Electron and Proton Spin Resonance Induced by Circularly Polarized Radiation: A Classical Derivation

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Classical electrodynamics is used to demonstrate electron and proton spin resonance induced by classical, monochromatic, circularly polarized radiation. The effect is present in $SU(2)$ symmetry as indicated by the minimal prescription, whose covering group is $O(3)$. The interaction Hamiltonian is shown to be,

$$H = -\alpha S_3 \sigma_Z \cdot \mathbf{k},$$

where α is the electron or proton polarizability; S_3 is the third Stokes parameter; σ_Z is the Pauli matrix; and $\mathbf{k}$ is a unit vector in Z.

Key words: Electron and proton spin resonance induced by radiation, $\mathbf{B}^{(3)}$ field.

1. Introduction

Sakurai [1] has given a clear explanation of the interaction of the electron spin magnetic moment with a static magnetic field in non–relativistic quantum mechanics. The minimal prescription is used to generate fundamental electromagnetic interactions from the kinetic energy operator in the $SU(2)$ group. This non–relativistic quantum theory, using the Schrödinger Pauli equation, is shown to give the correct g factor of the electron, *i.e.* two, without using the Dirac equation.

In this note, this method is extended to the non–relativistic classical level and used to show that classical, monochromatic, circularly polarized radiation induces electron (and proton) spin resonance through the interaction Hamiltonian,

$$H = -\alpha S_3 \sigma_Z \cdot \mathbf{k}\,. \tag{1}$$

Here, α is the polarizability,

$$\alpha = e^2/2m\omega^2\,, \tag{2}$$

where e/m is the charge to mass ratio of the Lorentz electron, and ω is the angular frequency of the radiation. The third Stokes parameter is [2-4] is,

$$S_3 = -i\left|\mathbf{E} \times \mathbf{E}^*\right|, \tag{3}$$

where $\mathbf{E}$ is the (complex) electric field strength of the radiation. Finally σ_Z is the Z axis Pauli matrix and $\mathbf{k}$ a unit vector in Z, the propagation axis of the radiation. Fundamental optical theory [2,3] shows that

$$S_0 = \pm S_3 \tag{4}$$

in circular polarization, where,

$$S_0 = \mathbf{E} \cdot \mathbf{E}^*, \tag{5}$$

is the zeroeth Stokes parameter, proportional to beam intensity I [4]. Electron spin resonance occurs between the states of in Eq. (1), and the effect is proportional to I/ω^2 from Eqs. (2) and (4). Simi-

larly, proton spin resonance can be induced by circularly polarized radiation, and its resonance frequency is similarly proportional to I/ω^2.

Equation (1) shows [5-7] that both electron and proton spin resonance can be made to occur in the infra red to visible range, with dramatic potential increase in resolution over currently available magnet based techniques of any kind.

2. Derivation of Eq.(1)

The classical derivation of Eq. (1) is simple and straightforward. It begins with the Newtonian kinetic energy of the free electron considered as a classical particle,

$$T = \frac{1}{2m}\mathbf{p}\cdot\mathbf{p}\,, \tag{6}$$

Here **p** is the linear momentum in the absence of the field. Following Sakurai [1], write Eq. (5) in the *SU*(2) basis defined by the Pauli matrices,

$$T = \frac{1}{2m}(\sigma\cdot\mathbf{p})(\sigma\cdot\mathbf{p}) = \frac{1}{2m}\mathbf{p}\cdot\mathbf{p}\,. \tag{7}$$

Now describe the fundamental electron to field interaction with the minimal prescription. The latter is the canonical momentum defined by the classical Lagrangian equivalent to the Lorentz force equation [8]. In the O(3) basis,

$$T = \frac{1}{2m}(\mathbf{p} - e\,\mathbf{A})\cdot(\mathbf{p} - e\,\mathbf{A}^*)\,, \tag{8}$$

and

$$\langle T\rangle = \frac{1}{2m}\mathbf{p}\cdot\mathbf{p} + \frac{e^2}{2m}\mathbf{A}\cdot\mathbf{A}^*\,, \tag{9}$$

is the mean kinetic energy of the electron in the field after averaging over many cycles in the laboratory frame. Here **A** is the complex vector potential of the field. The mean kinetic energy of interaction is therefore the Hamiltonian component,

$$H_{O(3)} = \frac{e^2}{2m}\mathbf{A}\cdot\mathbf{A}^* = \frac{e^2}{2m\omega^2}\mathbf{E}\cdot\mathbf{E}^*. \tag{10}$$

Therefore, in the *O*(3) group,

$$H_{O(3)} = \alpha S_0. \tag{11}$$

This result seemingly applies to all states of polarization. However, from Eq. (4), it is known that in circular polarization the S_3 parameter must be non–zero because S_0 is non–zero. The S_3 parameter is however, missing from Eq. (11).

