Hamiltonian of a many-electron atom in an external magnetic field and classical electrodynamics
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Résumé. — La précision croissante des expériences concernant l'effet Zeeman des atomes à plusieurs électrons nécessite une connaissance toujours plus approfondie des effets relativistes et radiatifs. L'extension de l'équation de Breit proposée par Hegstrom permet de rendre compte de ces effets jusqu'à l'ordre $1/c^3$ ; à la limite non relativiste, le hamiltonien trouvé est d'une grande complexité. Nous montrons dans cet article qu'il est possible de rendre compte — dans le cadre de l'électrodynamique classique — de la quasi-totalité de ses termes. Il apparaît ainsi que l'équation de Breit et son extension traduisent en fait essentiellement l'existence de deux phénomènes physiques simples et bien connus : i) l'interaction du moment magnétique de chaque particule avec le champ qu'elle subit dans son référentiel propre, ii) la précession de Thomas des spins des particules accélérées.

Abstract. — The increasing precision of experiments on the Zeeman effect of many electron atoms requires an ever increasing knowledge of relativistic and radiative effects. The generalization of the Breit equation as proposed by Hegstrom includes all these effects up to order $c^{-3}$. In the non relativistic limit the resulting Hamiltonian is quite intricate, but we show in this paper that it is possible to explain almost all of its terms within the frame of classical electrodynamics. In particular, picturing the atoms as point-like particles with intrinsic magnetic moments, we show that the physical phenomena underlying the Breit equation and its recent extension are mainly two well-known classical phenomena : i) the interaction of the magnetic moment of the constituent particles with the magnetic field they experience in their rest frame ; ii) the Thomas precession of the spins of the accelerated particles.

1. Introduction. — Increasing precision in the measurement of the Zeeman effect of atoms [1] has led to a revived interest in the theory of atomic systems interacting with external electromagnetic fields. In particular, the experimental accuracy of atomic $g$ factors requires an ever increasing knowledge of relativistic, radiative and nuclear-mass corrections in an external magnetic field. In the absence of a development from the fully covariant quantum field theory, we must use the generalized Breit equation including anomalous moment interactions, as first proposed by Hegstrom [2]. This generalized Hamiltonian, expected to be exact up to order $c^{-3}$, displays a rather striking feature : the anomalous part and the Dirac part of the magnetic moment do not seem to play a similar role, thus impeding a clear-cut interpretation of the various correcting terms. It happens however that the Hegstrom Hamiltonian can be understood with the help of classical electrodynamics and special relativity, and it is the object of this paper to show that the generalized Breit equation is mainly a consequence of two phenomena : the Thomas precession [3] of the spin of accelerated particles and the interaction of the magnetic moment of each particle with the magnetic field it experiences in its rest-frame.

The generalized Breit equation as proposed by Hegstrom is presented in section 2. Section 3 deals with the problem of the spin dynamics, and in particular with the relativistic definition of the spin, the Thomas precession, and the Hamiltonian suitable for a satisfying representation of the spin motion. In section 4, we collect these results, with the well known Darwin Hamiltonian for particles without spin. We determine the various electromagnetic fields acting on charges and magnetic moments and we obtain the Hamiltonian describing a many-electron atom, including all terms up to order $c^{-3}$. Except
for the Zitterbewegung term, the resulting Hamiltonian is the same as that deduced from the generalized Breit equation. We then discuss the physical origin of all the terms appearing in this Hamiltonian.

2. The generalized Breit equation in constant external magnetic field. — Within the formalism proposed by Hegstrom [2], the atom is considered as a system of Dirac particles with anomalous magnetic moments. Its evolution is governed by a generalized Breit equation and the corresponding Hamiltonian can be written as:

\[ \mathcal{H} = \sum_i \mathcal{K}_i + \sum_{i<j} U(i,j) \]  

(2.1)

where:

\[ \mathcal{K}_i = c^2 \beta_i m_i c^2 - \kappa_i \beta_i \sigma_i \cdot H_i - i \beta_i \sigma_i \cdot E_i, \]

and

\[ U(i,j) = e_i e_j r_{ij}^{-1} \left( 1 - \frac{\sigma_i \cdot \sigma_j}{2} - \frac{3 \sigma_i \cdot \sigma_j (\sigma_i \cdot r_{ij})}{2 r_{ij}^3} \right) + \]

\[ + \beta_i \beta_j \kappa_i \kappa_j c^{-2} \left( \frac{\sigma_i \cdot \sigma_j r_{ij}^3}{r_{ij}^5} - 3 \sigma_i \cdot \sigma_j (\sigma_i \cdot r_{ij}) + 3 \beta_i \beta_j \kappa_i \kappa_j c^{-2} \right) \]

Finally, \(\kappa_i\) is the anomalous part of the magnetic moment of the particle due to virtual radiative processes \(^{(1)}\) (the explicit value for electrons is given in refs. [4] and [5]).

