

# NEW TYPES OF ESR AND NMR SPECTROSCOPY FROM THE ECE2 THEORY.

by

M. W. Evans and H. Eckardt,

Civil List, AIAS and UPITEC


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[www.et3m.net](http://www.et3m.net) )

## ABSTRACT

The ECE2 unified field theory is used to develop new types of ESR and NMR spectroscopies of general utility in all atoms and molecules. The Lorentz covariance of the field equations of the theory means that all the equations of special relativity apply in a general spacetime that includes torsion and curvature. The novel resonance terms are expressed in terms of the  $W$  potential of ECE2 theory, which has the same units as the  $A$  potential of Maxwell Heaviside theory.

Keywords: generally covariant ECE2 unified field theory, new ESR and NMR spectroscopies.

UFT 329



## 1. INTRODUCTION

In recent papers of this series {1-12} the ECE2 generally covariant unified field theory has been developed in terms of the equations of special relativity, using the Lorentz covariance of the field equations of the theory. This is a novel type of Lorentz covariance which occurs in a mathematical space with torsion and curvature both always non zero. The ECE2 papers are UFT313-320, and UFT322-328 on [www.aias.us](http://www.aias.us). They are based on the development in UFT313 of the Bianchi identity with torsion - the Jacobi Cartan Evans (JCE) identity. They are also based on novel hypotheses which extend ECE theory, and on methods which reduce the field equations to a format that is identical with the Maxwell Heaviside field equations (MH). Note carefully that the ECE2 field equations are fundamentally different from the MH field equations because the former are written in a space with non zero torsion and non zero curvature, and are based on Cartan geometry. So the ECE2 field equations can be developed for gravitation and electromagnetism. The MH equations on the other hand are equations of the old type of special relativity, a theory that was developed in a mathematical space with no torsion and no curvature, the old concept of four dimensional space time. The new type of special relativity developed in ECE2 theory is very powerful, because it can be used to unify field theory, and to unify concepts of physics in many different ways.

In this paper ECE2 special relativity is used to demonstrate the existence of new types of ESR and NMR in all materials. This is a new subject capable of great development, both theoretically and experimentally. As usual this paper is a short synopsis of detailed calculations found in the accompanying notes to UFT329 on [www.aias.us](http://www.aias.us). Note 329(1) considers numerical corrections to the Sommerfeld and Dirac hamiltonians in ECE2 space, hamiltonians which originate in the ECE2 Einstein energy equation together with considerations of potential energy. The calculations of this note are based on the Dirac type of

rough approximation, which misses the hamiltonian that gives rise to the new effects of this paper. Note 329(2) gives some details of the Sommerfeld and Dirac hamiltonians in three dimensions, using spherical polar coordinates and the constants of motion defined in UFT270 and UFT271. The lagrangian and Euler Lagrange equations are defined. Section 2 of this paper is based on Notes 293(3) - 293(7). In which a careful and precise evaluation is made of the ECE2 hamiltonian, an evaluation which results in the discovery of new types of ESR and NMR.

In Section 3 some energy levels of the new hamiltonian are computed using the hydrogenic wave functions in the first approximation. This method is capable of great development in computational quantum chemistry using contemporary code libraries and supercomputers. In theory, several new types of spectroscopy of great utility emerge.

## 2. NEW ESR AND NMR

The new ESR and NMR emerge from the hamiltonian of ECE2 special relativity:

$$H = \left( p^2 c^2 + m^2 c^4 \right)^{1/2} + U \quad - (1)$$

where  $U$  is the potential energy,  $p$  the relativistic momentum,  $m$  the particle mass, and  $c$  the vacuum speed of light. In the hydrogen (H) atom, used as a simple illustration of the new theory, the potential energy is:

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

where  $e$  is the charge on the proton, and  $\epsilon_0$  the vacuum permittivity in S. I. Units. Here  $r$  is the distance between the proton and the electron of the H atom. The hamiltonian ( 1 ) can be rewritten as:

$$H_0 = H - mc^2 = \frac{p^2 c^2}{m(1+\gamma)} + U \quad (3)$$

in which:

$$\gamma = \left(1 - \frac{p_0^2}{m^2 c^2}\right)^{-1/2} \quad (4)$$

Here  $\gamma$  is the Lorentz factor defined by:

$$p_0^2 = 2m(H_0 - U) \quad (5)$$

where  $p_0$  is the classical particle momentum in the observer frame, related to the relativistic momentum  $p$  by:

$$\underline{p} = \gamma \underline{p}_0 \quad (6)$$

Note carefully that quantization takes place through the relativistic momentum as follows:

$$-i\hbar \underline{\nabla} \psi = \underline{p} \psi \quad (7)$$

where  $\psi$  is the wave function of the hydrogen atom. Therefore the relativistic quantum mechanical wave equation is constructed from Eq. (3), from which either the operator or classical function can always be used. Using the operator in the numerator and the classical function in the denominator produces the following relativistic quantum mechanical equation:

$$\langle H_0 \rangle = -\frac{\hbar^2 c^2}{m} \int \frac{\psi^* \nabla^2 \psi d\tau}{(1+\gamma)} + \int \psi^* U \psi d\tau \quad (8)$$

in which:

$$\underline{p}_0 = m \underline{v}_0 \quad - (9)$$

To a first approximation:

$$\left(1 - \frac{p_0^2}{m^2 c^2}\right)^{-1/2} \sim 1 + \frac{1}{2} \frac{p_0^2}{m^2 c^2} \quad - (10)$$

so the energy levels from Eq. ( 8 ) become:

$$\langle H_0 \rangle = -\frac{\hbar^2 c^2}{2m^2 c^2} \int \frac{\psi^* \nabla^2 \psi d\tau}{\left(2 + \frac{p_0^2}{2m^2 c^2}\right) mc^2} + \int \psi^* U \psi d\tau \quad - (11)$$

In the limit:

$$H_0 - U \ll mc^2 \quad - (12)$$

Eq. ( 11 ) reduces to the well known energy levels of the Schroedinger equation

$$\langle H_0 \rangle = -\frac{\hbar^2}{2m} \int \psi^* \nabla^2 \psi d\tau + \int \psi^* U \psi d\tau = -\frac{me^4}{32\pi^2 \epsilon_0^2 \hbar^2 n^2} \quad - (12)$$

for the H atom.

Using:

$$\left(2 + \frac{H_0 - U}{mc^2}\right)^{-1} = \frac{1}{2} \left(\frac{1 + \frac{H_0 - U}{2mc^2}}{1}\right)^{-1} \sim \frac{1}{2} \left(1 - \frac{H_0 - U}{2mc^2}\right) \quad - (13)$$

for:

$$H_0 - U \ll 2mc^2 \quad - (14)$$

Eq. ( 11 ) becomes:

$$\langle H_0 \rangle = \frac{-me^4}{32\pi^2 \epsilon_0^2 \hbar^2 n^2} + \frac{\hbar^2}{4m^2 c^2} \int \psi^* \nabla^2 ((H_0 - U)\psi) d\tau. \quad (15)$$

There is a shift in the energy levels of the H atom which is different for each principal quantum number  $n$ .

Now use the fact that  $H_0$ , the classical hamiltonian defined by:

$$H_0 = \frac{-me^4}{32\pi^2 \epsilon_0^2 \hbar^2 n^2} \quad (16)$$

is a constant of motion. Therefore

$$\langle H_0 \rangle = \frac{-me^4}{32\pi^2 \epsilon_0^2 \hbar^2 n^2} - \frac{\hbar^2}{4m^2 c^2} \int \psi^* \nabla^2 (U\psi) d\tau + \frac{\hbar^2 H_0}{4m^2 c^2} \int \psi^* \nabla^2 \psi d\tau \quad (17)$$

In the first approximation Eq. (16) can be used for  $H_0$  on the right hand side, so:

$$\langle H_0 \rangle = \frac{-me^4}{32\pi^2 \epsilon_0^2 \hbar^2 n^2} \left( 1 + \frac{\hbar^2}{4m^2 c^2} \int \psi^* \nabla^2 \psi d\tau \right) - \frac{\hbar^2}{4m^2 c^2} \int \psi^* \nabla^2 (U\psi) d\tau. \quad (18)$$

Details of the calculation are given in Note 329(3). In this note it is shown that the usual

Dirac approximation:

$$H \sim E \sim mc^2, \quad (19)$$

$$U \ll E \sim mc^2, \quad (20)$$

leads to:

$$\langle H_0 \rangle = \frac{-me^4}{32\pi^2 \epsilon_0^2 \hbar^2 n^2} - \frac{\hbar^2}{4m^2 c^2} \int \psi^* \nabla^2 (U\psi) d\tau \quad (21)$$

and misses the following term:

$$\langle H_0 \rangle_1 = \frac{-me^4}{32\pi^2 \epsilon_0^2 \hbar^2 n^3} \left( \frac{\hbar^2}{4m^2 c^4} \int \psi^* \nabla^2 \psi d\tau \right) \quad (22)$$

These energy levels can be evaluated by assuming that the wave functions in the first approximation are those from the Schrodinger equation. There are many code libraries of computational quantum chemistry with which to develop a more accurate subject.

