

NEW RESONANCE SPECTROSCOPIES FROM THE ECE FERMION EQUATION

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ABSTRACT

The ECE fermion equation is equivalent to the chiral form of the Dirac equation for some applications, which are illustrated in this paper by the inference of three new types of resonance spectroscopy from a the well known hamiltonian describing the interaction of an electron with the classical electromagnetic field. The three new types of spectroscopy are illustrated using the well known hydrogenic wavefunctions, correctly normalized with computer algebra. It is found that each new type of spectroscopy gives its own pattern of resonance frequencies characterized by the hydrogenic wavefunction being used.

Keywords: ECE theory, fermion equation, new resonance spectroscopies.

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1. INTRODUCTION

In the preceding paper of this series {1 - 10} the ECE fermion equation has been developed to give the new technique of electron spin orbit coupling resonance. The same techniques of using well known Pauli algebra in a different way are used in this paper to give three new types of spin resonance spectroscopy, which are illustrated with the hydrogenic wavefunctions correctly normalized with computer algebra. It is found that that each new type of spectrum has its own pattern of resonance, depending on the hydrogenic wavefunction used. In Section 2 the relevant part of the hamiltonian is defined for the interaction of the ECE electron with the classical electromagnetic field, and this is developed with original use of Pauli algebra as in the preceding paper. It is found that the hamiltonian results in three hitherto unknown types of spin resonance spectroscopy. These are developed with the hydrogenic wavefunctions, which are correctly normalized with computer algebra. In Section 3 the spectra are illustrated with computer algebra, and in theory give rise to different patterns of resonance for each hydrogenic wavefunction.

2. DEVELOPMENT OF THE HAMILTONIAN AND EXPECTATION VALUES OF ENERGY.

Consider the relevant part of the complete hamiltonian {1 - 10} of the ECE fermion equation:

$$H = -\frac{e}{2m} \left(\underline{\sigma} \cdot \underline{p} \underline{\sigma} \cdot \underline{A} + \underline{\sigma} \cdot \underline{A} \underline{\sigma} \cdot \underline{p} \right) \quad (1)$$

where $-e$ is the charge on the electron, m its mass, \underline{p} the linear momentum of the electron and \underline{A} the vector potential of the electromagnetic field in the standard approximation. In ECE physics \underline{A} is greatly developed {1 - 10} and this development will be incorporated in future

papers. Note carefully that Eq. (1) is the well known hamiltonian usually developed into the Zeeman effect, ESR, NMR and MRI. The new type of development given in this and the preceding paper is based on the Pauli algebra given by Merzbacher [11]:

$$\begin{aligned}\underline{\sigma} \cdot \underline{p} &= \frac{\underline{\sigma} \cdot \underline{r}}{r^2} \underline{\sigma} \cdot \underline{r} \underline{\sigma} \cdot \underline{p} \\ &= \frac{\underline{\sigma} \cdot \underline{r}}{r^2} \left(\underline{r} \cdot \underline{p} + i \underline{\sigma} \cdot \underline{r} \times \underline{p} \right) \quad - (2) \\ &= \frac{\underline{\sigma} \cdot \underline{r}}{r^2} \left(\underline{r} \cdot \underline{p} + i \underline{\sigma} \cdot \underline{L} \right)\end{aligned}$$

where the classical orbital angular momentum is defined by:

$$\underline{L} = \underline{r} \times \underline{p}. \quad - (3)$$

Therefore \underline{r} is the position vector, which does not appear in the usual development of the Zeeman effect and ESR.