For various reasons (and in particular because the only good wave functions we know are non-relativistic), it is desirable to reduce equation (2.1) to its non-relativistic limit. The result is [2]:

\[ \mathcal{H} = \sum_i m_i c^2 + \sum_{a=0}^7 \mathcal{K}_a \]

\[ \mathcal{K}_0 = \sum_i \frac{\pi_i^2}{2 m_i} + \sum_{i<j} \frac{e_i e_j}{r_{ij}} \]

\[ \mathcal{K}_1 = - \sum_i \frac{\pi_i^4}{8 m_i^3 c^2} \]

\[ \mathcal{K}_2 = - \sum_i \frac{\pi_i^4 e_i}{m_i c^2} (g_i - 1) \mu_0 \delta^3(r_{ij}) \]

\[ \mathcal{K}_3 = - \sum_{i<j} \frac{e_i e_j}{2 m_i m_j c^2} \left[ r_{ij}^{-1} \pi_i \cdot \pi_j + r_{ij}^{-3} (\pi_i \cdot r_{ij}) (\pi_j \cdot r_{ij}) \right] \]

\[ \mathcal{K}_4 = - \sum_i \frac{e_j}{m_j c^2} (g_i - 1) \mu_0 r_{ij}^{-3} s_i \cdot (r_{ij} \wedge \pi_i) \]

\[ \mathcal{K}_5 = \sum_i \frac{e_j}{m_j c^2} g_i \mu_0 r_{ij}^{-3} s_i \cdot (r_{ij} \wedge \pi_j) \]

\[ \mathcal{K}_6 = - \sum_{i<j} \frac{g_i \mu_0 \theta_i \theta_j \mu_0}{c^2} \left\{ \frac{8 \pi}{3} (s_i \cdot s_j) \delta^3(r_{ij}) + r_{ij}^{-3} \left[3(s_i \cdot r_{ij}) (s_j \cdot r_{ij}) - (s_i \cdot s_j) r_{ij}^2 \right]\right\} \]

\[ \mathcal{K}_7 = - \sum_i \theta_i \mu_0 s_i \cdot B_0 \left( 1 - \frac{\pi_i^2}{2 m_i^2 c^2} \right) - \sum_{i} (g_i - 2) \mu_0 s_i \cdot \left( \frac{\pi_i^2 - \pi_i \cdot \pi_j}{2 m_i^2 c^2} \right) \cdot B_0. \]

\(^{(1)}\) As far as radiative corrections are concerned, equation (2.1) assumes that the electron is a free one; in particular, this formalism does not account for the short-range modification of the Coulomb potential, responsible for the Lamb-shift. This effect manifests itself as an overall shift of order \(Z \alpha^2 R_s\) of the fine structure levels and for each multiplet as a relative shift of order \(\frac{\alpha^2}{Z} \log z R_s\) [6]. In a magnetic field similar effects lead to corrections of order \(\alpha^2 \mu_B B_0\) as discussed by Grotch and Hegstrom [7]. Except for these corrections, the Hamiltonian (2.1) is expected to be valid up to the order \(\alpha^3\), that is to say up to order \(\alpha^3 \mu_B B_0\) for the Zeeman effect.
In these expressions \( \mu_{oi} \) represents the ratio \( e_i/2m_i \); the Landé factor \( g_i \) of particle \( i \) is related to the anomalous part \( \kappa_i \) of the magnetic moment by:

\[
g_i \mu_{oi} = 2(\mu_{oi} + \kappa_i). \tag{2.7}
\]

Equation (2.6) is the starting point of the more elaborate calculations on the Zeeman effect of many-electron atoms [8, 9], and it would be gratifying to know the physics underlying the various terms appearing in this intricate Hamiltonian. There already exists a traditional interpretation of all these terms: \( \mathcal{K}_0 \) is the nonrelativistic Schrödinger Hamiltonian, \( \mathcal{K}_1 \) is the first relativistic correction to the kinetic energy, \( \mathcal{K}_2 \) the Darwin term due to the Zitterbewegung of the particles, \( \mathcal{K}_3 \) the interaction of the spin with the external magnetic field. Besides the great complexity of most of these terms, let us notice that the anomalous magnetic moment appears sometimes as \( g_i \), sometimes as \( g_i - 1 \) or \( g_i - 2 \). That means we cannot merely replace in the Pauli Hamiltonian the Dirac magnetic moment \( 2e \mu_i \sigma_i \) by the anomalous moment \( g_i \mu_i \sigma_i \). We are thus faced with a dilemma: either the anomalous part of a magnetic moment does not behave like the Dirac part, or the traditional interpretation of equation (2.6) is erroneous. In trying to answer these questions, we found it interesting to reconsider the problem of an atom in a magnetic field using a very simple relativistic but classical description where atoms are thought of as systems of point-like particles with magnetic moment proportional to an inner angular momentum. This is the purpose of the next two sections.

### 3. Relativistic dynamics of particles with intrinsic angular momentum

#### 3.1 INTRINSIC ANGULAR MOMENTUM AND INTRINSIC MAGNETIC MOMENT

In the framework of classical electrodynamics, a particle with spin is defined by its intrinsic angular moment \( \mathbf{S} \), together with an associated magnetic moment \( \mathbf{M} \) related to \( \mathbf{S} \) by:

\[
\mathbf{M} = g \mu_0 \mathbf{S} \quad \text{with} \quad \mu_0 = \frac{e}{2m}.
\tag{3.1}
\]

**a)** Equation (3.1) is a relation between three dimensional axial vectors and when guessing its four dimensional counterpart, two solutions are possible: the first one with four-vectors, the second one with antisymmetric four-tensors; the first choice is the most widely used by people interested in polarized beams (Bargman, Michel, Telegdi [10], Hagedorn [11] and others [12]), it has the merit of mathematical simplicity, the covariant equation for the polarization motion being rather easy to get [10]. However, as stressed by Hagedorn [11], the physical meaning of the polarization four-vector is ambiguous in any frame other than the rest-frame. For this reason, we have chosen the second solution and our point of view is based on the following hypothesis:

The intrinsic angular momentum of a particle is described by an antisymmetric 4-tensor \( \Sigma^{\mu
u} \); in a rest-frame of the particle the purely spatial part of \( \Sigma^{\mu
u} \) coincides with \( \mathbf{S} \) while the spatio-temporal part is null; i.e. in a rest frame:

\[
\mathbf{S} \equiv \left( \Sigma^{23}, \Sigma^{31}, \Sigma^{12} \right)
\]

\[
0 \equiv \left( \Sigma^{01}, \Sigma^{02}, \Sigma^{03} \right).
\]

This definition implies that in any frame

\[
\Sigma^{\mu\nu} \mathbf{u}_\nu = 0 \tag{3.2}
\]

where \( \mathbf{u}_\nu \) is the four velocity of the particle.

**b)** In an inertial frame \( F \) where the particle moves with velocity \( \mathbf{v} = c \mathbf{\beta} \), the spatio-temporal part of \( \Sigma^{\mu\nu} \) is non zero, and appears to represent (except for a factor \( -g \mu_0 c ) \) the electric dipolar moment associated with the moving magnetic moment. With the use of the Lorentz transformation of antisymmetric tensors, we easily get the components \( -c \mathbf{\beta} \mathbf{S} \) of \( \Sigma^{\mu\nu} \) in \( F \) from the rest-frame components \( \mathbf{0}, \mathbf{S} \).

The result is:

\[
\mathbf{S} = c \mathbf{\Omega} \times \mathbf{S} \tag{3.3}
\]

where:

\[
\mathbf{S} = \left( \Sigma^{23}, \Sigma^{31}, \Sigma^{12} \right)
\]

\[
c \mathbf{\Omega} = \left( \Sigma^{10}, \Sigma^{20}, \Sigma^{30} \right)
\]

\[
\mathbf{\beta} = \frac{\mathbf{v}}{c}, \quad \gamma = \frac{1}{\sqrt{1 - \beta^2}},
\]

and

\[
\mathbf{\Omega} = 1 - \frac{\gamma}{\gamma + 1} \mathbf{c} \mathbf{\beta} \tag{3.6}
\]

is the Lorentz contraction tensor. The advantage of the \( \Sigma \) formalism is clear: in any frame, \( \Sigma \) has a clear-cut physical interpretation, the associated vectors \( \mathbf{S} \) and \( \mathbf{\Omega} \) corresponding to usual quantities of electrodynamics, a point already stressed and thoroughly used by de Groot and Suttorp [13] (2).

#### 3.2 THE SPIN EQUATION OF MOTION, THE THOMAS PRECESSION

First consider the trivial case of a particle moving with a constant velocity relative to an inertial frame \( L_0 \); its motion is most simply

\(\footnote{The presence of the light velocity \( c \) in the tensor \( \Sigma^{\mu\nu} \) arises from our choice of the electrostatic system of units \( \left( \text{defined by } 4 \pi \epsilon_0 = 1 \text{ and } \mu_0 = 1/c^2 \right) \) in which the electromagnetic tensor \( F^{\mu\nu} \) is written as \( -cE/c, \mathbf{B} \), with \( E/c = (F^{10}, F^{20}, F^{30}) \) and \( \mathbf{B} = (F^{23}, F^{31}, F^{12}) \). We shall later see that this choice is particularly suitable whenever we want to develop the magnetic interaction terms in power of \( c^{-1} \).} \)

...
described in its inertial rest frame where it satisfies to the equation:

\[
\frac{dS}{d\tau} = M \wedge B
\]

where \(B\) is the magnetic field experienced by the particle and measured (like \(S, M\) and \(t\)) in the inertial rest frame.

In the general case where the particle is accelerating relative to \(L_0\), we do not have one single inertial rest frame, but rather a sequence of inertial rest frames, each member of the sequence being at a given proper time \(\tau\) an instantaneous rest frame of the particle. To define unambiguously this succession of rest frames, we must further specify the orientation of the axis of the successive rest frames. There are at least two possible sequences:

a) we can use a sequence in which all the successive instantaneous rest frames \(R(\tau)\) have their axis parallel to an arbitrary inertial frame \(L_0\) (for example the lab frame),

b) we can also use another sequence \(P(\tau)\), where \(P(\tau + d\tau)\) is deduced from \(P(\tau)\) by a pure Lorentz boost of velocity \(\delta v\) \([\delta v\ being\ the\ velocity\ of\ the\ particle\ at\ time\ \tau + d\tau\ as\ measured\ in\ P(\tau)]\).

In the absence of any external forces (no magnetic interactions), it is expected that the spin does not precess in the sequence \(P(\tau)\). But since the product of two pure Lorentz boosts is in general (for non collinear products) the product of a pure Lorentz boost by a rotation \([14]\), it happens that the sequence \(P(\tau)\) is rotating relative to \(R(\tau)\) and \(L_0\). If the spin is motionless in \(P(\tau)\), it will thus appear to be rotating in \(R(\tau)\) and \(L_0\): a phenomenon known as the Thomas precession \([3]\).

