H}_4 &= \sum_i \sum_{j\neq i} (e_j/m_j) g_i \mu_{0i} r_{ij}^{-3} \vec{S}_i \cdot \vec{r}_{ij}\times\vec{\pi}_j \,, \\ \mathcal{H}_5 &= -\sum_i g_i\mu_{0i}\vec{S}_i\cdot\vec{H}(1-\pi_i^2/2m_i^2) - \sum_i (g_i\mu_{0i} - e_i/m_i) \\ &\qquad \times (1/2m_i^2)\vec{S}_i\cdot(\pi_i^2\vec{1} - \vec{\pi}_i\vec{\pi}_i)\cdot\vec{H} \,, \\ \mathcal{H}_6 &= -\sum_{i<j} (e_i e_j/2m_i m_j)[r_{ij}^{-1}\vec{\pi}_i\cdot\vec{\pi}_j \\ &\qquad + \vec{r}_{ij}(r_{ij}^{-3}\vec{r}_{ij}\cdot\vec{\pi}_i)\cdot\vec{\pi}_j] \,, \\ \mathcal{H}_7 &= -\sum_{i<j} g_i\mu_{0i} g_j\mu_{0j}[(\tfrac{8}{3}\pi)\vec{S}_i\cdot\vec{S}_j\,\delta^3(\vec{r}_{ij}) \\ &\qquad + r_{ij}^{-5}(\vec{S}_i\cdot\vec{r}_{ij}\vec{S}_j\cdot\vec{r}_{ij} - \vec{S}_i\cdot\vec{S}_j r_{ij}^2)] \,, \end{aligned} \tag{21}$$

where

$$g_i\mu_{0i} = 2(e_i/2m_i + \kappa_i) \tag{22}$$

defines the g factor of particle i; μ_{0i} is taken to be the Bohr magneton $(e/2m_e)$ for electrons or the nu-

clear magneton ($e/2m_p$) for nuclei; $\vec{S}_i$ is the appropriate spin operator for particle i. Strictly speaking, the above result applies only to spin-$\frac{1}{2}$ particles, and thus excludes nuclei which do not have $S=\frac{1}{2}$. However, Bethe and Salpeter[15] have examined this and concluded that the Dirac theory for nuclei with $S\neq\frac{1}{2}$ gives correct results at least to order m_a^{-1}, where m_a is the nuclear mass, provided the observed nuclear magnetic moment and spin are substituted for the corresponding Dirac values in the Hamiltonian. This procedure can be followed for the nuclear-spin terms in Eq. (21).

Each of the terms appearing in the reduced Hamiltonian has a simple physical interpretation, and it seems appropriate to review them here. $\mathcal{H}_0$ is the nonrelativistic Schrödinger Hamiltonian, $\mathcal{H}_1$ is a relativistic correction to the kinetic energy, $\mathcal{H}_2$ is the Darwin term due to the *Zitterbewegung* of the particles, $\mathcal{H}_3$ describes the spin-orbit coupling, $\mathcal{H}_4$ describes the spin-other-orbit coupling, $\mathcal{H}_5$ describes the coupling of the spins to the external field (plus relativistic-mass corrections), $\mathcal{H}_6$ describes orbit-orbit coupling, and $\mathcal{H}_7$ describes the spin-spin coupling. Higher-order terms, which are important only for very heavy atoms, are neglected here. It is interesting to note that in $\mathcal{H}_2$, $\mathcal{H}_3$, and $\mathcal{H}_5$ the anomalous part of each magnetic moment behaves differently from the Dirac part. This means that for very accurate work (in order $\alpha^3\mu_0 H$) the radiative corrections to the magnetic moments cannot be accounted for simply by replacing, in the nonrelativistic Hamiltonian, the Dirac g factor $g=2$ with the experimental value.

The usual magnetic properties may be calculated from Eq. (21). For example, the lowest-order diamagnetic susceptibility is calculated from the magnetic part of $\mathcal{H}_0$, and the nuclear magnetic shielding of NMR spectroscopy from $\mathcal{H}_4$. The lowest-order contributions to atomic magnetic moments come from $\mathcal{H}_5$ and (for non-S states) $\mathcal{H}_0$, and higher-order corrections are obtained from $\mathcal{H}_3$, $\mathcal{H}_4$, and $\mathcal{H}_5$, and (for non-S states) $\mathcal{H}_1$ and $\mathcal{H}_6$.

