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NATURE OF THE DARWIN TERM AND $(Z\alpha)^4m^3/M^2$ CONTRIBUTION TO THE LAMB SHIFT FOR AN ARBITRARY SPIN OF THE NUCLEUS

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The contact Darwin term is demonstrated to be of the same origin as the spin-orbit interaction. The $(Z\alpha)^4m^3/M^2$ correction for the Lamb shift, which is generated by the Darwin term, is found for an arbitrary nonvanishing spin of the nucleus, both half-integer and integer. There is also a contribution of the same nature to the nuclear quadrupole moment.

1. The literature, including that of the pedagogical nature, abounds with assertions on the nature of the Darwin correction which are, in our view, at least doubtful. In particular, we cannot agree with the conclusion [1] that the Darwin term is absent for a particle with spin 1 (see also [2]). This subject is of real interest now for the interpretation of high precision experiments in atomic spectroscopy [3–5].

To study the problem we consider in this note the Born amplitude for scattering of a particle with an arbitrary spin in an external electromagnetic field. In the case of practical interest, that of an atom, this is the interaction of a nucleus with the electromagnetic field of an electron. We thus derive the general form of the Darwin term for an arbitrary nuclear spin and obtain the corresponding order $(Z\alpha)^4m^3/M^2$ correction to the Lamb shift (here and below m is the electron mass, and Z and M are, respectively, the charge and mass of the nucleus).

2. The wave function of a particle with an arbitrary spin can be written as (see, for example, §31 of Ref. [6])

$$\Psi = \begin{pmatrix} \xi \\ \eta \end{pmatrix}. \qquad (1)$$

The spinors,

$$\xi = \left\{ \xi^{\alpha_1 \alpha_2 \, .. \, \alpha_p}_{\dot\beta_1 \dot\beta_2 \, .. \, \dot\beta_q} \right\}$$

and

$$\eta = \left\{ \eta^{\beta_1 \beta_2 \, .. \, \beta_q}_{\dot\alpha_1 \dot\alpha_2 \, .. \, \dot\alpha_p} \right\}$$

are symmetric in the dotted and undotted indices separately, and

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$$p + q = 2I,$$

where I is the particle spin. For a particle of half-integer spin one can choose

$$p = I + \frac{1}{2}, \quad q = I - \frac{1}{2}.$$

In the case of integer spin it is convenient to use

$$p = q = I.$$

The spinors ξ and η are chosen in such a way that under reflection they go over into each other (up to a phase). At $p \neq q$ they are different objects which belong to different representations of the Lorentz group. If $p = q$, these two spinors coincide. Nevertheless, we will use the same expression (1) for the wave function of any spin; i.e., we will also introduce formally the object η for an integer spin, keeping in mind that it is expressed in terms of ξ. This will allow us to perform calculations in the same way for the integer and half-integer spins.

In the rest frame both ξ and η coincide with a nonrelativistic spinor ξ_0, which is symmetric in all indices; in the rest frame there is no difference between dotted and undotted indices. The Lorentz transformation of ξ_0, up to the terms $\sim (v/c)^2$ included, is

$$\xi = \left(1 + \frac{\mathbf{\Sigma v}}{2} + \frac{(\mathbf{\Sigma v})^2}{8}\right) \xi_0 \,,$$
$$\eta = \left(1 - \frac{\mathbf{\Sigma v}}{2} + \frac{(\mathbf{\Sigma v})^2}{8}\right) \xi_0 \,. \tag{2}$$

Here

$$\mathbf{\Sigma} = \sum_{i=1}^{p} \boldsymbol{\sigma}_i - \sum_{i=p+1}^{p+q} \boldsymbol{\sigma}_i \,,$$

and $\boldsymbol{\sigma}_i$ acts on the ith index of the spinor ξ_0 as follows:

$$\boldsymbol{\sigma}_i \, \xi_0 = (\boldsymbol{\sigma}_i)_{\alpha_i \beta_i} \, (\xi_0)_{\ldots \beta_i \ldots} \,. \tag{3}$$

In the Lorentz transformation (2) for ξ, after the action of the operator $\mathbf{\Sigma}$ on ξ_0 the first p indices are identified with the upper undotted indices and the next q indices with the lower dotted ones. The inverse situation takes place for η.

