DEVELOPMENT OF THE ESOR HAMILTONIAN

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ABSTRACT

The hamiltonian for electron spin orbit resonance is developed to show that it is richly structured in general and that it is an entirely new form of resonance spectroscopy. The development is made possible through a novel use of Pauli algebra. It is shown that the hamiltonian gives results that are different from those of the anomalous Zeeman effect. The hamiltonian is obtained from the ECE fermion equation or chiral Dirac equation, giving great confidence as to its eventual experimental verification.

Keywords: ECE fermion equation, electron spin orbit resonance (ESOR).

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1. INTRODUCTION

In the immediately preceding paper of this series of two hundred and fifty papers to date {1 - 10} the ECE fermion equation was used to produce a new form of resonance spectroscopy designated electron spin orbit resonance (ESOR). The new ESOR spectroscopy emerges from the fermion equation (or chiral Dirac equation) by novel use of Pauli algebra. In Section 2 the ESOR hamiltonian is developed and refined from the original hamiltonian of the fermion equation and shown to consist of two main parts, independent of and dependent on the position vector r. So the energy eigenvalues of the hamiltonian must be evaluated with this spatial dependence taken into account, resulting in a rich array of new results. In Section 3, some examples for hydrogen are given using computer algebra and graphics.

2. CALCULATION OF THE ESOR HAMILTONIAN

Consider the hamiltonian of the fermion equation (or chiral Dirac equation) in the usual approximation $\{1 - 10\}$:

$$Ent = \left(nc^{2} + e\phi + \frac{1}{dm} \stackrel{\sigma}{=} \cdot \left(p - eA\right) \left(1 + \frac{e\phi}{dmc^{2}}\right) \stackrel{\sigma}{=} \cdot \left(p - eA\right) \right) n' - (1)$$

.

Here m is the mass of an electron interacting with an electromagnetic field with scalar potential ϕ and vector potential A, and - e is the charge on the electron. The complete calculations are given in note 250(7) accompanying this paper on <u>www.aias.us</u>. Here we consider one term in the complete equation (1), i.e.:

$$H_{1}\phi = -\frac{e}{2m}\left(\underline{\sigma}\cdot\underline{A}\,\underline{\sigma}\cdot\underline{P}\,+\underline{\sigma}\cdot\underline{P}\,\underline{\sigma}\cdot\underline{A}\right)\phi - (a)$$

By regarding σ as a function this term can be developed as:

$$H_{i}\psi = -\frac{e}{dm}\left(\underline{A}\cdot\underline{p}+\underline{p}\cdot\underline{A}\cdot\underline{i}\sigma\cdot\underline{A}\times\underline{p}+\underline{i}\sigma\cdot\underline{p}\times\underline{A}\right)\psi - (3)$$

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using Pauli algebra {11}. For a uniform magnetic field:

$$\begin{array}{l}
\underline{A} = \frac{1}{2}\underline{B} \times \underline{\Gamma} - (4) \\
\text{so:} \quad \underline{H}_{1} \psi = -\frac{\varrho}{4m} \left(\underline{B} \times \underline{\Gamma} \cdot \underline{\rho} + \underline{\rho} \cdot \underline{B} \times \underline{\Gamma} \\
+ i \underline{\sigma} \cdot (\underline{B} \times \underline{\Gamma}) \times \underline{\rho} + i \underline{\rho} \times (\underline{B} \times \underline{\Gamma}) \right) \psi - (5) \\
\end{array}$$
By regarding p as a function:
$$\begin{array}{l}
\underline{A} = \frac{1}{2}\underline{B} \times \underline{\Gamma} - (4) \\
\underline{B} \times \underline{\Gamma} + \underline{\rho} \times \underline{\Gamma} + \underline{\rho} \times \underline{\Gamma} \\
\underline{B} \times \underline{C} \\
\underline{B} \underline{C} \\
\underline{B} \times \underline{C} \\
\underline{B} \times$$

$$\underline{B} \times \underline{r} \cdot \underline{P} = \underline{B} \cdot \underline{r} \times \underline{P} = \underline{B} \cdot \underline{L} - [6]$$

so the hamiltonian (3) becomes:

$$H_{1}\psi = -\frac{e}{2m} \sqsubseteq \cdot \underline{B}\psi + (i\underline{\sigma} \cdot \underline{A} \times \underline{p} + i\underline{\sigma} \cdot \underline{p} \times \underline{A})\psi.$$

$$-(7)$$

At this stage p is regarded as an operator, so the second term on the right hand side of Eq. (7) does not vanish. The use of p and 5 as functions or operators is arbitrary, and justified only by successful comparison with experimental data. From Eqs. (4) and