For the purposes of calculation, it is convenient to expand the Hamiltonian in terms of internal and (if the system is charged) c. m. coordinates. For a neutral atom, for example, $\mathcal{H}_0$ becomes

$$\mathcal{H}_0=\frac{\vec{K}^2}{2M}+\frac{1}{2\mu}\sum_i \vec{p}_{ia}^{\,2}-\sum_i\frac{Ze^2}{r_{ia}}+\sum_{i<j}\frac{e^2}{r_{ij}}$$
$$+\frac{1}{2m_a}\sum_i\sum_{j\neq i}\vec{p}_{ia}\cdot\vec{p}_{ja}+\frac{e}{M}\vec{K}\times\vec{H}\cdot\sum_i\vec{r}_{ia}$$
$$+\frac{e}{m_e}\left(1-\frac{m_e}{m_a}\right)\sum_i\vec{A}_{ia}\cdot\vec{p}_{ia}-\frac{e}{m_a}\sum_i\sum_{j\neq i}\vec{A}_{ia}\cdot\vec{p}_{ja}$$
$$+\frac{e^2}{2\mu}\sum_i\vec{A}_{ia}^{\,2}+\frac{e^2}{2m_a}\sum_i\sum_{j\neq i}\vec{A}_{ia}\cdot\vec{A}_{ja}\,, \qquad (23)$$

where a denotes the nucleus, μ is the reduced mass $m_e m_a/(m_e+m_a)$, and the summations are over electrons. Note that Eq. (23) contains nuclear-mass corrections to the Zeeman energy (for non-S states) of order $(m/M)\mu_B H$ obtained by Phillips many years ago.[16]

The magnetic-field-dependent part of the reduced Hamiltonian, except for the definition of $\vec{\pi}_i$ and the appearance of anomalous-moment terms, is identical to that of the early treatments.[3] Thus, for the calculation of atomic magnetic moments, for example, the present treatment will give the same results as the older treatments to order α^2. However, additional corrections of order $\alpha^2 m_e/M$ and α^3 can be calculated from Eq. (21). Experimental methods are now capable of measuring these small corrections.[1,4]

Finally, although the present treatment finds its most immediate application to the Zeeman effect in electronic atoms, we note that the results should also be applicable more generally, for example, to muonic atoms or even to molecules. To emphasize this generality I have employed a symmetric notation in Eq. (21).

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APPENDIX A

The magnetic field dependence of the radiative terms discussed in Sec. II is contained in the energy shift for the nth level,

$$\Delta E_n=\frac{2\alpha}{3\pi m^2}\int_0^\infty\frac{dk}{1+2k/m}$$
$$\times{\sum_{n'}}'\frac{\langle n'|\sum_i\vec{\pi}_i|n'\rangle\cdot\langle n'|\sum_i\vec{\pi}_i|n\rangle\,(E_{n'}-E_n)}{k+E_{n'}-E_n}\,, \qquad (A1)$$

which arises from self-energy and single transverse photon exchange in a nonrelativistic perturbative treatment. Here the $\vec{\pi}_i=\vec{p}_i-e\vec{A}_i$ are summed over the electrons in the atom, and $|n\rangle$ and E_n are the eigenfunctions and eigenvalues of the usual nonrelativistic Hamiltonian

$$\mathcal{H}_{\rm NR}=(1/2m)\sum_i p_i^{\,2}+V+\mu_B\vec{H}\cdot\sum_i(\vec{L}_i+2\vec{S}_i)$$
$$\equiv\mathcal{H}_{\rm NR}^{(0)}+\mathcal{H}_{\rm mag}\,. \qquad (A2)$$

I now outline a proof, due to Grotch[11] and generalized here to the many-electron case, that the magnetic field dependence of ΔE_n vanishes for S states in order $\alpha^3\mu_B H$. This magnetic field dependence may arise from two sources: (a) the magnetic field dependence of the operators $\vec{\pi}_i$ and (b) the magnetic field dependence of the energies $E_{n'}$. Considering first terms of type (a), employ

commutator identities such as

$$\left\langle n'\left|\sum_i \vec{p}_i\right|n\right\rangle (E_{n'}-E_n)=iZ\alpha\left\langle n'\left|\sum_i\left(\frac{\vec{r}_i}{r_i^3}\right)\right|n\right\rangle \tag{A3}$$

to write $\Delta E_n^{(a)}$ as

$$\Delta E_n^{(a)}=-\frac{iZ\alpha^2 e}{\pi m^2}\vec{H}\cdot\int_0^\infty \frac{dk}{1+2k/m} \times{\sum_{n'}}' \frac{\langle n|\sum_i \vec{r}_i|n'\rangle\times\langle n'|\sum_i(\vec{r}_i/r_i^3)|n\rangle}{k+E_{n'}-E_n}. \tag{A4}$$

