HYPERFINE SPIN ORBIT ESR FROM ECE2 SPECIAL RELATIVITY

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ABSTRACT

By replacing the restrictive Dirac approximation, new types of hyperfine spin orbit electron spin resonance (ESR) are developed systematically, revealing many new types of ESR hyperfine structure of great analytical utility. New schemes of quantization are proposed, schemes which depend on whether or not the wave function is relativistic. Order of magnitude estimates are made of the new type of hyperfine splitting, which is superimposed on the fine structure of spin orbit spectroscopy.

Keywords: ECE2 special relativity, ESR spin orbit hyperfine structure.

UFT 330

1. INTRODUCTION

In recent papers of this series {1 - 12} ECE2 theory has been developed from the Jacobi Cartan Evans identity of UFT313 and from hypotheses based on the fact that both torsion and curvature are in general non-zero. The vector format of ECE2 has been developed and its field equations of electromagnetism and gravitation shown to be Lorentz covariant in a space in which both torsion and curvature are non-zero. This unique property leads to the fact that the equations of special relativity can be used in a space in which both torsion and curvature are non zero. In the past, it was thought that special relativity is valid only in flat spacetime, where both torsion and curvature vanish. The new type of special relativity is characterized by a spin connection, indicating that it is part of a generally covariant unified field theory. So the distinction between special and general relativity is no longer needed When considering the interaction of electromagnetic radiation with an atom such as the hydrogen atom, the four potential in ECE2 can be written in terms of spin curvature, indicating that the space is not flat spacetime. In this paper several new types of hyperfine ESR structure are developed systematically in the simplest case, the H atom, whose orbitals are analytical as is well known.

This paper is a summary of the background notes to UFT330 on www.aias.us, and the background notes should be read with the paper. In Note 330(1) a review is given of conventional spin orbit theory in special relativity, indicating the existence of a new term that appears when the restrictive Dirac approximation is not used. This term was first discussed in UFT329. Note 330(2) develops new types of spin orbit fine structure, and Note 330(3) introduces new schemes of quantization, depending on whether or not the wave function is relativistic. The existence of two possible schemes of quantization seems not to have been realized in the literature of about ninety years. Note 330(4) begins the development of these schemes of quantization, and shows that the two schemes give rise to different spectra that can be searched for experimentally. Note 330(5) evaluates the expected magnitude of what is termed "spin orbit hyperfine structure". The various types of hyperfine structure are different for each atom or molecule, giving rise to several new types of analytically useful ESR. The same is true for NMR and MRI. Section 2 of this paper, UFT330, is based on Notes 330(6) and 330(7), in which the new term obtained by lifting the restrictions of the Dirac approximation is developed systematically. The results of this development are compared with a conventional development based on the Dirac approximation.

2. SYSTEMATIC DEVELOPMENT

From UFT329 and Eq. (10) of Note 330(1) the new hamiltonian term obtained by lifting the restrictive Dirac approximation is:

$$H_{01} = -\underline{\sigma}\cdot\underline{p}\,\frac{H_0}{4m^2c^2}\,\underline{\sigma}\cdot\underline{p} \qquad -(1)$$

in the SU(2) basis. It is important to note that $\underline{p}$ is the relativistic momentum defined by:

$$\underline{p} = \gamma\,\underline{p}_0 \qquad -(2)$$

where γ is the Lorentz factor and where $\underline{p}_0$ denotes the classical momentum. When an atom such as hydrogen (H) interacts with a magnetic field, or an electromagnetic field, the minimal prescription is applied to the relativistic four momentum. The vector potential $\underline{A}$ of the magnetic field is introduced in this way, to give:

$$H_{01} = -\underline{\sigma}\cdot\left(\underline{p} - e\underline{A}\right)\frac{H_0}{4m^2c^2}\,\underline{\sigma}\cdot\left(\underline{p} - e\underline{A}\right). \qquad -(3)$$

Here m is the mass of the electron, and c is the vacuum speed of light. The classical hamiltonian H_0 Is defined by the Schroedinger equation:

$$H_0 \phi = \left(-\frac{\hbar^2 \nabla^2}{2m} + U \right) \phi \quad -(4)$$

where ϕ are the classical hydrogenic wave functions, which are well known analytically. The definition (4) can be applied to any material as is well known.