In order to see the phenomenon from another point of view, we shall now report another demonstration of this precession. In this new demonstration we shall not use the rest frames \(P(\tau)\) and the rather intuitive assumptions we have just made; instead we shall use only the well defined \(R(\tau)\) frames and the fact that in these instantaneous rest frames, the spin remains a purely spatial quantity.

Thus we define the function \(S(\tau)\) which at each time \(\tau\) measures the orientation of the spin in the instantaneous rest frame \(R(\tau)\):

\[
S(\tau) = (\Sigma^{23}, \Sigma^{31}, \Sigma^{12})_{R(\tau)}
\]

the spatio-temporal part being in this succession of frames identically zero:

\[
cP(\tau) = (\Sigma^{10}, \Sigma^{20}, \Sigma^{30})_{R(\tau)} \equiv 0.
\]

At a particular time \(\tau_a\) there is a corresponding inertial frame \(R(\tau_a)\). At time \(\tau > \tau_a\) we shall denote as \(cP_a(\tau)\) the particle as judged from \(R(\tau_a)\) [all the quantities measured in \(R(\tau_a)\) will be affected with the subscript \(a\)]. At this time we have the following relation between the components of spin \([0, S(\tau)]\ in R(\tau) and in [\[-cP_a(\tau), S_a(\tau)]\ R(\tau_a) : \]

\[
[0, S(\tau)] = \Lambda(\beta(\tau)) \Lambda^{-1}(\beta(\tau_a)) [\[-cP_a(\tau), S_a(\tau)]
\]

(3.7)

where \(\Lambda(\beta(\tau))\) is the pure Lorentz boost which transforms coordinates of antisymmetric tensors from the laboratory frame \(L_0\) to the inertial frame \(R(\tau)\) moving with the velocity \(cP(\tau)\) with respect to \(L_0\). With the help of equations (3.3) and (3.6), equation (3.7) can be written in the form:

\[
S(\tau) = \gamma^{-1}(\tau) \gamma(\tau_a) \Omega^{-1}(\tau) \times \left[ \Omega(\tau_a) S_a(\tau) + \beta(\tau_a) \times (\beta(\tau) \wedge S(\tau)) \right] \]

(3.8)

\[
P(\tau) = 0.
\]

Deriving equation (3.8) with respect to \(\tau\) and taking the derivative at time \(\tau = \tau_a\) gives:

\[
\frac{dS(\tau)}{d\tau} \bigg|_{\tau=\tau_a} = \left[ \frac{dS_a(\tau)}{d\tau} \bigg|_{\tau=\tau_a} \right] + \frac{\gamma^2}{\gamma + 1} \frac{db}{d\tau} \wedge \beta \bigg|_{\tau=\tau_a} \wedge S(\tau_a). \tag{3.9}
\]

This equation shows us that the total rate of change of spin in the frame \(R(\tau)\) is the sum of the rate of change due to external interactions plus a purely kinematic term which takes into account the Thomas precession \((3)\). More precisely we can write (3.9) in the form:

\[
\frac{dS}{d\tau} = g\mu_b S \wedge B_R + \gamma \omega_T \wedge S \tag{3.10}
\]

where:

\[
\omega_T = \frac{\gamma^2}{\gamma + 1} \frac{db}{d\tau} \wedge \beta. \tag{3.11}
\]

\(B_R\) is the magnetic field experienced by the spin as judged from \(R(\tau)\) and \(d\beta/d\tau\) is the acceleration of the particle viewed from \(L_0\), given by the Lorentz force law.

Equation (3.10) introduces a good division between what we shall name magnetic interaction terms and purely kinematic ones, and therefore gives us a simple physical insight of the phenomena. On the other hand, the covariant character of the evolution law is totally hidden due to the particular choice of sequence \(R(\tau)\) with respect to \(L_0\). However, it is easy to derive

\((3)\) It is possible to make a demonstration very similar in form for any purely spatial quantity of \(R(\tau)\) (vector or pseudo-vector); that is consistent with the geometrical interpretation we give previously.
equation (3.10) from the following covariant equation [15]:

\[
\frac{d\Sigma^{\mu\nu}}{dt} = g_{\mu\nu}(F^{\alpha\gamma} \Sigma_{\alpha}^{\beta} - F^{\beta\gamma} \Sigma_{\alpha}^{\alpha}) + \\
+ \frac{1}{c^2} (g - 2) \mu_b (u^\alpha \Sigma^{\alpha\beta} - u^\beta \Sigma^{\alpha\alpha}) F_{\mu\nu} u^\mu \tag{3.12}
\]

where \( F^{\mu\nu} \) represents the antisymmetric tensor of electromagnetic fields. We have not followed this approach as it was our purpose to give the most pedestrian approach, with simple physical interpretation, but we draw attention to the fact that equations (3.10) and (3.12) have exactly the same physical content and the same limits, they are valid only for constant or slowly varying fields: a hypothesis we shall make throughout all this paper. As a final remark we must emphasize that equation (3.10) can equally well be derived from the B.M.T. equation which governs the evolution of four-vector \( S^\alpha \) (see by example refs. [14] and [16]).

### 3.3 Hamiltonian Form of Equation of Spin Motion.

Equation (3.10) with the Lorentz force law provides a complete description of the motion of a charged particle with intrinsic magnetic moment. From the Lorentz force law:

\[
\frac{du^\mu}{dt} = \frac{e}{m} F^{\mu\nu} u_\nu
\]

we easily obtain the acceleration of the particle in the lab frame as a function of the electro-magnetic fields acting on it:

\[
\frac{dB}{dt} = \frac{e}{\gamma mc} \left[ E_L + c B_L - \beta (\beta \cdot E_L) \right] \tag{3.13}
\]

and then the expression of the Thomas precession by (3.11).