We will use, however, Eq. (2) since it no longer distinguishes between the upper and lower or the dotted and undotted spinor indices. It allows us to introduce in a natural way the «standard» representation for the spinors, in close analogy with that for spin 1/2:

$$\phi = (\xi + \eta)/2, \quad \chi = (\xi - \eta)/2 \,.$$

In it the wave function is written as

$$\Psi = \begin{pmatrix} \left[1 + (\mathbf{\Sigma v})^2/8\right] \xi_0 \\ (\mathbf{\Sigma v}/2) \, \xi_0 \end{pmatrix} . \tag{4}$$

It is convenient to introduce the object

$$\overline{\Psi} = (\phi^{\star}, -\chi^{\star}).$$

Then

$$\overline{\Psi}\Psi = \phi^{\star}\phi - \chi^{\star}\chi = \xi_0^{\star}\,\xi_0$$

is an invariant. We will use the common noncovariant normalization of the particle number density

$$\rho = \frac{E}{M}\overline{\psi}\psi = 1, \tag{5}$$

where the wave function ψ is

$$\psi = \sqrt{\frac{M}{E}} \begin{pmatrix} [1 + (\mathbf{\Sigma v})^2/8]\;\xi_0 \\ (\mathbf{\Sigma v}/2)\;\xi_0 \end{pmatrix}. \tag{6}$$

Here E is the particle energy.

3. Let us go over now to the scattering amplitude itself. The order $1/M^2$ terms in it arise only in the time component of the electromagnetic current. Restricting the analysis to the form factors of the lowest multipolarity, electric F_e and magnetic G_m, we can write this component for an arbitrary spin as follows:

$$j_0 = F_e\,\frac{E+E'}{2M}\overline{\psi}'\psi + \frac{G_m}{2M}\psi'^{\star}\,\mathbf{\Gamma q}\,\psi, \tag{7}$$

where

$$\mathbf{q} = \mathbf{p}' - \mathbf{p}.$$

The matrix

$$\mathbf{\Gamma} = \begin{pmatrix} 0 & \mathbf{\Sigma} \\ -\mathbf{\Sigma} & 0 \end{pmatrix} \tag{8}$$

is a natural generalization of the corresponding expression for spin $1/2$ (which is valid in the spinor and standard representations):

$$\boldsymbol{\gamma} = \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ -\boldsymbol{\sigma} & 0 \end{pmatrix}. \tag{9}$$

This generalization is fairly obvious in the spinor representation. According to (9), here $\boldsymbol{\sigma}$ connects a dotted index in the initial spinor ψ with the undotted one in $\overline{\psi}$, and $-\boldsymbol{\sigma}$ connects an undotted index from ψ with dotted one of $\overline{\psi}$. This is exactly what $\mathbf{\Gamma}$ does. It is straightforward now to prove expression (8) for the standard representation. Let us mention also that Eq. (8) is confirmed by the final result, which reproduces correctly the spin-orbit interaction; the form of the latter is well-known for an arbitrary spin (see, e.g., § 41 of Ref. [6]).

The term with G_m in the current density is

$$\begin{aligned} j_{0\,m} &= \frac{G_m}{2M}\xi_0'^{\star}\left(1,\ \mathbf{\Sigma v}'/2\right)\begin{pmatrix} 0 & \mathbf{\Sigma q} \\ -\mathbf{\Sigma q} & 0 \end{pmatrix}\begin{pmatrix} 1 \\ \mathbf{\Sigma v}/2 \end{pmatrix}\xi_0 = \\ &= \frac{G_m}{4M^2}\xi_0'^{\star}\left(-(\mathbf{\Sigma q})^2 + 4i\,\mathbf{I}[\mathbf{qp}]\right)\xi_0\,. \end{aligned} \tag{10}$$

The spin operator is

$$\mathbf{I} = \frac{1}{2}\sum_{i=1}^{2I}\boldsymbol{\sigma}_i\,.$$

The first term, with F_e, in Eq. (7) reduces to an analogous structure:

$$\begin{aligned} j_{0\,ch} &= F_e\,\frac{E'+E}{2\sqrt{EE'}}\,\xi_0'^{\,*}\left(1+\frac{(\boldsymbol{\Sigma}\mathbf{v})^2}{8}+\frac{(\boldsymbol{\Sigma}\mathbf{v}')^2}{8}-\frac{(\boldsymbol{\Sigma}\mathbf{v}')(\boldsymbol{\Sigma}\mathbf{v})}{4}\right)\xi_0 = \\ &= F_e\,\xi_0'^{\,*}\left(1+\frac{(\boldsymbol{\Sigma}\mathbf{q})^2}{8M^2}-i\,\frac{\mathbf{I}[\mathbf{q}\mathbf{p}\,]}{2M^2}\right)\xi_0. \end{aligned} \tag{11}$$