(7) the hamiltonian can be written as:

$$H_{1} \psi = \left(-\frac{e}{2m} \sqsubseteq \cdot \underline{B} - \frac{e}{2m} \underbrace{\sigma} \cdot \underline{B} + \ldots\right) = -\frac{e}{2m} \left(\bigsqcup_{n=1}^{n} + 2\underbrace{S} \right) \psi$$

$$-(8)$$

The total angular momentum is conserved so the result ($\$) is rewritten as:

$$H_{1}\psi = -\frac{e}{2m}g_{\perp}^{T}\underline{J}\cdot\underline{B}\psi - (9)$$

where \Im_{L} is the Lande factor. A complete derivation of Eq. (\Im) is given in Note

250(2). Here J is defined by:

$$J = L + S, ..., 1L - S - (10)$$

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which is a Clebsch Gordan series. The conventional spin orbit term emerges from another term of the fermion hamiltonian:

$$H_{sor}\psi = \frac{e}{4mc^{2}} \frac{\sigma \cdot (p - eA)}{p - eA} \phi \frac{\sigma \cdot (p - eA)}{p$$

in which the first p is regarded as an operator but in which the second p is regarded as a function as in note 248(8) accompanying UFT248 on <u>www.aias.us.</u> So the conventional spin orbit hamiltonian is:

$$H_{so} = -\frac{ieh}{4m^2c^2} \left(\underline{\sigma} \cdot \underline{\nabla} \phi \underline{\sigma} \cdot \underline{P} \right) \psi - (12)$$

The standard assumption:

$$E = -\overline{\Sigma}\phi - (B)$$

is now used to find that:

$$H_{sor} \psi = -\frac{ieh}{4m^2c^2} \underbrace{\sigma \cdot E \sigma \cdot p}_{4m^2c^2} - (14)$$

At this point $\underline{\sigma}$ is regarded as a function so: $\underline{\sigma} \cdot \underline{E} \ \underline{\sigma} \cdot \underline{\rho} = \underline{E} \cdot \underline{\rho} + i \ \underline{\sigma} \cdot \underline{E} \times \underline{\rho} - (15)$

so the real valued part of the spin orbit hamiltonian is:

$$\hat{H}_{so} = \frac{e\hat{t}}{4m^2c^2} \cdot E \times p = (16)$$

Finally the standard Coulomb law is used:

$$E = -\nabla \phi = -\frac{e}{4\pi\epsilon_0 r^3} r - (17)$$

so:

$$H_{sor} = -\frac{e\hbar}{8\pi c^2 F_{om}^2 r^3} - (18)$$

where the classical angular momentum is:

$$\underline{L} = \underline{r} \times \underline{p} \cdot - (19) - (20)$$

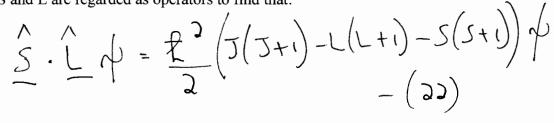
The complete conventional ESR hamiltonian is therefore:

$$\widehat{A} + = \left(\begin{array}{c} -\frac{k}{2m} & \underline{L} \cdot \underline{B} - e\underline{k} & \underline{\sigma} \cdot \underline{B} - \underline{g} & \underline{S} \cdot \underline{L} \end{array} \right) ,$$

where the spin orbit coupling constant is

$$e = \frac{e}{4\pi c^2 \epsilon_0 m^2 r^3} - (21)$$

Finally both S and L are regarded as operators to find that:



However, there are several other ways of developing the original hamiltonian of the

fermion equation, and ESOR is the result of one of these.