The hamiltonian (1) is quantized using:

$$\hat{H} \psi = -\frac{e}{2m} \frac{\hbar}{i} \left(\underline{\sigma} \cdot \underline{\nabla} \underline{\sigma} \cdot \underline{A} + \underline{\sigma} \cdot \underline{A} \underline{\sigma} \cdot \underline{\nabla} \right) \psi \quad - (4)$$

where \hbar is the reduced Planck constant and ψ the wavefunction. Note that [11]:

$$\underline{r} \cdot \underline{p} = \frac{\hbar}{i} r \underline{e}_r \cdot \underline{\nabla} = \frac{\hbar}{i} r \underline{e}_r \cdot \underline{e}_r \frac{d}{dr} = \frac{\hbar}{i} r \frac{d}{dr} \quad - (5)$$

where the radial unit vector is defined as:

$$\underline{e}_r = \frac{\underline{r}}{r}. \quad - (6)$$

Similarly:

$$\underline{\sigma} \cdot \underline{A} = \frac{\underline{\sigma} \cdot \underline{r}}{r^2} \left(\underline{r} \cdot \underline{A} + i \underline{\sigma} \cdot \underline{r} \times \underline{A} \right) \quad - (7)$$

For a uniform magnetic field:

$$\underline{A} = \frac{1}{2} \underline{B} \times \underline{r} \quad - (8)$$

in which case:

$$\underline{r} \cdot \underline{A} = 0 \quad - (9)$$

and:

$$\underline{\sigma} \cdot \underline{A} = i \frac{\underline{\sigma} \cdot \underline{r}}{r^2} \underline{\sigma} \cdot \underline{r} \times \underline{A} \quad - (10)$$

It follows (note 251(1) accompanying this paper on www.aias.us) that:

$$\begin{aligned} (\underline{\sigma} \cdot \underline{p} \underline{\sigma} \cdot \underline{A}) \psi &= \frac{\hbar}{r} \left(\underline{\sigma} \cdot \underline{r} \times \underline{A} \frac{\partial \psi}{\partial r} + \frac{\partial}{\partial r} (\underline{\sigma} \cdot \underline{r} \times \underline{A}) \psi \right) \\ &\quad - \frac{1}{r^2} \underline{\sigma} \cdot \underline{r} \times \underline{A} \underline{\sigma} \cdot \underline{L} \psi \quad - (11) \end{aligned}$$

where use has been made of the Leibnitz Theorem. Using Eq. (8) it follows that:

$$\begin{aligned} \frac{1}{r} \underline{r} \times \underline{A} &= \frac{1}{2r} \left(r^2 \underline{B} - \underline{r} (\underline{r} \cdot \underline{B}) \right) \quad - (12) \\ &= \frac{r}{2} \left(\underline{B} - \underline{e}_r (\underline{B} \cdot \underline{e}_r) \right) \end{aligned}$$

and that:

$$\frac{1}{r} \frac{\partial}{\partial r} \underline{r} \times \underline{A} = \underline{B} - \frac{1}{2r} \frac{\partial}{\partial r} \left(r^2 \underline{e}_r (\underline{e}_r \cdot \underline{B}) \right) = \underline{B} - \underline{e}_r (\underline{e}_r \cdot \underline{B}) \quad - (13)$$

It follows that:

$$\underline{\sigma} \cdot \underline{p} \underline{\sigma} \cdot \underline{A} \psi = \underline{\sigma} \cdot \underline{B}_1 \left(\frac{\hbar}{r} \psi + \frac{1}{2} r \frac{\partial \psi}{\partial r} - \frac{1}{2} \underline{\sigma} \cdot \underline{L} \psi \right) \quad - (14)$$

where the modified magnetic flux density is defined by:

$$\underline{B}_1 = \underline{B} - \underline{e}_r (\underline{e}_r \cdot \underline{B}) \quad - (15)$$

The hamiltonian (4) can therefore be defined as:

$$\hat{H}\psi = -\frac{e\hbar}{2m} \underline{\sigma} \cdot \underline{B}_1 \left(\psi + r \frac{d\psi}{dr} \right) + \frac{e}{2m} \underline{\sigma} \cdot \underline{B}_1 \underline{\sigma} \cdot \underline{L} \psi \quad (16)$$

giving three hitherto unknown resonance spectroscopies.

