

ECE2: TEST OF RELATIVISTIC QUANTUM MECHANICS BY ESR.

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ABSTRACT

It is shown that the rigorous relativistic quantum mechanics developed in the preceding series of papers can be tested directly with electron spin resonance. Two examples are given, a relativistic electron beam and the anomalous Zeeman effect in atoms and molecules. Therefore relativistic quantum mechanics can be tested at a foundational level using electron spin resonance, a critical test of the conventional solution of the Dirac equation.

Keywords: ECE2 theory, rigorous relativistic quantum mechanics, ESR, electron beam, anomalous Zeeman effect.

UFT 334

1. INTRODUCTION

In the immediately preceding series of papers of this series {1- 12} it has been shown that a rigorous approach to relativistic quantum mechanics leads to major new inferences at a foundational level. The usual approximation used in the solution of the Dirac equation has been shown to result in the vanishing of the classical hamiltonian, an unphysical result. Therefore, the precise results claimed for the Dirac equation are based on an unphysical approximation. These results are well known: the Thomas factor, the g factor of the electron, the anomalous Zeeman effect, spin orbit fine structure, electron spin resonance (ESR) and nuclear magnetic resonance (NMR). The rigorous solution leads to four classes of hamiltonian as discussed in immediately papers. Each class of hamiltonian leads to different spectral detail, depending on subjective use of operator, function and expectation value. It is concluded that relativistic quantum mechanics is not objective. The relevant equations can be derived from Cartan geometry within a rigorously objective unified field theory, but once having derived the equations from geometry, their solution is subjective. In this paper it is shown that electron spin resonance can be used to investigate the different types of spectra predicted by the rigorous solutions. The method is exemplified by a relativistic electron beam and the anomalous Zeeman effect in atoms and molecules.

This paper is as usual a summary of detailed calculations given in its accompanying notes (notes to UFT334 on www.aias.us). Note 334(1) gives details of anomalous Zeeman effect theory corrected with the class one hamiltonian of UFT333 on www.aias.us. Note 334(2) corrects the anomalous Zeeman effect with the class one hamiltonian. UFT334(3) calculates the electron spin resonance frequency in a relativistic electron beam corrected with the class one hamiltonian, and UFT334(4) calculates the electron spin resonance frequencies of the anomalous Zeeman effect corrected with the class one hamiltonian. These notes are

summarized in section 2.

2. ESR METHOD OF TESTING THE RIGOROUS HAMILTONIAN

Consider the class one hamiltonian of UFT333:

$$H = \frac{1}{m} \underline{\sigma} \cdot \underline{p}_0 \frac{\gamma^2}{1+\gamma} \underline{\sigma} \cdot \underline{p}_0 \quad - (1)$$

where m is the particle mass, \underline{p}_0 its classical linear momentum and where the Lorentz factor is:

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

where c is the vacuum speed of light. In the presence of a magnetic field:

$$\underline{p}_0 \rightarrow \underline{p}_0 - e \underline{A} \quad - (3)$$

where $-e$ is the charge on the electron and \underline{A} the vector potential, defined in ECE2 theory by

geometry as in UFT318. In the $O(3)$ basis the hamiltonian (1) becomes:

$$H = \frac{1}{m} \left(\frac{\gamma^2}{1+\gamma} \right) (\underline{p}_0 - e \underline{A}) \cdot (\underline{p}_0 - e \underline{A}) \quad - (4)$$

The vector potential can be written as:

$$\underline{A} = \frac{1}{2} \underline{B} \times \underline{r} \quad - (5)$$

for a uniform magnetic flux density \underline{B} , where \underline{r} is the position vector. By vector algebra:

$$\underline{B} \times \underline{r} \cdot \underline{p}_0 = \underline{r} \times \underline{p}_0 \cdot \underline{B} = \underline{L} \cdot \underline{B} \quad - (6)$$

where the orbital angular momentum is:

$$\underline{L} = \underline{r} \times \underline{p}_0. \quad - (7)$$

The orbital angular momentum term in the hamiltonian is:

$$H = -\frac{e}{m} \left(\frac{\gamma^2}{1+\gamma} \right) \underline{L} \cdot \underline{B} + \dots - (8)$$

and the Zeeman effect is modified to:

$$H_{\text{Ze}} = -\frac{e}{m} \left(\frac{\gamma^2}{1+\gamma} \right) L_z B_z \phi - (9)$$

As describe in Note 334(1) the energy levels of the H atom are modified in this rigorous

theory to:

$$E_H = -\frac{1}{2} m c^2 \left(\frac{\alpha}{n} \right)^2 - \left(\frac{\gamma^2}{1+\gamma} \right) \frac{e \hbar}{m} m_L B_z - (10)$$

where α is the fine structure constant and n the principal quantum number. In this equation:

$$m_L = -L, \dots, L - (11)$$

and \hbar is the reduced Planck constant. The magnetic flux density is aligned in the Z axis. The usual Zeeman effect is recovered in the non relativistic limit:

$$\frac{\gamma^2}{1+\gamma} \rightarrow \frac{1}{2} - (12)$$

when $v_0 \ll c$, and where v_0 the non relativistic classical velocity.