Using Pauli algebra {11}:

$$\frac{\sigma \cdot \rho}{f} = \frac{1}{\sqrt{2}} \frac{\sigma \cdot r}{\sigma} \left(\frac{r \cdot \rho}{f} + i \frac{\sigma}{\sigma} \cdot L \right) - (23)$$

$$\frac{\sigma \cdot A}{\sigma} = \frac{1}{\sqrt{2}} \frac{\sigma \cdot r}{\sigma} \left(\frac{r \cdot A}{\sigma} + i \frac{\sigma}{\sigma} \cdot \frac{r}{\sigma} \times A \right) - (24)$$

For a uniform magnetic field:

$$\underline{r} \cdot \underline{A} = 0 - (25)$$

$$\underline{r} \cdot \underline{A} = -\frac{1}{7^{2}} \cdot \underline{r} \cdot \underline{C} \cdot \underline{A} \times \underline{r} - (26)$$

$$\underline{r} \cdot \underline{A} = -\frac{1}{7^{2}} \cdot \underline{r} \cdot \underline{C} \cdot \underline{C} \cdot \underline{A} \times \underline{r} - (26)$$

$$\underline{\sigma} \cdot \underline{r} \times \underline{A} = -\frac{1}{7^{2}} \cdot \underline{r} \cdot \underline{r} \cdot \underline{C} \cdot \underline{C} \times \underline{A} - (27)$$

so:

A

and

as in note 250(7). Using these results it is found that:

$$H_{1} = -\frac{e}{2m} \left(\frac{\rho}{P} \cdot A + A \cdot \rho \right) \psi - (28)$$

$$= -\frac{e}{2m} \frac{\sigma}{P} \cdot A \times \Gamma \sigma \cdot L \psi$$

Now introduce the operator

-

$$S = \frac{1}{2} \frac{1}{5} \frac{1}{5} - (29)$$

so that:

$$H_{I}\psi = -\frac{\partial e}{f_{mr}^{2}} \cdot A \times r \leq \cdot \lfloor \psi - (3)$$

For a uniform magnetic field

$$A = \frac{1}{2}B \times (-(3))$$

so

$$\frac{A \times \underline{r}}{2} = \underline{l} \left(\underline{B} \times \underline{r} \right) \times \underline{r} = \frac{1}{2} \left(\underline{r} \left(\underline{r} \cdot \underline{B} \right) - \underline{r}^{2} \underline{B} \right) - \underline{r}^{2} \underline{B}$$

$$= (32)$$

giving the hamiltonian in the form:

$$H_{I}\psi = \frac{e}{Rm} \frac{\sigma}{\sigma} \cdot \left(\frac{B}{B} - \frac{c}{r} \cdot \frac{(r \cdot B)}{r^{2}}\right) \frac{s}{s} \cdot \frac{1}{L} \frac{d}{r^{2}}$$
$$= -\frac{e}{2m} \left(\frac{P \cdot A' + A \cdot P}{r}\right) \frac{d}{r^{2}} - \frac{(33)}{r^{2}}$$

Its expectation value is:

$$\langle \hat{H} \rangle = \frac{e}{E_m} \left[\gamma^* \hat{H} \gamma d\tau - (34) \right]$$

where the integration is carried out over all space and where the wavefunction is normalized:

$$\int \psi^* \psi \, d\tau = 1 - (35)$$

$$\int (\hat{J})^2 - \hat{L}^2 - \hat{S}^2) \psi - (35)$$

$$= f^2 (J(J+i) - L(L+i) - S(S+i)) \psi$$

Use the result:

S

Therefore as in note 250(9) the energy eigenvalues are:

$$E = e \frac{f}{2} \left(J(J+i) - L(L+i) - J(S+i) \right) \left(\frac{\sigma}{2} \cdot \frac{B}{2} - \int \frac{1}{2} \frac{\sigma}{2} \cdot \frac{F}{2} \cdot \frac{F}{2} \cdot \frac{B}{2} \cdot \frac{1}{2} \frac{\sigma}{2} - \frac{1}{2} \frac{\sigma}{2} \cdot \frac{B}{2} - \frac{1}{2} \frac{\sigma}{2} - \frac{1}{2} \frac{\sigma}{2} - \frac{1}{2} \frac{\sigma}{2} - \frac{1}{2} \frac{\sigma}{2} \frac{\sigma}{2} - \frac{1}{2} \frac{\sigma}{2} \frac{\sigma}{2} \frac{\sigma}{2} - \frac{1}{2} \frac{\sigma}{2} \frac{\sigma}{$$