The conventional development of the hamiltonian (4) is well known, and misses out the information given in Eq. (16):

$$\begin{aligned} \hat{H}\psi &= i\frac{e\hbar}{2m} \left(\underline{\nabla} \cdot (\underline{A}\psi) + \underline{A} \cdot \underline{\nabla}\psi \right) \\ &\quad - \frac{e\hbar}{2m} \underline{\sigma} \cdot (\underline{\nabla} \times (\underline{A}\psi)) + \underline{A} \times \underline{\nabla}\psi \quad (17) \\ &= -\frac{e\hbar}{2m} \underline{\sigma} \cdot \underline{B} + i\frac{e\hbar}{2m} \left((\underline{\nabla} \cdot \underline{A})\psi + 2\underline{\nabla}\psi \cdot \underline{A} \right) \end{aligned}$$

using the standard approximation:

$$\underline{B} = \underline{\nabla} \times \underline{A} \quad (18)$$

More details of these calculations are given in Note 251(1) on www.aias.us.

As in Note 251(2) on www.aias.us it is possible to identify three different types of hamiltonian:

$$\hat{H}_1 \psi = -\frac{e\hbar}{2m} \underline{\sigma} \cdot \underline{B}_1 \psi \quad (19)$$

$$\hat{H}_2 \psi = -\frac{e\hbar}{2m} \underline{\sigma} \cdot \underline{B}_1 r \frac{d\psi}{dr} \quad (20)$$

$$\hat{H}_3 \psi = \frac{e}{2m} \underline{\sigma} \cdot \underline{B}_1 \underline{\sigma} \cdot \underline{L} \psi \quad (21)$$

whose energy expectation values are:

$$E_1 = -\frac{e\hbar}{2m} \int \psi^* \underline{\sigma} \cdot \underline{B}_1 \psi d\tau \quad - (22)$$

$$E_2 = -\frac{e\hbar}{2m} \int \psi^* \underline{\sigma} \cdot \underline{B}_1 r \frac{d\psi}{dr} d\tau \quad - (23)$$

$$E_3 = \frac{e}{2m} \int \psi^* \underline{\sigma} \cdot \underline{B}_1 \underline{\sigma} \cdot \underline{L} \psi d\tau \quad - (24)$$

where integration takes place over all space with the Born normalization {11}:

$$\int \psi^* \psi d\tau = 1. \quad - (25)$$

The energy expectation values can be illustrated on the simplest level with the hydrogenic wavefunctions. These are correctly normalized with computer algebra and the first few tabulated in Section 3. The method is illustrated in all detail in Note 251(3) and some details of the principles given here for the hydrogenic wavefunction:

$$\psi = N \alpha e^{-\alpha r} \quad - (26)$$

If the magnetic field is aligned in Z then:

$$\underline{\sigma} \cdot \underline{B}_1 = \sigma_z B_z - \frac{z B_z}{r^2} \underline{\sigma} \cdot \underline{r} = \frac{B_z}{r^2} \left(z^2 \sigma_z + y 2 \sigma_y + x z \sigma_x \right) \quad - (27)$$

However the only well defined component of spin angular momentum in quantum mechanics is {11}:

$$\hat{S}_z \psi = \pm \frac{1}{2} \hbar \psi \quad - (28)$$

so the only term of relevance in Eq. (27) is:

$$\underline{\sigma} \cdot \underline{B}_1 = \left(1 - \left(\frac{z}{r} \right)^2 \right) \sigma_z B_z \quad - (29)$$

In spherical polar coordinates:

$$1 - \left(\frac{z}{r}\right)^2 = 1 - \cos^2 \theta = \sin^2 \theta \quad - (30)$$

and it follows that the expectation values of energy are:

$$E_1 = -\frac{e\hbar}{2m} \sigma_z B_z \int \psi^* \sin^2 \theta \psi d\tau \quad - (31)$$

$$E_2 = -\frac{e\hbar}{2m} \sigma_z B_z \int \psi^* \sin^2 \theta r \frac{\partial \psi}{\partial r} d\tau \quad - (32)$$

$$E_3 = \frac{e}{2m} \sigma_z B_z \int \psi^* \sin^2 \theta \underline{\sigma} \cdot \underline{L} \psi d\tau \quad - (33)$$

