

## OPTICAL NMR FROM THE DIRAC EQUATION: A REPLY TO BUCKINGHAM AND PARLETT

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Received March 8, 1996

The Dirac equation of the fermion in a circularly polarized electromagnetic field produces optical NMR shifts of the same order of magnitude as observed in the recent experiments of Warren *et al.* By decreasing the frequency of the irradiation field the Dirac equation shows that electromagnetically induced NMR lines can be observed in the infrared or visible range in theory. A recent paper by Buckingham and Parlett [9] is criticized in detail.

Key words: optical NMR,  $\mathbf{B}^{(3)}$  field, Dirac equation.

### 1. INTRODUCTION

In his original derivation of the half integral spin of the electron, Dirac assumed [1] that the electromagnetic

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potential vector  $\mathbf{A}$  was a real quantity, so that the cross product  $\mathbf{A} \times \mathbf{A}$  is zero identically. This is adequate for a the conjugate product  $\mathbf{A} \times \mathbf{A}^*$  is non-zero [2]. It has magnetic symmetry and is responsible for inverse Faraday induction [3-6]. In this note we use  $\mathbf{A} \times \mathbf{A}^*$  in Dirac's original derivation [1] to adequately reproduce the order of magnitude of optically induced NMR shifts observed recently by Warren *et al.* [7,8], using visible frequencies. The agreement of experiment and data is strongly indicative of the usefulness of this technique, especially if the visible frequency laser used by Warren *et al.* [7,8] is replaced by a radio frequency field. In this case the Dirac equation of one fermion in the field indicates theoretically the possibility of NMR in the infra red or visible.

A recent paper by Buckingham and Parlett [9] is criticized using these results from the original Dirac equation [1].

## 2. NMR OF ONE FERMION IN A CIRCULARLY POLARIZED RADIATION FIELD

There is no reason to assume that NMR and/or ESR must always be practiced with static magnetic fields or that a Pauli spinor must always interact with a static magnetic field. The conjugate product  $\mathbf{A} \times \mathbf{A}^*$  of an electromagnetic wave has magnetic symmetry and produces magnetic resonance from the Dirac equation of one fermion in the field. The wave equation for a fermion in a static magnetic field [10], expected from analogy with the classical Hamiltonian, is [1]

$$((p_0 + eA_0^2) - (\mathbf{p} + e\mathbf{A})^2 - m^2c^2)\psi = 0, \quad (1)$$

where  $p_\mu := (p_0, \mathbf{p})$  is the energy-momentum four-vector and the potential four-vector is  $A_\mu := (A_0, \mathbf{A})$ . The charge and mass of the fermion are  $e$  and  $m$ , respectively, and  $c$  is the speed of light in vacuo. Equation (1) was written by Dirac for a real  $\mathbf{A}$ . For a complex  $\mathbf{A}$ , it becomes

$$((p_0 + eA_0)(p_0 + eA_0^*) - (\mathbf{p} + e\mathbf{A}) \cdot (\mathbf{p} + e\mathbf{A}^*) - m^2c^2)\psi = 0, \quad (2)$$

where it has been assumed that  $A_0$  is also complex. In order to make his theory of the electron resemble Eq. (1) as closely as possible, Dirac carries out a product of factors

for real  $\mathbf{A}$  [1]. For complex  $\mathbf{A}$ , we obtain [10] an equation that replaces Eq. (31), Chap. 11, of Ref. (1). The conjugate product  $\mathbf{A} \times \mathbf{A}^*$  originates in the term  $e^2(\boldsymbol{\sigma} \cdot \mathbf{A}^*)(\boldsymbol{\sigma} \cdot \mathbf{A})$  on using the expansion

$$(\boldsymbol{\sigma} \cdot \mathbf{B})(\boldsymbol{\sigma} \cdot \mathbf{C}) = \mathbf{B} \cdot \mathbf{C} + i(\boldsymbol{\sigma} \cdot \mathbf{B} \times \mathbf{C}), \quad (3)$$

as given by Dirac [1]. Straightforward calculation [10] then shows that the eigenvalue of the interaction energy between the field and one fermion is

$$W := E\eta - mc^2 \sim \frac{e^2 c^2 (\boldsymbol{\sigma} \cdot \mathbf{A})(\boldsymbol{\sigma} \cdot \mathbf{A}^*)}{E\eta + mc^2 + e c A_0} - e c A_0. \quad (4)$$