From equation (3.10), it is straightforward to obtain the Hamiltonian of the motion in \( R(t) \) using the heuristic definition [17, 18] of Poisson brackets:

\[
\{ S_\mu, S_\nu \} = \epsilon_{\mu\nu\lambda} S_\lambda \quad (3.14)
\]

With the help of (3.14), (3.10) and (3.13) lead to the equation of motion of spin in \( R(t) \) with the form:

\[
\frac{dS}{dt} = \{ S, \mathcal{K}_R \}
\]

with

\[
\mathcal{K}_R = -\mu_b S \cdot B_R + \gamma \omega_T \cdot S \tag{3.15}
\]

and

\[
\omega_T = \frac{\gamma}{\gamma + 1} mc [E_L + c B_L] \wedge \beta.
\]

Finally, to obtain the equations of motion and the corresponding Hamiltonian in the lab frame \( L_0 \) we have only to use the pure Lorentz boost given in (3.3). By deriving equation (3.3), we obtain:

\[
\frac{dS}{dt} = \left( \frac{d}{dt} \gamma \Omega \right) \cdot S + \gamma \Omega \cdot \frac{dS}{dt}
\]

\[
\frac{d\mathcal{F}}{dt} = \left( \frac{d\gamma \mathcal{F}}{dt} \right) \wedge S + \frac{\gamma \mathcal{F}}{c} \wedge \frac{dS}{dt}
\]

the first terms on the right hand sides represent the rate of change of \( S \) and \( \mathcal{F} \) due to the time-variation of the Lorentz boost which transforms \( L_0 \) in \( R(t) \), they are just partial derivative of \( S \) and \( \mathcal{F} \); using moreover equation (3.15), we can write equations (3.16) as:

\[
\frac{dS}{dt} = \frac{d}{dt} \frac{\partial S}{\partial t} + \Omega \cdot \{ S, \mathcal{K}_R \}
\]

\[
\frac{d\mathcal{F}}{dt} = \frac{d}{dt} \frac{\partial \mathcal{F}}{\partial t} + \frac{\mathcal{F}}{c} \wedge \{ S, \mathcal{K}_R \}
\]

Taking (3.14) into account, we then get:

\[
\frac{dS}{dt} = \frac{\partial S}{\partial t} + \left\{ S, \frac{1}{\gamma} \mathcal{K}_R \right\}
\]

\[
\frac{d\mathcal{F}}{dt} = \frac{\partial \mathcal{F}}{\partial t} + \left\{ \mathcal{F}, \frac{1}{\gamma} \mathcal{K}_R \right\}
\]

which bring out the fact that the Hamiltonian which governs the equation of motion of spin in the lab frame is:

\[
\mathcal{K}_{lab} = + \frac{1}{\gamma} \mathcal{K}_R = - \frac{1}{\gamma} \mu_b S \cdot B_R + \omega_T \cdot S \tag{3.19}
\]

**Remarks:** 1) The factor \( 1/\gamma \) introduced between (3.15) and (3.19) merely takes into account the change of time scale between the lab frame and the rest frame of the particle \( dt = \gamma \, dx \).

2) It is intentional that we keep in expression (3.19) the expression of spin components in the rest frame since they are the only intrinsic quantities with simple commutation rules; we must also emphasize that the same point of view prevails in quantum mechanics. Moreover note that in Blount's quantum mechanical picture [19] we have an equation of motion very similar to (3.19) (see equally ref. [20], chap. 8).

3) As in the initial equation (3.10), we shall distinguish in Hamiltonian (3.19) the magnetic interaction from the kinematic effects. At this point it is interesting to rewrite the magnetic part in terms of quantities of the lab frame \( (\mathcal{S}, \mathcal{F}, B_L, E_L) \); we then get:

\[
\mathcal{K}_{mag} = - \frac{1}{\gamma} \mu_b (S \cdot B_L) = - \frac{1}{\gamma} \mu_b (S \cdot B_L + \mathcal{F} \cdot E_L)
\]
This last form is physically interesting, it accounts for the interaction in the lab frame of the dipolar magnetic moment with the magnetic field, and for that of the dipolar electric moment with the electric field. But in fact, it will be simpler in following calculations to use the composite form:

\[ \mathcal{K}_{\text{mag}} = -g_{\mu_B} \left[ \mathbf{B}_L \cdot \Omega \cdot \mathbf{S} + E_L \cdot \left( \frac{\mathbf{p} \times \mathbf{S}}{c} \right) \right] \]  

(3.21)

4. We finally obtain the kinematic part due to Thomas precession in the form:

\[ \mathcal{K}_{\text{Th}} = \frac{e}{m} \gamma \mathbf{S} \cdot (\mathbf{1} \beta^2 - \mathbf{B} \mathbf{B}) \mathbf{B}_L - \frac{e}{mc} \gamma \mathbf{S} \cdot (\mathbf{B} \times \mathbf{E}_L). \]  

(3.22)

In this last form, we can rediscover the well known contribution of the Thomas precession to the spin-orbit interaction, but we have also in addition a non negligible contribution to the Zeeman effect.