The spin angular momentum operator is defined {11} as:

$$\underline{\hat{S}} = \frac{1}{2} \hbar \underline{\hat{\sigma}} \quad - (34)$$

from which the spin orbit operator is well known to be:

$$\underline{\hat{S}} \cdot \underline{\hat{L}} \psi = \frac{\hbar^2}{2} (j(j+1) - l(l+1) - s(s+1)) \psi \quad - (35)$$

where the Clebsch Gordan series gives:

$$j = l + s, l + s - 1, \dots, |l - s| \quad - (36)$$

$$m_j = m_l + m_s \quad - (37)$$

In these expressions:

$$\sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \quad - (38)$$

and spin resonance can be induced between the states of σ_z . The three different types of

resonance spectra are:

$$\omega_1 = \frac{eB_z}{m} \int \psi^* \sin^2 \theta \psi d\tau \quad - (39)$$

$$\omega_2 = \frac{eB_z}{m} \int \psi^* r \sin^2 \theta \frac{\partial \psi}{\partial r} d\tau \quad (40)$$

$$\omega_3 = \frac{eB_z}{m} (j(j+1) - l(l+1) - s(s+1)) \int \psi^* \sin^2 \theta \psi d\tau \quad (41)$$

In computing Eq. (41) use is made of the Clebsch Gordan equation (37) as described in Section 3 so the wavefunction corresponds to the quantum numbers in the correct way. In each case the resonance frequencies depend on the wavefunction being considered, leading to three new types of richly structured spectroscopies and opening up a new area of computational quantum chemistry.

In spherical polar coordinates:

$$d\tau = r^2 dr \sin \theta d\theta d\phi \quad (42)$$

so the integrals are evaluated as follows using computer algebra as in Section 3:

$$\int \psi^* \sin^2 \theta \psi d\tau = \int_{r=0}^{\infty} \int_{\theta=0}^{\pi} \int_{\phi=0}^{2\pi} \psi^* r^2 \sin^4 \theta \psi dr d\theta d\phi \quad (43)$$

and

$$\int \psi^* r \sin^2 \theta \frac{\partial \psi}{\partial r} d\tau = \int_{r=0}^{\infty} \int_{\theta=0}^{\pi} \int_{\phi=0}^{2\pi} \psi^* r^3 \sin^4 \theta \frac{\partial \psi}{\partial r} dr d\theta d\phi \quad (44)$$

In general:

$$\psi = \psi(r, \theta, \phi) \quad (45)$$

In note 251(5) on www.aias.us these results are distinguished carefully from the Zeeman effect, which is described by:

$$\hat{H} \psi = -\frac{e\hbar^2}{2m} g_L m_J B_z \psi \quad (46)$$

where g_L is the well known Landé factor {11}. The Zeeman effect is derived from the standard development of the hamiltonian (4) and gives an entirely different spectrum.

Some sample hand calculations are given in Notes 251(3) and 251(4) using the useful definite integrals:

$$\int_0^{\infty} r^n e^{-ar} dr = \frac{n!}{a^{n+1}} \quad (47)$$

$$\int_0^{\pi} \cos^n \theta \sin \theta d\theta = \frac{1 + (-1)^n}{n+1} \quad (48)$$

$$\int_0^{2\pi} \cos^2 \phi d\phi = \pi \quad (49)$$

Two examples suffice to end this section, using one of the simplest types of hydrogenic wavefunction:

$$\psi = N x e^{-dr} \quad (50)$$

where N is the normalization:

$$N = \left(\frac{d^5}{\pi} \right)^{1/2} \quad (51)$$

and in spherical polar coordinates:

$$x = r \sin \theta \cos \phi \quad (52)$$

The energy expectation value is:

$$E_1 = -\frac{e\hbar^2}{2m} \sigma_z B_z \left(\int \psi^* \psi (1 - \cos^2 \theta) d\tau \right) \quad (53)$$