In Dirac's approximation [1],  $E\eta = mc^2$ ; and assuming that  $A_0 = 0$  (the conventional Coulomb gauge), one gets

$$W = \frac{e^2}{2m} (\mathbf{A} \cdot \mathbf{A}^* + i \boldsymbol{\sigma} \cdot \mathbf{A} \times \mathbf{A}^*). \quad (5)$$

The interaction term  $i \boldsymbol{\sigma} \cdot \mathbf{A} \times \mathbf{A}^*$  therefore emerges directly from the Dirac equation and is responsible for radiation induced fermion (e.g., nuclear) magnetic resonance. The  $\mathbf{B}^{(3)}$  field of Evans and Vigier [11-15] is defined as

$$\mathbf{B}^{(3)*} := -i \frac{e}{\hbar} \mathbf{A} \times \mathbf{A}^* := -i \frac{e}{\hbar} \mathbf{A}^{(1)} \times \mathbf{A}^{(2)}, \quad (6)$$

giving the interaction energy between fermion and magnetic field in the standard form

$$E\eta_{int} = -\frac{e}{m} \left( \frac{\hbar}{2} \boldsymbol{\sigma}^{(3)} \right) \cdot \mathbf{B}^{(3)*}, \quad (7)$$

i.e., in the same form as that between the spinor and a static magnetic field.

In terms of intensity ( $I$ ,  $W \text{ m}^{-2}$ ), otherwise known as power density, and beam angular frequency ( $\omega$ ,  $\text{rad s}^{-1}$ ), the  $\mathbf{B}^{(3)}$  field from Eq. (6) is [10]

$$\mathbf{B}^{(3)} = \frac{e\mu_0 c}{\hbar} \frac{I}{\omega^2} \mathbf{e}^{(3)} = 5.723 \times 10^{17} \frac{I}{\omega^2} \mathbf{e}^{(3)}, \quad (8)$$

where  $\mu_0$  is the permeability in vacuo and  $\mathbf{e}^{(3)}$  is a unit vector in the (3) axis of frame ((1), (2), (3)) [11-15].

### 3. COMPARISON WITH EXPERIMENTAL DATA

Fermion resonance occurs at a probe angular frequency  $\omega_{\text{res}}$  defined by transitions from the negative to the positive states of the spinor  $\sigma^{(3)}$  in Eq. (7):

$$\hbar\omega_{\text{res}} = \frac{e^2 c^2 B^{(0)2}}{2m\omega^2} (1 - (-1)). \quad (9)$$

The resonance frequency of the probe field is therefore, for one fermion,

$$\omega_{\text{res}} = \left( \frac{e^2 \mu_0 c}{\hbar m} \right) \frac{I}{\omega^2}, \quad (10)$$

that is, inversely proportional to the square of the angular frequency. For proton ( $^1H$ ) resonance we adjust this result empirically [10] for the different Landé factors of the proton (5.5857) and the electron (2.002), and multiply (10) by the ratio 5.5857/2.002, giving

$$\omega_{\text{res}}(^1H) = 1.532 \times 10^{25} \frac{I}{\omega^2}. \quad (11)$$