The different origin of the terms of similar form appearing in (3.21), and (3.22) now clearly explains the appearance of the various factors \( g, (g - 1), (g - 2) \) in (2.6) which was a priori so puzzling.

4. Classical Hamiltonian of a many-electron atom in a constant magnetic field. — In order to get this Hamiltonian we first recall the calculation of the spin-independent terms (Darwin Hamiltonian).

4.1. The Darwin Hamiltonian. — Let us consider a particle \( i \) without spin, moving in an electromagnetic field deriving from the potentials \( \mathbf{A}, \varphi \). Its Hamiltonian may be written as:

\[ \mathcal{K}_i = \sqrt{m_i^2 c^4 + e^2 (\mathbf{p}_i - e_i \mathbf{A}_i)^2} + e_i \varphi_i \]  

(4.1)

where \( m_i, e_i \) and \( \mathbf{p}_i \) are respectively the mass, charge and momentum of particle \( i \). The expansion in powers of \( c^{-1} \) leads to the standard expression:

\[ \mathcal{K}_i = m_i c^2 + \frac{(\mathbf{p}_i - e_i \mathbf{A}_i)^2}{2 m_i} - \frac{1}{8 m_i^2 c^2} (\mathbf{p}_i - e_i \mathbf{A}_i)^4 + e_i \varphi_i + \cdots \]  

(4.2)

\( \mathbf{A}_i \) and \( \varphi_i \) are the potentials of the overall electromagnetic fields acting on particle \( i \) (i.e. the fields created by other particles \( j \neq i \) plus the external field \( \mathbf{B}_0 \)). To obtain the Darwin Hamiltonian, we must choose the Coulomb gauge (\( \text{div} \mathbf{A} = 0 \)). Then, following a method proposed by de Groot and Suttorp [20], we expand the potential and fields in power of \( c^{-1} \) and express their values at time \( t \) as a function of the values at the same time \( t \) of the dynamic variables of the source particles. This method has the remarkable advantage of implicitly taking the retardation effect into account. The results are given in table I. We have kept in the expansion of \( \mathbf{A} \) the terms up to the order \( c^{-3} \). The term \( A^{(3)} \) leads to well known difficulties (radiation damping) connected with energy dissipation within the atomic system [21]. Such a radiative process cannot be coherently taken into account unless we quantize the electromagnetic field, we shall henceforth neglect it.

When the potentials given in table I are introduced into the Hamiltonian (4.2), we get, up to order \( c^{-2} \):

\[ \mathcal{K}_i = m_i c^2 + \frac{\pi_i^2}{2 m_i} - \frac{1}{8 m_i^2 c^2} \sum_{j \neq i} \frac{e_i e_j}{r_{ij}} - \sum_{j \neq i} \frac{e_i e_j}{2 m_i m_j c^2} \frac{\pi_i \pi_j + (\pi_i \mathbf{n}) (\pi_j \mathbf{n})}{r_{ij}} \]  

(4.3)

with the mechanical moment now defined as:

\[ \pi_i = \mathbf{p}_i - e_i \mathbf{A}_0(r_i) \]

and

\[ \mathbf{A}_0(r_i) = \frac{1}{2} (\mathbf{B}_0 \times \mathbf{r}_i) \]

**Table I**

Potentials and fields created at point \( i \) by a particle \( j \) in motion

electrostatic units

\[ \left( \frac{1}{4 \pi \varepsilon_0} = 1, \frac{\mu_0}{4 \pi} = \frac{1}{c^2} \right) \]

**Potentials (Coulomb gauge)**

\[ \varphi_i = \varphi_i^{(0)} + \frac{e_i}{r_{ij}} \]

\[ A_i^{(0)} = \sum_j A_j^{(0)} = 0 \]

\[ A_i^{(2)} = \frac{e_i}{2 \varepsilon_c} \mathbf{B}_j + \frac{n(n \mathbf{B}_j)}{r_{ij}} \]

with \( n = \frac{r_{ij}}{r_{ij}}, \mathbf{B}_j = \frac{n}{c} \mathbf{B}_j \)

**Fields**

\[ \mathbf{E}_i = \sum_j \mathbf{E}_j^{(0)} \]

\[ \mathbf{E}_i^{(0)} = e_i \frac{\mathbf{n}}{r_{ij}} \]

\[ \mathbf{E}_i^{(1)} = 0 \]

\[ \mathbf{E}_i^{(2)} = \frac{e_i}{2 \varepsilon_c} \left( \mathbf{B}_j - 3(n \mathbf{B}_j) - \frac{e_i}{2 r_{ij} c} (\mathbf{B}_j + n(n \mathbf{B}_j)) \right] \]

\[ \mathbf{B} = \sum_j \mathbf{B}_j^{(0)} \]

\[ \mathbf{B}_j^{(0)} = 0 \]

\[ \mathbf{B}_j^{(1)} = \frac{e_i}{r_{ij}} \mathbf{B}_j \]

\[ \mathbf{B}_j^{(2)} = \frac{e_i}{r_{ij} c} \mathbf{B}_j \]
It is noticeable that this Hamiltonian, where all terms up to order $c^{-2}$ have been included, is exactly the Darwin Hamiltonian [22]. Besides the relativistic kinetic energy correction, it involves a correction to the instantaneous electrostatic interaction often referred to in terms of a magnetic interaction between the orbit of the moving particles. Let us stress that, if we can neglect the radiative terms $A^{(3)}$, this Hamiltonian remains exact up to the order $c^{-3}$.