Then, choosing $\vec{H}$ to be in the z direction and defining

$$T_{\pm1}^{(1)}=\mp\sum_i \frac{x_i\pm iy_i}{\sqrt{2}},$$

$$Q_{\pm1}^{(1)}=\mp\sum_i \frac{x_i\pm iy_i}{r_i^3\sqrt{2}}, \tag{A5}$$

one obtains

$$\Delta E_n^{(a)}=-\frac{\alpha^2 ZeH}{\pi m^2}\int_0^\infty \frac{dk}{1+2k/m}{\sum_{n'}}'(k+E_{n'}-E_n)^{-1} \times(\langle n|T_1^{(1)}|n'\rangle\langle n|Q_1^{(1)}|n'\rangle^* -\langle n|T_{-1}^{(1)}|n'\rangle\langle n|Q_{-1}^{(1)}|n'\rangle^*). \tag{A6}$$

Now $T^{(1)}$ and $Q^{(1)}$ are irreducible tensor operators whose matrix elements may be evaluated using the Wigner–Eckart theorem. In an L-S coupling scheme one obtains

$$\Delta E_{nLM_L}^{(a)}=-\frac{\alpha^2 ZeH}{\pi m^2}\int_0^\infty \frac{dk}{1+2k/m}\sum_{n'L'M_L'}(k+E_{n'L'}-E_{nL})^{-1}\langle nL||T^{(1)}||n'L'\rangle\langle nL||Q^{(1)}||n'L'\rangle^* \times\left\{\begin{pmatrix} L & 1 & L' \\ -M_L & 1 & M_L'\end{pmatrix}^2-\begin{pmatrix} L & 1 & L' \\ -M_L & -1 & M_L'\end{pmatrix}^2\right\}. \tag{A7}$$

For an S state, $L=M_L=0$, $L'=1$, and the difference of squares of the 3-j symbols vanishes. Thus, $\Delta E_{n00}^{(a)}=0$ in order $\alpha^3\mu_B H$.

Now consider contributions of type (b). In this case, $\Delta E_n^{(b)}$ is

$$\Delta E_n^{(b)}=\frac{2\alpha}{3\pi m^2}\int_0^\infty \frac{dk}{1+2k/m} \times{\sum_{n'}}' \frac{\langle n|\sum_i \vec{p}_i|n'\rangle\cdot\langle n'|\sum_i \vec{p}_i|n\rangle(E_{n'}-E_n)}{k+E_{n'}-E_n}. \tag{A8}$$

Denoting the magnetic-field-dependent part of E_n by ϵ_n so that $E_n=E_n^{(0)}+\epsilon_n$, and expanding the energy denominator of Eq. (A8) in powers of H, we obtain for the term linear in H

$$\Delta E_n^{(b)}=-\frac{2\alpha}{3\pi m^2}\int_0^\infty dk \times{\sum_{n'}}' \frac{\langle n|\sum_i \vec{p}_i|n'\rangle\cdot\langle n'|\sum_i \vec{p}_i|n\rangle(E_{n'}^{(0)}-E_n^{(0)})(\epsilon_{n'}-\epsilon_n)}{(k+E_{n'}^{(0)}-E_n^{(0)})^2}. \tag{A9}$$

Performing the k integration, one obtains

$$\Delta E_n^{(b)}=-\frac{2\alpha}{3\pi m^2}{\sum_{n'}}'\langle n|\sum_i \vec{p}_i|n'\rangle\cdot\langle n'|\sum_i \vec{p}_i|n\rangle(\epsilon_{n'}-\epsilon_n). \tag{A10}$$