For comparison, the conventional Dirac approximation (see UFT329) leads to the well known spin orbit term:

$$H_{02} = \underline{\sigma} \cdot \left(\underline{p} - e\underline{A} \right) \frac{U}{4m^2c^2} \underline{\sigma} \cdot \left(\underline{p} - e\underline{A} \right) \quad -(5)$$

where the potential energy between the proton and electron of the H atom is:

$$U = \frac{-e^2}{4\pi \epsilon_0 r} . \quad -(6)$$

Here e is the charge on the proton, ϵ_0 the S. I. vacuum permittivity, and r the magnitude of the distance between the proton and the electron. Now apply the relativistic quantization:

$$p^\mu \phi_r = i\hbar \partial^\mu \phi_r \quad -(7)$$

where the relativistic four momentum is:

$$p^\mu = \left(\frac{E}{c}, \underline{p} \right) \quad -(8)$$

and where:

$$\partial^\mu = \left(\frac{1}{c} \frac{\partial}{\partial t}, -\underline{\nabla} \right) . \quad -(9)$$

Here E is the relativistic energy:

$$E = \gamma m c^2 . \quad -(10)$$

In the almost ninety year old development of the Dirac equation, the following quantization is used, (as explained in some previous UFT papers):

$$H_{01}\phi_r = i\hbar\,\underline{\sigma}\cdot\underline{\nabla}\,\frac{H_0}{4m^2c^2}\,\underline{\sigma}\cdot\underline{p}\,\phi_r \quad -(11)$$

The relativistic momentum is used both as an operator and a function. Eq. (11) is the result of lifting the Dirac approximation. The latter gives a number of well known and important results, notably the g factor of the electron, the Thomas factor, spin orbit fine structure, ESR, and also NMR and MRI, antiparticles and correct probabilities. In ECE theory the Dirac equation is developed into the fermion equation, which removes negative energies and the need for the unobservable Dirac sea. So Eq. (11) is well justified. In a rough first approximation, assume that the true relativistic wave function can be approximated by the non relativistic, hydrogenic wave functions. In H, this approximation is justified because spin orbit splitting in H is very small, but observable and important.

There are two types of hamiltonian:

$$H_{011}\phi = \frac{i\hbar}{4m^2c^2}\,H_0\,\phi\,\underline{\sigma}\cdot\underline{\nabla}\,\underline{\sigma}\cdot\underline{p} \quad -(12)$$

and

$$H_{012}\phi = \frac{i\hbar H_0}{4m^2c^2}\,\underline{\sigma}\cdot\underline{p}\,\underline{\sigma}\cdot\underline{\nabla}\,\phi \quad -(13)$$

because H_0 is a constant of motion. Using Pauli algebra:

$$\underline{\sigma}\cdot\underline{\nabla}\,\underline{\sigma}\cdot\underline{p} = \underline{\nabla}\cdot\underline{p} + i\,\underline{\sigma}\cdot\underline{\nabla}\times\underline{p} \quad -(14)$$

and

$$\underline{\sigma}\cdot\underline{p}\;\underline{\sigma}\cdot\underline{\nabla}\phi=\underline{p}\cdot\underline{\nabla}\phi+i\underline{\sigma}\cdot\underline{p}\times\underline{\nabla}\phi. \quad -(15)$$

Therefore:

$$\mathrm{Re}\,H_{011}\phi=-\frac{\hbar}{4m^2c^2}H_0\phi\;\underline{\sigma}\cdot\underline{\nabla}\times\underline{p} \quad -(16)$$

and

$$\mathrm{Re}\,H_{012}\phi=-\frac{\hbar H_0}{4m^2c^2}\;\underline{\sigma}\cdot\underline{p}\times\underline{\nabla}\phi. \quad -(17)$$

so there are two types of new hamiltonian.