If the pump frequency  $\omega$  is about  $5,000 \text{ cm}^{-1}$  in the visible, and if  $I$  is chosen to be a moderate 10 W per square centimeter, the resonance frequency  $\omega_{\text{res}}$  from Eq. (11) is about 1.7 Hz. This is in good qualitative agreement with the data by Warren *et al.* [7,8], who observed shifts as large as about 2 Hz for a laser of intensity about 3 watts  $\text{cm}^{-2}$ , shifts which changed direction with the sense of circular polarization of the beam. However, the overall pattern of results [7,8] was complicated and the shifts were small, because, understandably, a visible frequency was used. Equation (11) now shows that much greater shifts are expected for the same intensity

(I) at radio frequencies [10]. Qualitative agreement with data is all that can be reasonably expected from Eq. (11), which is for one unshielded fermion.

The Ar<sup>+</sup> laser frequencies used by Warren *et al.* [7,8] were 528.7 nm, 488 nm, and 476.5 nm, giving resonance frequencies from Eq. (11) of, respectively, 0.12 Hz, 0.10 Hz, and 0.09(8) Hz for I of 10 watts cm<sup>2</sup>. These are many orders of magnitude greater than those in the received phenomenology of Buckingham and Parlett [9] but are at the extreme edge of contemporary detection capability. Equation (11) (essentially the Dirac equation) shows that for <sup>13</sup>C the shifts would be more than an order of magnitude smaller, and therefore undetectable, because of the inverse mass dependence and smaller Landé factor of <sup>13</sup>C. This is again in qualitative agreement with the experimental results [7,8].

#### 4. CRITICISM OF REMARKS BY BUCKINGHAM AND PARLETT [9]

Buckingham and Parlett [9] have given a simple phenomenological theory of the optical NMR phenomenon which leads to results that are several orders of magnitude smaller than the data observed by Warren *et al.* [7,8]. These authors apparently believe that the results by Warren *et al.* [7,8] are artifacts, because their phenomenology produces shifts many orders of magnitude too low. In so doing they do not consider the Dirac equation, which is a precise equation of the relativistic quantum field theory. They assert that the correct mechanism must be one based on the antisymmetric electronic polarizability: essentially a perturbation calculation for the chemical shift. These authors have not met the challenge posed by the data of Warren *et al.* [7,8], and have preferred to restate well known phenomenology which does not explain anything new. It is erroneously asserted [9] that  $\mathbf{B}^{(3)}$  defined by Eq. (6) violates  $\hat{C}$  symmetry, whereas it has been shown already [10-15] that the B cyclics trivially conserve  $\hat{C}$  symmetry. A variation of the conjugate product is used [9] in the context of the well known inverse Faraday effect [3-6], but these authors have failed to understand that  $\mathbf{A} \times \mathbf{A}^*$  interacts directly with the nuclear spinor (Eq. (5)). In the same way, ordinary NMR depends on the interaction of a static magnetic field with a nuclear spinor. Superimposed on this main mechanism is the chemical shift, for which a fairly adequate explanation is given [9], but without reference to several other theories already in the literature [16-20].

## ACKNOWLEDGEMENTS

Doctor Debabrata Goswami is thanked for a copy of his Ph.D. Thesis (Princeton, 1994) and the Warren group for many interesting discussions. The paper by Buckingham and Parlett appeared in print without the author's prior knowledge, and the author was given no opportunity to reply. Several attempts at replying or commenting by the present author have been blocked by the staff of *Science*. Buckingham and Parlett believe that their phenomenology implies the artifactual nature of ONMR, whereas the opposite is implied by rigorous relativistic quantum field theory. The issue should be resolved by the use of radio frequencies ( $\omega$ ) in Eq. (10). The Dirac equation produces ONMR for one unshielded fermion. We need only use a non-zero  $\mathbf{A} \times \mathbf{A}^*$ , which in a slightly different form is also used by Buckingham and Parlett. The present author initiated the subject of ONMR in a well-known paper of 1991 [17], at which point in time nothing was known about the interaction of  $\mathbf{A} \times \mathbf{A}^*$  with the nuclear Pauli spinor.

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