In spherical polar coordinates:

$$\chi = i \sin \theta \cos \phi - (38)$$

$$\chi = i \sin \theta \sin \phi - (38)$$

$$\chi = i \cos \theta$$

integration of a function f over all space means that:

If the magnetic field is aligned in Z then in Cartesian coordinates:

$$\frac{\sigma \cdot r}{r} \cdot B = \frac{\sigma^2 z^2 B_z}{z^2 + y^2 + z^2} - (40)$$

If it is assumed on average that:

$$\left\langle \frac{\chi^2 + \chi^2 + 2}{\chi^2 + 2} \right\rangle^{=}$$

then Eq. (37) reduces to

$$E = \frac{1}{3} \frac{ef}{m} \sigma_z B_z \left(J(J+i) - L(L+i) - J(S+i) \right)^{-(42)}$$

and electron spin orbit resonance (ESOR) occurs at:

spin orbit resonance (ESOR) occurs at:

$$\omega = \frac{d}{3} \frac{e}{m} B_{Z} \left(J \left(J + I \right) - L \left(L + I \right) - S \left(S + I \right) \right) - \left(4J \right)$$

 $\frac{1}{3} - (41)$

In spherical polar coordinates:

$$\frac{X_{3}+\lambda_{3}+2}{2}$$

so:

In spherical polar coordinates:

$$\frac{7^{3}}{3^{3}+7^{3}+7^{3}} = \cos^{2}\theta - (44)$$
so:

$$\int \sqrt{\frac{5 \cdot \Gamma}{7^{3}}} = \beta_{2} \sqrt{2} \int \int \sqrt{\frac{1}{7}} \sqrt{\frac{1}{7$$

It is seen that this part of the hamiltonian is r dependent and must be evaluated for each wavefunction ψ . It is well known that the only analytical wavefunctions are the hydrogenic wavefunctions. So computer algebra is used in Section 3 to evaluate a few results. 1 1/2 . dora (- 5) For example the $d p_1$ orbital is:

$$\frac{1}{|a_{p_2}|^2} = \frac{1}{|a_{p_2}|^2} = \frac{1}{|a_{p_2}|^2} \left(\frac{1}{|a_{m_2}|^2} \right) \frac{r}{a_0} \left(\frac{1}{|a_{m_2}|^2} \right) \frac{r}{|a_{m_2}|^2} \left(\frac{1}{|a_{m_2}|^2$$

so in this case:

$$\int \frac{d}{\sqrt{\frac{\sigma \cdot r}{r}}} \frac{r}{r} \cdot \frac{\beta}{r} d\tau = \frac{\sigma_z \beta_z}{16 \alpha_0^5} \int_{0}^{1/4} \frac{\sigma_z \beta_z}{r} \left(\frac{-r}{\alpha_0} \right) dr \left(\frac{\sigma_z \beta_z}{r} \right) \frac{dr}{r} \left(\frac{\sigma_z \beta_z}{r} \right) \frac{dr}{r}$$

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However for other orbitals this part of the hamiltonian gives non - zero eigenvalues of energy in general, and a richly structured spectrum.

3. NUMERICAL EVALUATION WITH HYDROGENIC WAVEFUNCTIONS

Section by Dr. Horst Eckardt

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Development of the ESOR Hamiltonian

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3 Numerical evaluation with Hydrogenic wave functions

The Hydrogenic wave functions in spherical coordinates are defined by

$$\psi(r,\theta,\phi) = R_{nl}(r) Y_{lm}(\theta,\phi)$$
(48)

where n is the principal quantum number and l, m are the quantum numbers of angular momentum. R_{nl} are the radial parts of the wave functions and Y_{lm} the spherical harmonics which represent the angular part. The spherical harmonics are listed in [12] up to l = 3. The radial wave functions are in some tabular works given with wrong normalization constants and therefore listed here in Table 1. Normalization has been checked by executing the integral

$$N = \int_0^\infty R_{nl}(r)^2 r^2 dr.$$
 (49)