Using the minimal prescription:

$$\underline{p}\rightarrow\underline{p}-e\underline{A} \quad -(18)$$

in the presence of an electromagnetic field, several new types of spin orbit ESR fine structure are obtained. For example:

$$H_{ESR}\phi=\frac{e\hbar H_0\phi}{4m^2c^2}\;\underline{\sigma}\cdot\underline{\nabla}\times\underline{A}=\frac{e\hbar H_0\phi}{4m^2c^2}\;\underline{\sigma}\cdot\underline{B} \quad -(19)$$

whose energy levels are:

$$\langle H_{ESR}\rangle=\frac{e\hbar}{4m^2c^2}\langle H_0\rangle\;\underline{\sigma}\cdot\underline{B} \quad -(20)$$

where for the H atom:

$$\langle H_0\rangle=\frac{-e^4}{32\pi^2\epsilon_0^2\hbar^2c^2n^2}. \quad -(21)$$

This is the same result as Eq. (8) of Note 329(6), providing a cross check of concepts and algebra. The expectation value of Eq. (21) can be reexpressed as:

$$\langle H_0 \rangle = -\frac{\hbar c}{2}\left(\frac{\alpha}{r_B}\right)\frac{1}{n^2} \quad -(22)$$

where r_B is the Bohr radius and α the fine structure constant.

The conventional ESR hamiltonian is:

$$\langle H_{ESRo} \rangle = -\frac{e\hbar}{2m}\,\underline{\sigma}\cdot\underline{B} \quad -(23)$$

so the magnitude of this new type of spin orbit hyperfine structure is:

$$\langle H_{ESR} \rangle = \frac{1}{4}\left(\frac{\hbar}{mc}\right)\left(\frac{\alpha}{r_B}\right)\frac{1}{n^2}\langle H_{ESRo} \rangle = \frac{1.33128\times 10^{-5}}{n^2}\langle H_{ESRo} \rangle \quad -(24).$$

in the H atom. This is within range of ESR and NMR spectrometers and if found, would be very useful in the analytical laboratory. In the H atom it depends on the principal quantum number n, but in more complex atoms and molecules it would produce a richer spectral structure. The Dirac approximation misses all this detail.

Two more types of spectra can be obtained using:

$$H_0\phi = \left(-\frac{\hbar^2\nabla^2}{2m} - \frac{e^2}{4\pi\epsilon_0}\frac{r}{r^2}\right)\phi \quad -(25)$$

and:

$$H_{012}\phi = \frac{i\hbar}{4m^2c^2}\,\underline{\sigma}\cdot\underline{\nabla}\left(H_0\phi\right)\underline{\sigma}\cdot\underline{p} \quad -(26)$$

to give:

$$H_{012}\phi = \frac{ie^2\hbar}{16\pi\epsilon_0 r^3}\,\underline{\sigma}\cdot\underline{r}\,\underline{\sigma}\cdot\underline{p}\,\phi - \frac{i\hbar^3}{8m^3c^2}\,\underline{\sigma}\cdot\underline{\nabla}\left(\nabla^2\phi\right)\underline{\sigma}\cdot\underline{p}. \quad -(27)$$

The first part of this expression gives the conventional spin orbit term:

$$\mathrm{Re}\, H_{so}\phi = \frac{e^2\hbar}{16\pi\epsilon_0 m^2 c^2 r^3}\, \underline{\sigma}\cdot\underline{L}\,\phi \quad -(28)$$

where the orbital angular momentum is:

$$\underline{L} = \underline{r}\times\underline{p}. \quad -(29)$$

Note carefully as in Notes 330(1) to 330(5) that $\underline{p}$ is the relativistic momentum, so $\underline{L}$ in Eq. (29) is the relativistic angular momentum:

$$\underline{L} = \gamma\,\underline{L}_0 \,. \quad -(30)$$

So additional spin orbit fine structure appears as developed in Notes 330(1) to 330(5).