The transition rules in Eq. (10) are:

$$\Delta n \text{ any}, \Delta L = 1, \Delta m_L = 0, \pm 1 - (13)$$

In this equation:

$$\frac{\gamma^2}{1+\gamma} = \left(1 - \frac{p_0^2}{m^2 c^2} + \left(1 - \frac{p_0^2}{m^2 c^2} \right)^{1/2} \right)^{-1} \quad - (14)$$

so if p_0^2 is regarded as a function the usual Zeeman effect is shifted. However if

expectation values in the H atom are used:

$$\frac{p_0^2}{m^2 c^2} = \left\langle \frac{p_0^2}{m^2 c^2} \right\rangle = \left(\frac{\alpha}{n} \right)^2 = \frac{5.3144 \times 10^{-5}}{n^2} \quad - (15)$$

the expected energy levels become:

$$E_H = -\frac{1}{2} m c^2 \left(\frac{\alpha}{n} \right)^2 - \left(1 - \left(\frac{\alpha}{n} \right)^2 + \left(1 - \left(\frac{\alpha}{n} \right)^2 \right)^{1/2} \right)^{-1} \frac{e \hbar}{m} m_L B_z \quad - (16)$$

and the Zeeman spectrum is split into hyperfine structure as in immediately preceding papers.

There is no way of knowing which is the correct choice, so an experimental method is needed to investigate this fundamental problem. This method, based on ESR, is developed in this section.

First quantize the hamiltonian (4) as follows (see Note 334(2) for details):

$$H \psi = i e \frac{\hbar}{m} \left(\frac{\gamma^2}{1+\gamma} \right) \underline{\sigma} \cdot \underline{\nabla} \underline{\sigma} \cdot \underline{A} \psi + \dots \quad - (17)$$

so:

$$\text{Re } H \psi = -\frac{e \hbar}{m} \left(\frac{\gamma^2}{1+\gamma} \right) \underline{\sigma} \cdot \underline{B} + \dots \quad - (18)$$

where:

$$\underline{B} = \underline{\nabla} \times \underline{A} \quad - (19)$$

Define the well known spin angular momentum by:

$$\underline{S} = \frac{\hbar}{2} \underline{\sigma} \quad - (20)$$

to obtain the rigorous anomalous Zeeman effect hamiltonian:

$$H = -\frac{e}{m} \left(\frac{\gamma^2}{1+\gamma} \right) (\underline{L} + 2\underline{S}) \cdot \underline{B} \quad - (21)$$

In the non relativistic limit:

$$\frac{\gamma^2}{1+\gamma} \rightarrow \frac{1}{2} \quad - (22)$$

it reduces to the well known result {1 - 12}:

$$H \rightarrow -\frac{e}{2m} (\underline{L} + 2\underline{S}) \cdot \underline{B} \quad - (23)$$

Eq. (21) can be expressed {1 - 12} as:

$$H = -\frac{e}{m} \left(\frac{\gamma^2}{1+\gamma} \right) g_J \underline{J} \cdot \underline{B} \quad - (24)$$

where the Landé factor is:

$$g_J = 1 + \frac{J(J+1) + S(S+1) - L(L+1)}{2J(J+1)} \quad - (25)$$

The J quantum number of Sommerfeld is:

$$J = L + S, \dots, |L - S| \quad - (26)$$

with:

$$\begin{aligned} J_z \psi &= \hbar m_J \psi, \\ m_J &= -J, \dots, J \end{aligned} \quad - (27)$$

and:

$$J^2 \psi = \hbar^2 J(J+1) \psi \quad - (28)$$

Therefore the energy levels of the H atom are:

$$E_H = -\frac{1}{2} mc^2 \left(\frac{\alpha}{n}\right)^2 - \frac{e\hbar}{m} \left(\frac{\gamma^2}{1+\gamma}\right) g_J m_J B_Z \quad - (29)$$

with selection rules:

$$\left. \begin{aligned} \Delta J &= 0, \pm 1; \quad J=0 \rightarrow J=0 \\ \Delta m_J &= 0, \pm 1, \\ \Delta n &= \text{any} \end{aligned} \right\} - (30)$$

Again, there is no way of knowing if the relativistic factor $\gamma^2 / (1+\gamma)$ should be a function or an expectation value. This question can be answered only with experimental data, namely electron spin resonance (ESR).