Then evaluate

$$\langle n'|\sum_i \vec{p}_i|n\rangle(\epsilon_{n'}-\epsilon_n)=\left\langle n'\left|\left[\mathcal{H}_{\rm mag},\sum_i \vec{p}_i\right]\right|n\right\rangle =(ie/2m)\left\langle n'\left|\vec{H}\times\sum_i \vec{p}_i\right|n\right\rangle \tag{A11}$$

and use closure to finally obtain

$$\Delta E_n^{(b)}=-(i\alpha e/3\pi m^3)\vec{H}\cdot\left\langle n\left|\sum_i \vec{p}_i\times\sum_i \vec{p}_i\right|n\right\rangle=0. \tag{A12}$$

Therefore, $\Delta E_n^{(b)}=0$ in order $\alpha^3\mu_B H$ for all states in general, and for S states in particular.

APPENDIX B

I show that, for a neutral system, the sum

$$\sum_i e_i\vec{A}_i$$

is independent of $\vec{R}$. Using the definition of $\vec{A}_i$ and Eq. (5), the above summation becomes (note that $\vec{r}_{aa}=\vec{A}_{aa}=0$ in the following equations)

$$\sum_i e_i\tfrac{1}{2}\vec{H}\times\left[\vec{R}+\vec{r}_{ia}-\sum_{j\neq i}\left(\frac{m_j}{M}\right)\vec{r}_{ja}\right] =\left(\sum_i e_i\right)\vec{A}(\vec{R})+\sum_i e_i\vec{A}_{ia}-\left(\sum_i e_i\right)\sum_{j\neq i}\left(\frac{m_j}{M}\right)\vec{A}_{ja}.$$

If the sum of charges is zero, we have

$$\sum_i e_i\vec{A}_i=\sum_i e_i\vec{A}_{ia}.$$

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Linear Polarization of Low-Energy-Electron Bremsstrahlung*

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The linear polarization of bremsstrahlung from thin targets ($\sim 50\ \mu g/cm^2$) of Al, Cu, Ag, and Au was measured for incident electron energies of 50, 75, and 100 keV. The polarization was measured as a function of photon energy at four emission angles ($\theta = 22.5°$, 45°, 90°, and 135°). Data presented were obtained with a Compton polarimeter having a large asymmetry ratio (from 35 to 150) and high resolution. The results have been found to be in general agreement with the predictions of various bremsstrahlung calculations.

I. INTRODUCTION

Bremsstrahlung exhibits linear polarization. Several calculations[1-4] of the polarization of electron bremsstrahlung have been carried out since the original nonrelativistic theory of Sommerfeld[5] was published. The most recent work is the relativistic calculation by Tseng and Pratt,[6] which covers the incident electron energy range of 5 keV to 1 MeV. Most calculations have been for single electron interactions and must be compared to experimental results obtained using very thin targets. Most measurements of linear polarization at low energies have been made using relatively thick targets.[7-18] Furthermore, when thin targets were employed, quantitative data were obtained only in limited spectral regions because x-ray detectors of relatively poor resolution were used.[19-26]

For bremsstrahlung, the linear polarization P is defined by the expression

$$P(T_0, k, \theta, Z) = \frac{I_\perp(T_0, k, \theta, Z) - I_\parallel(T_0, k, \theta, Z)}{I_\perp + I_\parallel}\ , \tag{1}$$

where $I_\perp$ is the bremsstrahlung intensity component with polarization perpendicular to the reaction plane (the plane containing the direction vectors of both the incident electron and the photon), and $I_\parallel$ is the bremsstrahlung intensity component with polarization parallel to the reaction plane. $I_\perp$, $I_\parallel$, and, therefore, P are functions of electron energy T_0, photon energy k, emission angle θ, and target atomic number Z.

This paper reports measurement of the linear polarization of low-energy bremsstrahlung as a function of k for (a) incident electron energies of 50, 75, and 100 keV, (b) emission angles of 22.5°, 45°, 90°, and 135°, and (c) target atomic numbers of 13, 29, 47, and 79. The measurements were obtained using thin solid targets and a high-resolution Compton polarimeter.

II. EXPERIMENTAL

Apparatus

Part of the experimental arrangement is shown schematically in Fig. 1. The electron beam from a 150-kV accelerator was momentum analyzed and focused to a 5-mm-diam spot on target. The target chamber was a hollow right-circular cylinder of Al, 15 cm long and 10 cm in diam. A 2.54-cm-high Be x-ray port 47 mg/cm^2 thick, subtended