As shown in detail in Note 329(4), the new hamiltonian in the SU(2) basis is:

$$H_{01} = -\frac{1}{4m^2 c^2} \underline{\sigma} \cdot \underline{p} H_0 \underline{\sigma} \cdot \underline{p} \quad (23)$$

which leads to the energy level shifts:

$$H_{01} = \frac{\hbar^2 H_0}{4m^2 c^2} \nabla^2 \psi \quad (24)$$

In the old type of special relativity, developed in a space with non-zero torsion and curvature, the effect of an external magnetic field as in ESR and NMR is described by the minimal prescription:

$$\underline{p} \rightarrow \underline{p} - e\underline{A} \quad (25)$$

where A is the vector potential. So the hamiltonian (23) in the presence of a magnetic field becomes:

$$H_{01} = -\frac{H_0}{4m^2 c^2} \underline{\sigma} \cdot (\underline{p} - e\underline{A}) \underline{\sigma} \cdot (\underline{p} - e\underline{A}) \quad (26)$$

which quantizes to

$$H_{01} \psi = -\frac{H_0}{4m^2 c^2} \left( -\hbar^2 \nabla^2 + e^2 A^2 + i\hbar e (\underline{\nabla} \cdot \underline{A} + \underline{A} \cdot \underline{\nabla}) \right) \psi \quad (27)$$

giving many effects as described in Notes for UFT250, and UFT252. As shown in detail in

Note 329(5) the quantization scheme that leads to the new ESR and NMR is:

$$H_{01} \psi = -\frac{H_0}{4m^2c^2} \underline{\sigma} \cdot (-i\hbar \underline{\nabla} - e\underline{A}) \underline{\sigma} \cdot (\underline{p} - e\underline{A}) \psi \quad (28)$$

where  $\underline{p}$  is the relativistic momentum. As shown in Note 329(6) the hamiltonian of relevance

is:

$$H_{ESR} \psi = -\frac{ie\hbar H_0}{4m^2c^2} \underline{\sigma} \cdot \underline{\nabla} \underline{\sigma} \cdot \underline{A} \psi \quad (29)$$

Using the Pauli algebra:

$$\underline{\sigma} \cdot \underline{\nabla} \underline{\sigma} \cdot \underline{A} = \underline{\nabla} \cdot \underline{A} + i \underline{\sigma} \cdot \underline{\nabla} \times \underline{A} \quad (30)$$

its real and physical part is:

$$\text{Re}(H_{ESR}) \psi = \frac{e\hbar H_0}{4m^2c^2} \underline{\sigma} \cdot \underline{B} \psi \quad (31)$$

where

$$\underline{B} = \underline{\nabla} \times \underline{A} \quad (32)$$

is the magnetic flux density defined in the old theory by:

$$\underline{\sigma} \cdot \underline{\nabla} \times \underline{A} = \underline{\sigma} \cdot \underline{B} \quad (33)$$

Using Eq. ( 16 ) in the first approximation, the new ESR and NMR hamiltonian is:

$$\langle \text{Re}(H_{ESR}) \rangle = \frac{-e^5}{128\pi^2 \epsilon_0^2 \hbar mc^2 \hbar^2} \underline{\sigma} \cdot \underline{B} \quad (34)$$

In ECE2 theory (UFT317), the magnetic flux density is defined by:



$$\underline{B} = \underline{\nabla} \times \underline{W} = \underline{\nabla} \times \underline{A} + 2\underline{\omega} \times \underline{A} \quad (35)$$

so the minimal prescription becomes:

$$p^\mu \rightarrow p^\mu - e \underline{W}^\mu \quad (36)$$

where

$$\underline{W}^\mu = \left( \frac{\phi}{W}, c \underline{W} \right) \quad (37)$$

and:

$$\underline{B} = \underline{\nabla} \times \underline{W} = W^{(0)} \underline{R}(\text{spin}) \quad (38)$$

as in UFT317. Therefore as shown in detail in Note 329(7), the new hamiltonian is defined by

spin curvature as follows:

$$Re(H_{ESR}) \psi = \frac{e \hbar H_0 W^{(0)}}{4m^2 c^2} \underline{\sigma} \cdot \underline{R}(\text{spin}) \psi \quad (39)$$

This is true also for all types of well known ESR, NMR and MRI, which can be used to measure the ECE2 spin curvature experimentally.