Consider a relativistic electron beam in which electrons can be accelerated to close to the speed of light, and apply a magnetic flux density to the beam in the Z axis. In the non relativistic limit of slow moving electrons, the real part of the interaction hamiltonian between an electron and the external magnetic field is:

$$\text{Re} H_{\text{ESR}} \psi = -\frac{e}{m} S_z B_Z \psi \quad - (31)$$

where:

$$S_z \psi = m_s \hbar \psi \quad - (32)$$

and

$$m_s = -S, \dots, S = -\frac{1}{2}, \frac{1}{2} \quad - (33)$$

Using the transition rule:

$$\Delta m_s = \pm 1 \quad - (34)$$

for absorption of radiation produces the well known ESR frequency:

$$\omega_{\text{ESR}} = \frac{e}{m} B_z. \quad - (35)$$

For relativistic electrons however:

$$\text{Re} H_{\text{ESR}} \psi = -\frac{e\hbar}{m} \left(\frac{\gamma^2}{1+\gamma} \right) \underline{\sigma} \cdot \underline{B} \psi = -2 \frac{e}{m} \left(\frac{\gamma^2}{1+\gamma} \right) \underline{S} \cdot \underline{B} \psi \quad - (36)$$

and the ESR resonance frequency of a relativistic electron beam is:

$$\omega_{\text{ESR}} = 2 \left(\frac{\gamma^2}{1+\gamma} \right) \frac{e}{m} B_z. \quad - (37)$$

This frequency is directly measurable. In this case the relativistic factor is always:

$$\frac{\gamma^2}{1+\gamma} = \left(1 - \frac{p_0^2}{m^2 c^2} + \left(1 - \frac{p_0^2}{m^2 c^2} \right)^{1/2} \right)^{-1} \quad - (38)$$

The experimentally measurable momentum of the electron in the beam is the relativistic momentum:

$$\underline{p} = \gamma \underline{p}_0 \quad - (39)$$

from which the non relativistic p_0^2 of the Lorentz factor may be found as follows:

$$p_0^2 = p^2 / \gamma^2 = p^2 \left(1 - \frac{p_0^2}{m^2 c^2} \right) \quad - (40)$$

so:

$$p_0^2 = p^2 / \left(1 + \frac{p^2}{m^2 c^2} \right) \quad - (41)$$

Therefore the experiment consists of measuring the ESR frequency of a relativistic electron beam together with the relativistic linear momentum of the beam. This provides a simple and direct test of the foundations of rigorously relativistic quantum mechanics.

ESR can also be used to test the rigorously relativistic version of Eq. (23), in

which:

$$H = -\frac{e}{2m} (\underline{L} + 2\underline{S}) \cdot \underline{B} = -\frac{e}{2m} g_J \underline{J} \cdot \underline{B}, \quad (42)$$

$$\underline{J} = \underline{L} + \underline{S}. \quad (43)$$

Therefore the spin part of the hamiltonian (20) is:

$$H_{ESR} = -\frac{e}{2m} g_J \underline{S} \cdot \underline{B} \quad (44)$$

If the magnetic field is aligned in the Z axis:

$$H_{ESR} = -\frac{e}{2m} g_J S_z B_z \quad (45)$$

where:

$$S_z \psi = m_s \hbar \psi \quad (46)$$

and:

$$m_s = \pm 1/2, \quad (47)$$

so the ESR resonance frequency of the anomalous Zeeman effect is:

$$\omega_{ESR} = \frac{1}{2} g_J \frac{e B_z}{m} \quad (48)$$

where:

$$J = L + S, L + S - 1, \dots, |L - S| \quad (49)$$

by the Clebsch Gordan Theorem.

So in the anomalous Zeeman effect the ESR spectrum of one electron is split by the Landé factor g_J . This is the most useful feature of ESR in analytical chemistry.

For a free electron in an electron beam:

$$J = S, L = 0 \quad - (50)$$

so:

$$g_J = 1 + \frac{2S(S+1)}{2S(S+1)} = 2, \quad - (51)$$

the Landé factor of a free electron, or g factor of the electron. Note carefully that this factor of two is obtained from the Dirac equation if and only if the Dirac approximation is used:

$$H := H_0 + mc^2 = mc^2, H_0 = 0, \quad - (52)$$

as in immediately preceding papers. In the rigorously correct theory of this section, the ESR frequency becomes:

$$\omega_{\text{ESR}} = \left(\frac{\gamma^2}{1+\gamma} \right) \left(1 + \frac{J(J+1) + S(S+1) - L(L+1)}{2J(J+1)} \right) \frac{eB_z}{m} \quad - (53)$$

where:

$$J = L + S, \dots, |L - S| \quad - (54)$$

and if we use expectation values in the H atom:

$$\frac{\gamma^2}{1+\gamma} = \left(1 - \left(\frac{\alpha}{n} \right)^2 + \left(1 - \left(\frac{\alpha}{n} \right)^2 \right)^{1/2} \right)^{-1} \quad - (55)$$

So the ESR splittings of the anomalous Zeeman effect in the H atom can be observed directly by ESR using Eqs. (53) to (55).

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