Thus the total charge density is

$$j_0 = \xi_0'^{\,*}\left(F_e-(2G_m-F_e)\frac{(\boldsymbol{\Sigma}\mathbf{q}\,)^2}{8M^2}+(2G_m-F_e)\,i\,\frac{\mathbf{I}[\mathbf{q}\mathbf{p}\,]}{2M^2}\right)\xi_0.$$

We disregard for now the charge radius of the nucleus, so that

$$F_e = F_e(0) = 1.$$

The dependence of the spin-orbit interaction on the gyromagnetic ratio g is universal for any spin, this ratio enters through the factor $g-1$. Therefore, our magnetic form factor is normalized as follows

$$G_m(0) = \frac{g}{2}.$$

Let us split now $(\boldsymbol{\Sigma}\mathbf{q})^2$ into the contact and quadrupole parts:

$$\Sigma_i\Sigma_j\,q_iq_j \;=\; \frac{\mathbf{q}^2}{3}\Sigma_i\Sigma_i + (q_iq_j - \frac{1}{3}\mathbf{q}^2\delta_{ij})\Sigma_i\Sigma_j. \tag{12}$$

The contact term in (12) is

$$\begin{aligned} \boldsymbol{\Sigma}\boldsymbol{\Sigma} &= \left(\sum_{i=1}^{p}\boldsymbol{\sigma}_i\right)^2 - 2\left(\sum_{i=1}^{p}\boldsymbol{\sigma}_i\right)\left(\sum_{i=p+1}^{p+q}\boldsymbol{\sigma}_i\right) + \left(\sum_{i=p+1}^{p+q}\boldsymbol{\sigma}_i\right)^2 = \\ &= 3(p+q)+2\left(\frac{p(p-1)}{2}+\frac{q(q-1)}{2}-pq\right) = 4I(1+\zeta), \end{aligned} \tag{13}$$

$$\zeta = \begin{cases} 0, & \text{integer spin,} \\ 1/4I, & \text{half-integer spin.} \end{cases}$$

In deriving Eq. (13) we used the symmetry in any pair of spinor indices, α_1, α_2 (see Eq. (3)). This symmetry means that the corresponding spins, 1 and 2, add up into the total spin $S = 1$. Therefore,

$$(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_2)\,\xi_0 = \xi_0\,.$$

The interaction operator is proportional to the Fourier transform of the Born amplitude (see, e.g., § 83 of [6]). We thus obtain from (13) the following contact interaction between a nucleus of charge Z and electron:

$$U(\mathbf{r}) = \frac{2\pi}{3}\frac{Z\alpha}{M^2}(g-1)\,I\,(1+\zeta)\,\delta(\mathbf{r})\,. \tag{14}$$

The corresponding energy correction is

$$\Delta E_n = \frac{2}{3}\frac{m^3}{M^2}(g-1)I(1+\zeta)\,\frac{(Z\alpha)^4}{n^3}\delta_{0\ell}. \tag{15}$$

For the hydrogen atom ($I = 1/2$) this correction was obtained long ago in Ref. [7].

Let us consider now the quadrupole part of (12). Using again the complete symmetry of ξ_0, one can easily calculate the corresponding quadrupole interaction:

$$U_2(\mathbf{r}) = -\frac{1}{6}\,\nabla_i\nabla_j\frac{e}{r}\,\delta Q_{ij}\,. \tag{16}$$

Here

$$\delta Q_{ij} = -\frac{3}{4}\frac{Ze\,(g-1)}{M^2}\Lambda\left\{I_i\,I_j + I_j\,I_i - \frac{2}{3}\delta_{ij}\,I(I+1)\right\}, \tag{17}$$

$$\Lambda = \begin{cases} 1/(2I-1), & \text{integer spin,} \\ 1/2I, & \text{half-integer spin.} \end{cases}$$

Expression (17) is a correction to the nuclear quadrupole moment. Its existence for $I = 1$ was pointed out in Ref. [1].

This correction to the quadrupole moment can be estimated as

$$\delta Q \approx -0.22\,(g-1)\,\frac{Z\,I}{A^2}\;e\,\text{mbarn}\,.$$

For the deuteron ($Z = 1,\ A = 2,\ g = 2\mu_d = 1.714,\ Q = 2.86\,e$ mbarn) it is $-0.04\,e$ mbarn.