The spin-independent part of the Hamiltonian of a many electron atom can now be deduced by summing the different terms (4.3) for each component of this atom, provided we do not take the interaction terms into account twice. (At this level of approximation, this Hamiltonian appears necessarily as a sum over the individual $\mathcal{J}_i$, a feature which may not persist at higher approximations because of three-body interactions.)

\textbf{4.2 SPIN-DEPENDENT PART OF THE HAMILTONIAN. —} In section 3, we proved that the spin-dependent part of the interaction of a particle $i$ with an electromagnetic field can be described by a Hamiltonian composed of a magnetic part $H_{\text{mag}}^i$ and a kinetic part $\mathcal{J}_{\text{Kth}}^i$.

\textit{a) Calculation of $\mathcal{J}_{\text{mag}}^i$.}

Gathering the results of table I (fields of moving charges) and appendix (fields of moving magnetic dipoles) and limiting ourselves to terms up to order $c^{-2}$, we obtain from the initial expression (3.21):

\begin{equation}
\mathcal{J}_{\text{mag}}^i = -\alpha_{i0} \left[ B_i \cdot \left( 1 - \frac{\pi_i \pi_i}{2 m_i^2 c^2} \right) \cdot r_i + E_{\text{i}} \cdot \frac{\pi_i \wedge S_i}{m_i c^2} \right]
\end{equation}

and the final result:

\begin{equation}
\mathcal{J}_{\text{mag}}^i = -\alpha_{i0} S_i \cdot \left( 1 - \frac{\pi_i \pi_i}{2 m_i^2 c^2} \right) \cdot B_0
\end{equation}

\begin{equation}
-\alpha_{i0} \sum_{j \neq i} \frac{e_j}{m_j c^2} S_j \cdot \left( \frac{\pi_j \wedge r_{ij}}{r_{ij}^3} \right) - \alpha_{i0} \sum_{j \neq i} \frac{e_j}{m_j c^2} \left\{ \frac{\pi_i \wedge S_i}{m_i^3} \right\}
\end{equation}

The physical origin of all the above terms is now clear and we can successively distinguish the interaction of the magnetic moment of particle $i$ with the external magnetic field and with the magnetic field of the moving charges $j$, then the interaction between the motional induced electric moment with the electric fields produced by the $j$ particles and finally the interaction between magnetic moments (4).

\textit{b) Calculation of the kinetic part $H_{\text{Kth}}^i$.}

To determine $H_{\text{Kth}}^i$ from (3.22) up to the order $c^{-3}$, it is sufficient to consider the expressions of $E_i$ and $B_i$ up to the order $c^{-1}$ and we obtain:

\begin{equation}
\mathcal{J}_{\text{Kth}}^i = -\frac{e_i}{2 m_i^3 c^2} \sum_{j \neq i} \left[ \left( \frac{e_j r_{ij}}{r_{ij}^3} \right) \wedge \pi_i \right] \cdot S_i + \left( \frac{\pi_i}{m_i} \wedge B_0 \right) \wedge r_{ij} \cdot S_i \right].
\end{equation}

We see that the Thomas precession plays an important role in the spin orbit interaction and also that it is responsible for a correction to the Zeeman effect.

\textbf{4.3 COMPLETE HAMILTONIAN. —} Gathering the spin-independent Hamiltonian (4.3), the magnetic Hamiltonian $\mathcal{J}_{\text{mag}}^i$ (4.5) and the Thomas Hamiltonian (4.6) and summing over the particles, we obtain the atomic Hamiltonian. Except for the Zitterbewegung term, the result is identical to the Hamiltonian deduced from the generalized Breit equation and given in (2.6).

The obvious advantage of our classical derivation is to allow us to give a clear-cut interpretation of the various terms: the Schrödinger Hamiltonian $\mathcal{J}_s$ and the relativistic kinetic correction $\mathcal{J}_l$ are well known. $\mathcal{J}_s$ appears as a purely quantum term that can be understood as the interaction with the mean potential seen by delocalized electrons. $\mathcal{J}_l$ expresses the orbit-orbit interaction: it is not only due to simple interaction between the two orbits considered as magnetic

(*) It is possible to improve the calculation so as to get the contact potential between magnetic moments. This is achieved by ascribing a tiny volume to the magnetic moment as can be seen for example in Cohen-Tannoudji et al. [23].
moments but most exactly includes retardation effects in the Coulomb interaction.

The so-called spin-orbit term $\mathcal{K}_a$ results from two different effects: the first one has a magnetic origin and appears as the interaction of the electric moment (originating in the moving magnetic moment) with the electric field of the nucleus and electrons, while the second one has a purely kinematic origin, related to the Thomas precession of the intrinsic angular momentum in the accelerated frame; this is at the origin of the presence of the $(g - 1)$ factor.

The so-called spin-orbit term $\mathcal{K}_4$ results from two different effects: the first one has a magnetic origin and appears as the interaction of the electric moment (originating in the moving magnetic moment) with the electric field of the nucleus and electrons, while the second one has a purely kinematic origin, related to the Thomas precession of the intrinsic angular momentum in the accelerated frame; this is at the origin of the presence of the $(g - 1)$ factor.

The so-called spin-other orbit interaction $\mathcal{K}_5$ is purely magnetic and expresses the interaction of the magnetic moment with the magnetic field created by the other moving electrons.