The norm evaluates to N = 1 in all cases. The energy eigenvalues of Eq.(37) respectively Eq.(45) can be written as a sum of two terms E_1 and E_2 :

$$E = E_1 + E_2, \tag{50}$$

$$E_1 = \frac{e \ h}{2 \ m} F_J \ \sigma_Z \ B_Z,\tag{51}$$

$$E_2 = \frac{e \hbar}{2 m} F_J \sigma_Z B_Z \int_0^{2\pi} \int_0^{\pi} \int_0^{\infty} \psi^* \cos^2 \theta \ \psi \ r^2 \ \sin \theta \ dr \ d\theta \ d\phi \tag{52}$$

with the quantum number function

$$F_J = J(J+1) - L(L+1) - S(S+1).$$
(53)

The results are listed in Table 2. The energies are given in units of $e\hbar/(2m)$. There is no contribution from S states. The numerical factor in eV is

$$\frac{e\ \hbar}{2\ m} = 3.63695 \cdot 10^{-4}\ eV. \tag{54}$$

This is only a very small spectral correction. It has to be multiplied by the results given in Table 2 to obtain the quantum-number dependent energy values.

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| n | l | R_{nl} |
|---|---|--|
| 1 | 0 | $2\left(\frac{Z}{a_0}\right)^{\frac{3}{2}}e^{-\frac{rZ}{a_0}}$ |
| 2 | 0 | $\frac{\left(\frac{Z}{a_0}\right)^{\frac{3}{2}}}{2^{\frac{3}{2}}} \left(2 - \frac{rZ}{a_0}\right) e^{-\frac{rZ}{2a_0}}$ |
| 2 | 1 | $\frac{Z}{2\sqrt{6}a_0} \left(\frac{Z}{a_0}\right)^{\frac{3}{2}} r e^{-\frac{r Z}{2 a_0}}$ |
| 3 | 0 | $\frac{\left(\frac{Z}{a_0}\right)^{\frac{3}{2}}}{3^{\frac{5}{2}}} \left(\frac{4r^2 Z^2}{9a_0^2} - \frac{4rZ}{a_0} + 6\right) e^{-\frac{rZ}{3a_0}}$ |
| 3 | 1 | $\frac{2Z}{27\sqrt{6}a_0} \left(\frac{Z}{a_0}\right)^{\frac{3}{2}} r \left(4 - \frac{2rZ}{3a_0}\right) e^{-\frac{rZ}{3a_0}}$ |
| 3 | 2 | $\frac{4 Z^2}{81 \sqrt{30} a_0^2} \left(\frac{Z}{a_0}\right)^{\frac{3}{2}} r^2 e^{-\frac{r Z}{3 a_0}}$ |

Table 1: Radial wave functions for Hydrogenic orbitals.