and one of the integrals to be evaluated is:

$$\begin{aligned}
 \bar{T} &= \frac{1}{\pi} \int_0^{\infty} r^4 e^{-2dr} dr \int_0^{\pi} \sin^3 \theta \cos^2 \theta d\theta \int_0^{2\pi} \cos^2 \phi d\phi \\
 &= \frac{3}{4} \int_0^{\pi} \sin^3 \theta \cos^2 \theta d\theta \\
 &= \frac{3}{4} \left(\int_0^{\pi} \cos^2 \theta \sin \theta d\theta - \int_0^{\pi} \cos^4 \theta \sin \theta d\theta \right) \\
 &= \frac{1}{3}. \quad \text{--- (54)}
 \end{aligned}$$

Obviously, hand calculation becomes impractical very quickly, so the energy expectation values given in Eqs. (39) to (41) are evaluated by computer algebra in Section 3 and the results tabulated.

The second example is the evaluation of:

$$\bar{E}_2 = -\frac{e\hbar}{2m} \sigma_z B_z \int \psi^* r \sin^2 \theta \frac{\partial \psi}{\partial r} d\tau \quad \text{--- (55)}$$

where a differentiation of the wavefunction must be carried out with respect to r :

$$\frac{\partial \psi}{\partial r} = N \sin \theta \cos \phi e^{-dr} (1-dr) \quad \text{--- (56)}$$

Therefore:

$$\bar{E}_2 = -\frac{e\hbar}{2m} N^2 \sigma_z B_z \int r \sin^4 \theta \cos^2 \phi (1-dr) e^{-2dr} d\tau \quad \text{--- (57)}$$

Using the standard integral:

$$\int \sin^4 \theta d\theta = \frac{3\theta}{8} - \frac{\sin 2\theta}{4} + \frac{\sin 4\theta}{32} \quad \text{--- (58)}$$

it is found that:

$$E_2 = -\frac{3\pi e\hbar d^5 \sigma_z B_z}{16} \int_0^\infty r(1-dr)e^{-2dr} dr \quad (59)$$

In these calculations:

$$\int_0^\infty r e^{-2dr} dr = \frac{1}{4d^2}, \quad \int_0^\infty r^2 e^{-2dr} dr = \frac{1}{4d^3} \quad (60)$$

For this particular wavefunction it is found that:

$$E_2 = 0 \quad (61)$$

but as shown in Section 3, the energy expectation values^s are non zero in general, giving a new type of spin resonance spectrum.

3. COMPUTATION OF ENERGY EXPECTATION VALUES OF THE HYDROGENIC WAVEFUNCTIONS, AND RESONANCE FREQUENCIES.

Section by Dr. Horst Eckardt.

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New resonance spectroscopies from the ECE fermion equation

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3 Computation of energy expectation values of the Hydrogenic wave functions, and resonance frequencies

The expectation values of energies E_1 - E_3 defined in section 2 (Eqs.(31-33)) are evaluated by computer algebra. The operator $\boldsymbol{\sigma} \cdot \mathbf{L}$ is replaced with the quantum number eigenvalues as given by Eq. (41). Basis of evaluation are the analytically given Hydrogen-like wave functions as used in paper 250. The constant factors of the energy eigenvalues have been compiled in the following list, extended by their numerical values in electron Volts (eV). To obtain the full energy expectation values, the results listed in the tables have to be multiplied by these values.

$$E_1 = E_2 = -\frac{e \hbar}{2 m} \sigma_Z B_Z = -3.63695 \cdot 10^{-4} \sigma_Z B_Z, \quad (62)$$

$$E_3 = -E_1. \quad (63)$$

The frequencies factors in Hz (Eqs.(39-41)) then are given by

$$\omega_1 = \omega_2 = \omega_3 = \frac{e B_Z}{m} = 1.75882 \cdot 10^{11} B_Z. \quad (64)$$

From Table 1 it can be seen that E_1 and E_2 give only minor corrections of spectra as expected. In Table 2 the energy eigenvalues E_3 have been listed. In contrast to Table 1, these energies depend on the relativistic quantum numbers which lead to a common factor

$$F_j := j(j+1) - l(l+1) - s(s+1). \quad (65)$$

It can be seen that this factor changes sign so that corrections in both directions appear. The corrections are small again according to Eq.(63). The spectral energy differences (Eqs.(39-41)) of section 2) are in the range of $10^{11} Hz$ and therefore detectable.