In addition there is a second new term from Eq. (27):

$$\mathrm{Re}\, H_2\phi = \frac{\hbar^3}{8m^3c^2}\, \underline{\sigma}\cdot\underline{\nabla}\left(\nabla^2\phi\right)\times\underline{p}. \quad -(31)$$

In the presence of an electromagnetic field this term gives:

$$\mathrm{Re}\, H_2\phi = -\frac{e\hbar^3}{8m^3c^2}\, \underline{\sigma}\cdot\underline{\nabla}\left(\nabla^2\phi\right)\times\underline{A} \quad -(32)$$

whose energy levels are:

$$\langle H_2\rangle = -\frac{e\hbar^3}{8m^3c^2}\, \underline{\sigma}\cdot\int\phi^*\underline{\nabla}\left(\nabla^2\phi\right)d\tau\times\underline{A} \quad -(33)$$

This is also a new type of spin orbit hyperfine structure in ESR and NMR.

Some of these new spectra are developed numerically in Section 3.

Finally in this Section, Note 330(7) gives a detailed summary of some hyperfine structure that emerges from the conventional Dirac approximation. As shown in Note 330(7) the conventional development gives rise to results such as :

$$\langle \mathrm{Re}\, H_{SO1} \rangle = \frac{e\hbar}{8\pi\epsilon_0 m c^2} \left\langle \frac{1}{r^3} \right\rangle \underline{\sigma} \cdot \underline{m}_{ind} \quad -(34)$$

where $\underline{m}_{ind}$ is the induced magnetic dipole moment in an electromagnetic field. This is related directly to the $\underline{B}^{(3)}$ field {1-12} as follows:

$$\underline{B}^{(3)} \propto \underline{m}_{ind.} \quad -(35)$$

In the H atom:

$$\left\langle \frac{1}{r^3} \right\rangle = \frac{1}{a_0^3 L\left(L+\frac{1}{2}\right)(L+1)n^3} \quad -(36)$$

where L is the angular momentum quantum number, and n the principal quantum number. In more complex atoms and molecules this expectation value has a much richer structure. This should also be present in ESR, NMR and MRI. Again this would be very useful for analysis and medicine.

As discussed in Note 330(7) there is also the conventional type two hamiltonian:

$$\langle H_{SO2} \rangle = \frac{e^3\hbar}{16\pi\epsilon_0 m^2 c^2} \left\langle \frac{1}{r} \right\rangle \underline{\sigma} \cdot \underline{B}. \quad -(37)$$

In H:

$$\langle U \rangle = \int \phi^* U \phi \, d\tau = -\frac{e^4 m}{16\pi^2 \epsilon_0^2 \hbar^2 n^2}$$

so the energy levels are:

$$\langle H_{SO2} \rangle = \frac{-}{4mc^2} \left(\frac{e^5}{16\pi^2 \epsilon_0^2 \hbar c^2} \right) \frac{\underline{\sigma} \cdot \underline{B}}{n^2} \quad -(38)$$

and should also be observable. Otherwise the Dirac equation is refuted.

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3 Computation of some expectation values

Most of the relevant terms for Hydrogen have already been computed in paper 329, section 3. Her we present some additional results. In Table 1 the expectation values of $1/r^3$ and $1/r^4$ and their ratio are compiled. We used again the non-relativistic wave functions of Hydrogen as an approximation as described earlier. For quantum number $l = 0$, the expectation values do not exist, which can be seen from the denominator of Eq.(36) for $\langle 1/r^3 \rangle$. The ratio is a multiple of Z/a_0 where a_0 is the Bohr radius. This means that spectroscopic terms of $\langle 1/r^4 \rangle$ are smaller but relevant.

Another expectation value appearing in the new spectroscopy is according to Eq.(33):

$$\langle \mathbf{I}_2 \rangle = \int \psi^* \boldsymbol{\nabla}(\nabla^2 \psi) \, d\tau. \tag{39}$$

We present the radial component of this term in Table 2, together with the kinetic energy

$$\langle E_{\mathrm{kin}} \rangle = -\hbar \int \psi^* (\nabla^2 \psi) \, d\tau. \tag{40}$$

The kinetic energy is positive and only depends on the main quantum number. The integral itself is negative. The radial component of the term (39) exists only for s states and is proportional to $(Z/a_0)^3$.