As previously found $\mathcal{K}_6$ is a purely magnetic interaction between the magnetic moments of electrons.

Finally, $\mathcal{K}_7$ represents the interaction of the spin with the external magnetic field; its previous expression (2.6) can be advantageously replaced by the more explicit form:

$$\mathcal{K}_7 = - \sum_i g_i \mu_{0i} S_i \left( 1 - \frac{\pi_i^2}{2 m_i^2 c^2} \right) \cdot B_0 +$$

$$+ \sum_i \mu_{0i} \frac{\pi_i^2}{m_i^2 c^2} (B_{0i} \cdot S_{1i})$$

(4.7)

where $B_{0i}$ and $S_{1i}$ represent the components of $B_0$ and $S_i$ perpendicular to the velocity of the particle $i$. In this new expression, we see the interaction of the spin with the magnetic field as seen in the rest frame and a relativistic correction of purely kinematic origin (which gives a contribution to the Margenau correction). This overall relativistic effect appears as an anisotropic modification of the Thomas precession in a magnetic field. (It has been shown in a somewhat different way in reference [24] that this correction reduces for a Dirac electron to the so-called relativistic mass correction.)

It is thus remarkable that despite its intrinsic and well known limitations (radiation damping), classical electrodynamics is able to offer a clear explanation of all the relativistic terms up to order $c^{-3}$ appearing in the Hamiltonian (2.6) derived from the generalized Breit equation.

Appendix: Retarded potentials and fields created by moving magnetic moments. — A moving magnetic dipole reveals itself not only as a contracted magnetic moment:

$$\mu_i = g_i \mu_{0i} \gamma_i \cdot \Omega_i \cdot S_i$$

(A.1)

but also as an electric dipole:

$$\nu_i = \frac{\gamma_i}{c} \beta_i \wedge g_i \mu_{0i} S_i = \frac{1}{c} \beta_i \wedge \mu_i$$

(A.2)

Consequently a set of particles with spin will be described by a magnetization density:

$$M(R(t)) = \sum_i \mu_i \delta^3(R_i - R)$$

(A.3)

together with a polarization density:

$$P(R(t)) = \sum_i \frac{\beta_i \wedge \mu_i}{c} \delta^3(R_i - R) = \sum_i \frac{\nu_i}{c} \delta^3(R_i - R)$$

(A.4)

and in the presence of a charge density $\rho$ and current density $j$ the Maxwell equations in vacuum may be written as:

$$\nabla \cdot E = 4\pi (\rho - \nabla \cdot P)$$

$$\nabla \times E = \frac{4\pi}{c^2} \left( j + \frac{\partial P}{\partial t} - \nabla \cdot M \right)$$

(A.5)

$$\nabla \times B = 0$$

$$\nabla \cdot E + \frac{\partial B}{\partial t} = 0.$$
Thus \( \pi \) and \( \pi^* \) are given by the corresponding formulas:

\[
\pi(R, t) = \int \frac{P(R', t')}{r(t')} \delta \left( t - t' - \frac{r(t')}{c} \right) \, dt' \quad (A.13)
\]
and

\[
\pi^*(R, t) = \int M(R', t') \delta \left( t - t' - \frac{r(t')}{c} \right) \, dt' \quad (A.14)
\]

where \( r(t') = |R - R'| \).

Following a method developed by de Groot and Suttorp [20], we expand the delta function in a Taylor series around \( t = t' \) and we obtain the expressions for the superpotentials created at point \( i \) by the set of particles \( j \neq i \), in the form of power series in \( c^{-1} \). (What is remarkable is that each term of the series is synchronous i.e. it involves the values of \( M \) and \( P \) at the very time \( t \) the potentials \( \pi \) and \( \pi^* \) are calculated.)

The first terms of the series are:

\[
\pi^{(0)} = \pi^{(1)} = 0 \quad (A.15)
\]

\[
\pi^{(2)} = \sum_{j \neq i} \frac{v_j}{r_{ij}} \quad (A.16)
\]

from which we successively obtain the potentials \( \varphi \) and \( A \):

\[
\begin{aligned}
\varphi^{(0)} &= \varphi^{(1)} = 0 \\
\varphi^{(2)} &= \sum_{j \neq i} \frac{v_j r_{ij}}{r_{ij}^3} \\
\varphi^{(3)} &= 0 \\
A^{(0)} &= A^{(1)} = 0 \\
A^{(2)} &= \sum_{j \neq i} \frac{\mu_j \wedge r_{ij}}{c^2 r_{ij}^3} \\
A^{(3)} &= 0
\end{aligned}
\]

and the fields \( E \) and \( B \):

\[
\begin{aligned}
E^{(0)} &= E^{(1)} = 0 \\
B^{(0)} &= B^{(1)} = 0 \\
E^{(2)} &= \frac{1}{c^2} \sum_{j \neq i} \left\{ \frac{3 (\mathbf{p}_j \cdot \mathbf{r}_{ij}) r_{ij}}{r_{ij}^3} - \frac{\mathbf{p}_j}{r_{ij}^3} \right\} \\
B^{(3)} &= 0
\end{aligned}
\]

References


[18] A more elaborate foundation of classical Hamiltonian formalism has been developed by BARUT, A. O., in Electrodynamics and Classical Theory of Fields and Particles (McMillan Comp., N. Y.) 1964, chap. II.
[22] DARWIN, C. G., Phil. Mag. 39 (1920) 537.