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n	l	m_l	E_1	E_2
1	0	0	$\frac{2}{3}$	-1
2	0	0	$\frac{2}{3}$	-1
2	1	0	$\frac{2}{5}$	$-\frac{3}{5}$
2	1	± 1	$\frac{4}{5}$	$-\frac{6}{5}$
3	0	0	$\frac{2}{3}$	-1
3	1	0	$\frac{2}{5}$	$-\frac{3}{5}$
3	1	± 1	$\frac{4}{5}$	$-\frac{6}{5}$
3	2	0	$\frac{10}{21}$	$-\frac{5}{7}$
3	2	± 1	$\frac{4}{7}$	$-\frac{6}{7}$
3	2	± 2	$\frac{6}{7}$	$-\frac{9}{7}$

Table 1: Energies E_1 and E_2 .

n	l	m_l	j	s	m_s	m_j	F_j	E_3
1	0	0	1/2	1/2	-1/2	-1/2	0	0
1	0	0	1/2	1/2	1/2	1/2	0	0
2	0	0	1/2	1/2	-1/2	-1/2	0	0
2	0	0	1/2	1/2	1/2	1/2	0	0
2	1	-1	3/2	1/2	-1/2	-3/2	1	$\frac{4}{5}$
2	1	-1	3/2	1/2	1/2	-1/2	1	$\frac{4}{5}$
2	1	0	1/2	1/2	-1/2	-1/2	-1	$-\frac{2}{5}$
2	1	0	3/2	1/2	1/2	1/2	1	$\frac{2}{5}$
2	1	1	1/2	1/2	-1/2	1/2	-1	$-\frac{4}{5}$
2	1	1	3/2	1/2	1/2	3/2	1	$\frac{4}{5}$
3	0	0	1/2	1/2	-1/2	-1/2	0	0
3	0	0	1/2	1/2	1/2	1/2	0	0
3	1	-1	3/2	1/2	-1/2	-3/2	1	$\frac{4}{5}$
3	1	-1	3/2	1/2	1/2	-1/2	1	$\frac{4}{5}$
3	1	0	1/2	1/2	-1/2	-1/2	-1	$-\frac{2}{5}$
3	1	0	3/2	1/2	1/2	1/2	1	$\frac{2}{5}$
3	1	1	1/2	1/2	-1/2	1/2	-1	$\frac{4}{5}$
3	1	1	5/2	1/2	1/2	3/2	1	$\frac{4}{5}$
3	2	-2	5/2	1/2	-1/2	-5/2	2	$\frac{12}{7}$
3	2	-2	5/2	1/2	1/2	-3/2	2	$\frac{12}{7}$
3	2	-1	3/2	1/2	-1/2	-3/2	-2	$-\frac{8}{7}$
3	2	-1	5/2	1/2	1/2	-1/2	2	$\frac{8}{7}$
3	2	0	3/2	1/2	-1/2	-1/2	-2	$-\frac{20}{21}$
3	2	0	5/2	1/2	1/2	1/2	2	$\frac{20}{21}$
3	2	1	3/2	1/2	-1/2	1/2	-2	$-\frac{8}{7}$
3	2	1	5/2	1/2	1/2	3/2	2	$\frac{8}{7}$
3	2	2	3/2	1/2	-1/2	3/2	-2	$-\frac{12}{7}$
3	2	2	5/2	1/2	1/2	5/2	2	$\frac{12}{7}$

Table 2: Energies E_3 with $F_j = j(j+1) - l(l+1) - s(s+1)$.