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n	l	$\langle 1/r^3 \rangle$	$\langle 1/r^4 \rangle$	$\frac{\langle 1/r^4 \rangle}{\langle 1/r^3 \rangle}$
1	0	–	–	–
2	0	–	–	–
2	1	$\frac{Z^3}{24\, a_0^3}$	$\frac{Z^4}{24\, a_0^4}$	$\frac{Z}{a_0}$
3	0	–	–	–
3	1	$\frac{Z^3}{81\, a_0^3}$	$\frac{10\ Z^4}{729\ a_0^4}$	$\frac{10\ Z}{9\ a_0}$
3	2	$\frac{Z^3}{405\, a_0^3}$	$\frac{2\ Z^4}{3645\ a_0^4}$	$\frac{2\ Z}{9\ a_0}$

Table 1: Expectation values $\langle 1/r^3 \rangle$, $\langle 1/r^4 \rangle$ and their ratio.

n	l	$\langle E_{\mathrm{kin}} \rangle$	$\langle I_2 \rangle_r$
1	0	$\frac{\hbar\, Z^2}{a_0^2}$	$\frac{10\, \sqrt{\pi}\, Z^3}{a_0^3}$
2	0	$\frac{\hbar\, Z^2}{4\, a_0^2}$	$\frac{11\, \sqrt{\pi}\, Z^3}{8\, a_0^3}$
2	1	$\frac{\hbar\, Z^2}{4\, a_0^2}$	0
3	0	$\frac{\hbar\, Z^2}{9\, a_0^2}$	$\frac{4\, \sqrt{\pi}\, Z^3}{3^{\frac{5}{2}}\ \sqrt{6}\, a_0^3}$
3	1	$\frac{\hbar\, Z^2}{9\, a_0^2}$	0
3	2	$\frac{\hbar\, Z^2}{9\, a_0^2}$	0

Table 2: Expectation values of kinetic energy and special term of Eq.(33).

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REFERENCES

{1} M. W. Evans, H. Eckardt, D. W. Lindstrom and S. J. Crothers, "Principles of ECE Theory" (open source on www.aias.us as UFT281 to UFT288, New Generation in prep).

{2} M. W. Evans, "Collected Scientometrics" (open source as UFT307 and New Generation 2015).

{3} M. W. Evans, S. J. Crothers, H. Eckardt and K. Pendergast, "Criticisms of the Einstein Field Equation" (CEFE, open source as UFT301, Cambridge International 2010).

{4} L Felker, "The Evans Equations of Unified Field Theory" (UFT302, Abramis 2007).

{5} H. Eckardt, "The ECE Engineering Model" (UFT303, collected equations).

{6} M. W. Evans, H. Eckardt and D. W. Lindstrom, "Generally Covariant Unified Field Theory" (Abramis 2005 to 2011 in seven volumes and open source as the relevant UFT papers)

{7} M .W. Evans, Ed. J. Found. Phys. Chem., (Cambridge International 2011, open source as the relevant UFT papers).

{8} M .W. Evans, Ed. "Definitive Refutations of the Einsteinian General Relativity" (Cambridge International 2012, open source on www.aias.us).

{9} M .W. Evans and L. B. Crowell, "Classical and Quantum Electrodynamics and the B(3) Field" (World Scientific, 2001, open source Omnia Opera section of www.aias.us).

{10} M. W. Evans and S. Kielich., Eds "Modern Nonlinear Optics" (Wiley Interscience, New York 1992, 1993, 1997 and 2001, hardback, softback e book), in two editions and six volumes.

{11} M. W. Evans and J.-P. Vigier, "The Enigmatic Photon", (Kluwer, Dordrecht, 1994 to 2002), hardback and softback, open source Omnia Opera www.aias.us.

{12} M . W. Evans and A. A. Hasanein, "The Photomagneton in Quantum Field Theory" (World Scientific, 1994).