Second Order Effects of Nuclear Magnetic Fields

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Using the Dirac equation, we consider the contributions to atomic levels of terms quadratic in $\not{A}$. $\not{A}$ may be, for example, the nuclear magnetic dipole field. We show that a consistent quantum mechanical treatment cancels all terms arising from $[A_i, A_j] \neq 0$. This resolves a disagreement between hyperfine structure corrections calculated nonrelativistically and relativistically.

In this note we will consider the contributions to atomic levels of terms quadratic in $\not{A}$, where $\not{A}$ is, for example, a nuclear magnetic dipole field. We will see that if $A_i$ and $A_j$ do not commute, a correct quantum mechanical treatment nevertheless cancels all terms arising from this noncommutativity. This result explains the disagreement between various...
hyperfine structure (hfs) calculations.

Consider an electron moving in the field of a fixed nucleus. Its motion is given by the Dirac equation,

$$\left[ m + q \cdot \left( p + eA \right) - e\phi \right] \psi = E\psi,$$

(1)

where $\phi$ is the nuclear Coulomb potential. Treating

$$\nabla \cdot \phi = \frac{\partial A}{\partial t},$$

as perturbation, for a state $i$ we obtain to order $A^2$

$$\Delta E_i = \langle i|\psi|1 > + \sum_{m=\pm \frac{1}{2}} \langle i|\psi|n > < n|\psi|1 > (E_n - E_i)^{-1} ,$$

(2)

where $n$ is summed over all positive and negative energy Coulomb states but $1$.

If $i$ is a positive energy state, the Pauli approximation gives

$$\Delta E_i = \langle i|\psi_+|1 > + \sum_{m=\pm \frac{1}{2}} \langle i|\psi_+|n > < n|\psi_+|1 > (E_n - E_i)^{-1}$$

$$\quad + \sum_{m=\pm \frac{1}{2}} \langle i|\psi_-|n > < n|\psi_-|1 > (E_n - E_i)^{-1}$$

(3)

where

$$\psi_\pm = (a/m)\gamma_1 \pm (a/2m)\gamma_5.$$

In the negative energy case we can replace $(E_n - E_i)$ by $2m$ and then sum over
all states, including the positive energy levels. Thus this term becomes
\[ (e^2/2m) < i|V^2|i > , \]
and
\[ \Delta E_1 = < i|V^2|i > + \sum_{n \neq 0} < i|V_n|i > < n|V_0|i > (E_0 - E_n)^{-1} \]
\[ + (e^2/2m) < i|A^2 + ig \cdot A \times i|i > . \]

All the terms in Eq. (5) are familiar from the usual Foldy–Wouthuysen and Pauli reductions except for the one proportional to
\[ g: A \times A + \sigma_i A_j A_k \epsilon_{ijk} . \]
This vanishes if A is a classical field, i.e., if \( A_j \) and \( A_k \) commute. However, if \( A \) contains the nuclear spin operator, then
\[ [A_j, A_k] \neq 0 . \]

The point that we wish to make is that if (6) holds, \( \Delta \) is not a classical field despite the static nature of the source. A proper quantum mechanical treatment, in terms of Feynman graphs or old fashioned non-covariant quantum electrodynamics, does not lead to Eq. (5).

Figure 1 shows the two Feynman graphs quadratic in \( \Delta \). With \( k, k', \)
\( p = 2\Delta \), the crossed diagram is smaller by \( 2\Delta \) than the uncrossed diagram for positive energy states. However, for negative energy states these diagrams differ to lowest order only in the ordering of the operators. The uncrossed diagram gives
\[ (e^2/2m) \sigma_1 \sigma_j A_j = (e^2/2m) (E^2 + g \cdot A) \]
\[ (\sigma_j A_j) . \]
and the crossed one gives

\[
(e^2/\hbar m) \alpha_1 \alpha_j A_j A_1 = (e^2/\hbar m)(A^2 - 1g \cdot A \times A)
\]  \hspace{1cm} (8)

Thus we see that the \( \sigma \cdot A x A \) term in Eq. (5) is incorrect and should be omitted.

It is precisely this term which is responsible for the disagreement between various hfs calculations. A nonrelativistic calculation has been published of the second order perturbation theory contributions to

\[
R = (8\nu_2 - \nu_1)/\nu_1
\]  \hspace{1cm} (9)

where \( \nu_1 \) and \( \nu_2 \) are the hfs \( \frac{\hbar c}{2} \) the 1s and 2s levels of a one electron atom. The result is

\[
R_s = -(1 - \frac{2}{3} \text{ln} 2), \quad R_d = -\frac{1}{3}(-\frac{17}{10} - \frac{5}{3} \text{ln} 2)
\]  \hspace{1cm} (10)

in units of \( g \sigma^2 m/N \) for \( s \) and \( d \) intermediate states respectively, where \( g \) is the nuclear \( g \)-factor and \( N \) is the proton mass. Reference 3 also quotes a result based upon the Dirac equation,

\[
R_s' = -(\frac{17}{12} - \frac{1}{3} \text{ln} 2).
\]  \hspace{1cm} (11a)

Another calculation using the Dirac equation has yielded this value for \( R_s' \), and
\[ R_{q}^* = - \left( \frac{11}{30} \right) - \frac{1}{3} \sqrt{2} \] (4b)

It is easy to show that \( R_{q}^* + R_{q}^* \) goes over into \( R_{q} + R_{q} \) if one subtracts off the last term of Eq. (5).

We may remark that this cancellation is well known in other contexts, e.g., the Bethe-Salpeter equation and the Breit interaction.

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REFERENCES

4. L.L. Foldy has pointed out to me that Eq. (11a) is \( R_a^* \), not \( R_a^* + R_a^\prime \).
6. See Sec. 4 of W.A. Newcomb and E.E. Salpeter, Phys. Rev. 97, 1146 (1955);
7. See, for example, reference 2, p. 259.
Fig. 1. The Feynman graphs quadratic in $A$. 

FIGURE CAPTION
FIG. 1