### 3. COMPUTATION OF ENERGY LEVELS

Section by Dr. Horst Eckardt

# New types of ESR and NMR spectroscopy from the ECE2 theory

M. W. Evans\*<sup>‡</sup>; H. Eckardt<sup>†</sup>  
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## 3 Computation of energy levels

According to eq.(18), the relativistic expectation value of the Hamiltonian can be approximated by

$$\langle H_0 \rangle = E_0 + \langle H_0 \rangle_{s-o} + \langle H_0 \rangle_1 \quad (40)$$

where the three parts are the non-relativistic energy eigenvalues

$$E_0 = -\frac{e^4}{32 \pi^2 \epsilon_0^2 n^2 m c^2}, \quad (41)$$

the spin-orbit contribution of Dirac theory

$$\langle H_0 \rangle_{s-o} = f \int \psi^* \nabla^2 (U\psi) d\tau, \quad (42)$$

and the new additional part

$$\langle H_0 \rangle_1 = -f E_0 \int \psi^* \nabla^2 \psi d\tau, \quad (43)$$

both with the factor

$$f = -\frac{\hbar^2}{4m^2 c^2}. \quad (44)$$

The integrals are evaluated for the Hydrogen wave functions in three dimensions, for details see UFT papers 250 and 308. The Laplace operator in three dimensions with spherical coordinates  $(r, \theta, \phi)$  is

$$\nabla^2 \psi = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial \psi}{\partial r} \right) + \frac{1}{r^2 \sin(\theta)} \frac{\partial}{\partial \theta} \left( \sin(\theta) \frac{\partial \psi}{\partial \theta} \right) + \frac{1}{r^2 \sin^2(\theta)} \frac{\partial^2 \psi}{\partial \phi^2}. \quad (45)$$

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\*email: [emyrone@aol.com](mailto:emyrone@aol.com)

<sup>†</sup>email: [mail@horst-eckardt.de](mailto:mail@horst-eckardt.de)

$n$	$l$	Integral $\langle H_0 \rangle_{s-o}$	Integral $\langle H_0 \rangle_1$
1	0	$-\frac{Z^4}{a_0^3}$	$-\frac{Z^2}{a_0^2}$
2	0	$-\frac{Z^4}{16 a_0^3}$	$-\frac{Z^2}{4a_0^2}$
2	1	$\frac{5Z^4}{48 a_0^3}$	$-\frac{Z^2}{4a_0^2}$
3	0	$-\frac{Z^4}{81 a_0^3}$	$-\frac{Z^2}{9a_0^2}$
3	1	$\frac{Z^4}{27 a_0^3}$	$-\frac{Z^2}{9a_0^2}$
3	2	$\frac{7Z^4}{405 a_0^3}$	$-\frac{Z^2}{9a_0^2}$

Table 1: Energy shifts of Integrals (42) and (43).

Additional parameters appearing in the wave functions are the atomic number  $Z$  and the Bohr radius  $a_0$ . The Coulomb energy has been assumed as

$$U = -\frac{Ze^2}{4\pi\epsilon_0 r}. \quad (46)$$

For Hydrogen we have  $Z = 1$ , for higher  $Z$  values these are very crude approximations.

The integral values appearing in Eqs.(42, 43) have been computed analytically and are listed in Table 1. The ordinary spin-orbit terms depend on the  $n$  and  $l$  quantum numbers, not on  $m_l$ . Surprisingly, the additional term  $\langle H_0 \rangle_1$  does not depend on the angular quantum number  $l$ , only on the main quantum number  $n$ . Obviously a factor of  $1/n^2$  is contained in the result. It should be noticed that this factor also appears in  $E_0$  but has not been multiplied here for the integral values. Test runs with a Laplace operator (45) without angular parts showed that  $\langle H_0 \rangle_1$  becomes dependent on the  $l$  quantum number then. In spectroscopies which are angle-sensitive, we expect that the new term will show an  $l$  dependence.

The numerical values of energy shifts in eV are shown in Table 2. The corrections  $\langle H_0 \rangle_1$  are smaller than those of the Dirac term of spin-orbit coupling. Nonetheless the 1s state is shifted significantly by the new term. This is in the order of magnitude of  $10^{-4}$  eV and should be observable by spectroscopy. From Table 1 it is seen that the new effects grow with atomic number  $Z^2$  while the ordinary spin-orbit terms grow with  $Z^4$ . Therefore these corrections will be less significant for heavier elements.

$n$	$l$	$E_0$	$\langle H_0 \rangle_{s-o}$	$\langle H_0 \rangle_1$	$\langle H_0 \rangle$
1	0	-13.6056919	0.0003623	0.0001811	-13.6051485
2	0	-3.4014230	0.0000226	0.0000113	-3.4013890
2	1	-3.4014230	-0.0000075	0.0000038	-3.4014268
3	0	-1.5117435	0.0000045	0.0000022	-1.5117368
3	1	-1.5117435	-0.0000045	0.0000012	-1.5117468
3	2	-1.5117435	-0.0000009	0.0000004	-1.5117440

Table 2: Energy shifts of Eqs.(42, 43) and total energies in eV.

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