4. Let us return now to the discussion of the contact term. There is some ambiguity in its definition related to the nuclear charge radius. The contribution of the latter produces a contact interaction and enters physical observables in a sum with the expression $(g-1)\mathbf{q}^2\times \times I(1+\zeta)/(6M^2)$. In particular, the elastic cross-section of the electon-nucleus scattering at small $\mathbf{q}^2$, up to the terms $\mathbf{q}^2/M^2$ included, is

$$\begin{aligned}\frac{d\sigma}{d\Omega} = \frac{\alpha^2}{4\epsilon^2}\frac{\cos^2(\theta/2)}{\sin^4(\theta/2)}\frac{1}{1+2\sin^2(\theta/2)\,\epsilon/M}\times \\ \times\left\{\left[1-\frac{1}{6}\langle r^2\rangle_F\,\mathbf{q}^2-(g-1)\frac{\mathbf{q}^2}{6M^2}I(1+\zeta)\right]^2+\right. \\ \left.+\frac{4}{3}G_m^2\,I(I+1)\left[2\,\mathrm{tg}^2(\theta/2)+1\right]\right\},\end{aligned} \tag{18}$$

where $\langle r^2\rangle_F$ is defined in terms of the expansion of the form factor F_e

$$F_e(q^2) \approx 1 - \frac{1}{6}\langle r^2\rangle_F \mathbf{q}^2. \tag{19}$$

We note here that the expression in square brackets in Eq. (18) reduces for the proton ($I = 1/2$) to

$$1 - \frac{1}{6}\langle r^2\rangle_F \mathbf{q}^2 - (g-1)\frac{\mathbf{q}^2}{8M^2}, \tag{20}$$

and for the deuteron ($I = 1$) to

$$1 - \frac{1}{6}\langle r^2\rangle_F \mathbf{q}^2 - (g-1)\frac{\mathbf{q}^2}{6M^2}. \tag{21}$$

However, the proton charge radius is usually defined differently from that in Eq. (20), i.e., in terms of the expansion of the so-called Sachs form factor

$$G_e = F_e - \frac{\mathbf{q}^2}{4M^2} G_m .$$

Obviously, the charge radius defined in terms of the form factor G_e is

$$-\frac{1}{6}\langle r^2\rangle_G = \frac{\partial G_e}{\partial \mathbf{q}^2} = -\frac{1}{6}\langle r^2\rangle_F - \frac{g}{8M^2}.$$

Correspondingly, expression (20) is usually rewritten as

$$1 - \frac{1}{6}\langle r^2\rangle_G \mathbf{q}^2 + \frac{\mathbf{q}^2}{8M^2}, \tag{22}$$

and the Darwin correction for the proton is defined as

$$\frac{\mathbf{q}^2}{8M^2},$$

but not as

$$-\frac{(g-1)\mathbf{q}^2}{8M^2}.$$

We could redefine the electric form factor for the deuteron from F_e to G_e in such a way that here

$$-\frac{1}{6}\langle r^2\rangle_G = \frac{\partial G_e}{\partial \mathbf{q}^2} = -\frac{1}{6}\langle r^2\rangle_F - \frac{g}{6M^2},$$

so that the Darwin correction for the deuteron becomes

$$\frac{\mathbf{q}^2}{6M^2},$$

instead of

$$-\frac{(g-1)\mathbf{q}^2}{6M^2}.$$

However, for a deuteron the common definition of the charge radius is neither F_e nor G_e but

$$-\frac{1}{6}\langle r^2\rangle_D = -\frac{1}{6}\langle r^2\rangle_F - \frac{g-1}{6M^2}.$$

Of course, under this definition the whole Darwin term is swallowed up by $\langle r^2\rangle_D$. No wonder that the authors of Ref. [1], using $\langle r^2\rangle_D$ instead of $\langle r^2\rangle_E$ or $\langle r^2\rangle_G$, have concluded that for the deuteron, in contrast with the proton, the Darwin correction is absent.

Clearly, this distinction between the deuteron and the proton is based only on a rather arbitrary definition of the charge radius of the former; this distinction has no physical meaning and has nothing to do with the nature of the Darwin term.

5. In summary, the Darwin interaction exists for any nonvanishing spin and is of the same nature as the spin-orbit interaction. In particular, like the spin-orbit interaction, the Darwin term is not directly related to the so-called Zitterbewegung. Of course, there is a certain difference between the spin-orbit and contact energy corrections. The former has a classical limit together with $\langle 1/r^3\rangle$, while the latter which is proportional to $|\psi(0)|^2$, does not. However, this fact has nothing to do with relativity and negative energies, and therefore is certainly unrelated to the Zitterbewegung.

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