References

 $[12] \ http://mathworld.wolfram.com/SphericalHarmonic.html$

| n | L | M_L | J | S | M_S | M_J | F_{j} | E_1 | E_2 | $E_1 + E_2$ |
|----------|---|-------|---------------------|-----|-------|---------------------|---------|-------|------------------|------------------|
| 1 | 0 | 0 | 1/2 | 1/2 | -1/2 | -1/2 | 0 | 0 | 0 | 0 |
| 1 | 0 | 0 | 1/2 | 1/2 | 1/2 | -1/2 | 0 | 0 | 0 | 0 |
| 2 | 0 | 0 | 1/2 | 1/2 | -1/2 | -1/2 | 0 | 0 | 0 | 0 |
| 2 | 0 | 0 | 1/2 | 1/2 | 1/2 | -1/2 | 0 | 0 | 0 | 0 |
| 2 | 1 | -1 | $\mathbf{3/2}$ | 1/2 | -1/2 | -3/2 | 1 | 1 | $\frac{1}{5}$ | $\frac{6}{5}$ |
| 2 | 1 | -1 | $\mathbf{3/2}$ | 1/2 | 1/2 | -1/2 | 1 | 1 | $\frac{1}{5}$ | $\frac{6}{5}$ |
| 2 | 1 | 0 | 1/2 | 1/2 | -1/2 | -1/2 | -1 | -1 | $-\frac{3}{5}$ | $-\frac{8}{5}$ |
| 2 | 1 | 0 | $\mathbf{3/2}$ | 1/2 | 1/2 | 1/2 | 1 | 1 | $\frac{3}{5}$ | $\frac{8}{5}$ |
| 2 | 1 | 1 | 1/2 | 1/2 | -1/2 | 1/2 | -1 | -1 | $-\frac{1}{5}$ | $-\frac{6}{5}$ |
| 2 | 1 | 1 | 3/2 | 1/2 | 1/2 | 3/2 | 1 | 1 | $\frac{1}{5}$ | $\frac{6}{5}$ |
| 3 | 0 | 0 | 1/2 | 1/2 | -1/2 | -1/2 | 0 | 0 | 0 | 0 |
| 3 | 0 | 0 | 1/2 | 1/2 | 1/2 | -1/2 | 0 | 0 | 0 | 0 |
| 3 | 1 | -1 | $\mathbf{3/2}$ | 1/2 | -1/2 | -3/2 | 1 | 1 | $\frac{1}{5}$ | $\frac{6}{5}$ |
| 3 | 1 | -1 | $\mathbf{3/2}$ | 1/2 | 1/2 | -1/2 | 1 | 1 | $\frac{1}{5}$ | $\frac{6}{5}$ |
| 3 | 1 | 0 | 1/2 | 1/2 | -1/2 | -1/2 | -1 | -1 | $-\frac{3}{5}$ | $-\frac{8}{5}$ |
| 3 | 1 | 0 | 3 / 2 | 1/2 | 1/2 | 1/2 | 1 | 1 | $\frac{3}{5}$ | $\frac{8}{5}$ |
| 3 | 1 | 1 | 1/2 | 1/2 | -1/2 | 3 / 2 | -1 | -1 | $-\frac{1}{5}$ | $-\frac{6}{5}$ |
| 3 | 1 | 1 | 5/2 | 1/2 | 1/2 | -5/2 | 1 | 1 | $\frac{1}{5}$ | $\frac{6}{5}$ |
| 3 | 2 | -2 | 5/2 | 1/2 | -1/2 | -5/2 | 2 | 2 | $\frac{2}{7}$ | $\frac{16}{7}$ |
| 3 | 2 | -2 | 5/2 | 1/2 | 1/2 | -3/2 | 2 | 2 | $\frac{2}{7}$ | $\frac{16}{7}$ |
| 3 | 2 | -1 | 3 / 2 | 1/2 | -1/2 | -3/2 | -2 | -2 | $-\frac{6}{7}$ | $-\frac{20}{7}$ |
| 3 | 2 | -1 | 5/2 | 1/2 | 1/2 | -1/2 | 2 | 2 | $\frac{6}{7}$ | $\frac{20}{7}$ |
| 3 | 2 | 0 | 3 / 2 | 1/2 | -1/2 | -1/2 | -2 | -2 | $-\frac{22}{21}$ | $-\frac{64}{21}$ |
| 3 | 2 | 0 | 5/2 | 1/2 | 1/2 | 1/2 | 2 | 2 | $\frac{22}{21}$ | $\frac{64}{21}$ |
| 3 | 2 | 1 | 3/2 | 1/2 | -1/2 | 1/2 | -2 | -2 | $-\frac{6}{7}$ | $-\frac{20}{7}$ |
| 3 | 2 | 1 | 5/2 | 1/2 | 1/2 | 3 / 2 | 2 | 2 | $\frac{6}{7}$ | $\frac{20}{7}$ |
| 3 | 2 | 2 | 3/2 | 1/2 | -1/2 | 3 / 2 | -2 | -2 | $-\frac{2}{7}$ | $-\frac{16}{7}$ |
| 3 | 2 | 2 | 5/2 | 1/2 | 1/2 | 5/2 | 2 | 2 | $\frac{2}{7}$ | $\frac{16}{7}$ |

Table 2: Energies E_1 , E_2 and E in units of $e\hbar/(2m)$.