The solution to this self–inconsistency is given by writing Eq. (8) in the homomorphic *SU*(2) symmetry,

$$T = \frac{e^2}{2m}\sigma\cdot(\mathbf{p} - e\mathbf{A})\sigma\cdot(\mathbf{p} - e\mathbf{A}^*)\,, \tag{12}$$

giving, after averaging over many cycles of the electromagnetic field,

$$\langle T\rangle = \frac{e^2}{2m}\mathbf{p}\cdot\mathbf{p} + \frac{e^2}{2m}\sigma\cdot\mathbf{A}\sigma\cdot\mathbf{A}^*. \tag{13}$$

The mean interaction kinetic energy in *SU*(2) is the Hamiltonian component,

$$H_{SU(2)} = \frac{e^2}{2m}\sigma\cdot\mathbf{A}\sigma\cdot\mathbf{A}^*\,. \tag{14}$$

Using the rules for Pauli matrix algebra given by Sakurai [1] we find that

$$H_{SU(2)} = \frac{e^2}{2m}(\mathbf{A}\cdot\mathbf{A}^* + i\sigma\cdot\mathbf{A}\times\mathbf{A}^*). \tag{15}$$

This classical interaction Hamiltonian differs from its homomorph, Eq. (10), and can be expressed as

$$H_{SU(2)} = \alpha(S_0 - S_3\sigma_Z\cdot\mathbf{k}). \tag{16}$$

3. Discussion

The Hamiltonian (16) consistently accounts for the presence of $S_3 = \pm S_0$ in circularly polarized radiation, whereas the homomorphic Hamiltonian (11) does not. The existence of electron spin resonance is deduced from the usual resonance equation,

$$\hbar\omega = \alpha S_3\sigma_Z\cdot\mathbf{k}, \tag{17}$$

where $\hbar$ is the Dirac constant and ω the electron spin resonance probe beam frequency. It is easily deduced [5-7] that resonance occurs at

$$\omega_{res}(\text{proton}) = 1.007\times10^{28}\, I/\omega^2 \tag{18}$$

for the unshielded electron. Repeating for the unshielded proton, we find [5],

$$\omega_{res}(\text{proton}) = 1.532\times10^{25}\, I/\omega^2, \tag{19}$$

after making due allowance for the different empirically observed g factors of the electron (2.002) and the proton (5.5857).

It is a simple matter to show that both *ESR* and *NMR* spectra occur in the infra red or visible range by adjusting I/ω^2 using pulsed or *CW* radiation. In theory, this produces a dramatic increase in instrumental resolution over anything possible with permanent magnets.

The Hamiltonian for radiatively induced electron or proton resonance is

$$H = -\alpha S_3\sigma_Z\cdot\mathbf{k}, \tag{20}$$

and should be incorporated as an operator in quantum perturbation theory [9] or quantum electrodynamics [10] to develop the theory in atoms, molecules and proteins. It should be possible to simulate new instruments based on the new theory by calculating the free induction decay expected in the presence and absence of the permanent magnet. These developments apply in principle to a vast new area of investigation, both theoretical and experimental. In $\mathbf{B}^{(3)}$ theory [5-7], the interaction Hamiltonian is,

$$H = \frac{e\hbar}{2m}\sigma_Z\cdot\mathbf{B}^{(3)}, \tag{21}$$

and has the same form exactly as the Hamiltonian of a fermion in a static magnetic field [9]. It can be used in the same way in time dependent and independent perturbation theory with $\mathbf{B}^{(3)}$ defined [11] in the vacuum as

$$\mathbf{B}^{(3)} := -i\frac{e}{\hbar}\mathbf{A}\times\mathbf{A}^*. \tag{22}$$

Note finally that the linear term,

$$H_L := -i\frac{e}{2m}\sigma\cdot(\mathbf{A}\times\mathbf{p} + \mathbf{p}\times\mathbf{A}^*), \tag{23}$$

in Eq. (23) is the Rabi-Anderson-Ernst term [11] used to produce free induction decay in *FT NMR* spectrometers. The real part of the linear term is,

$$Re(H_L) - \frac{ec}{m\omega}\frac{B^{(0)}}{\sqrt{2}}\vec{\sigma}\cdot(i\cos\phi - j\cos\phi)\times\mathbf{p}\,, \tag{24}$$

where the usual monochromatic electromagnetic phase is :

$$\phi = \omega t - \kappa Z\,, \tag{24a}$$

where κ is the wavevector at instant t and coordinate Z. The term (24) aligns spins in preparation for free induction decay through a 90° or 180° pulse, or a pulse sequence, as usual. The simple classical Hamiltonian (12) therefore gives this well known effect in addition to the *RFR* term, Eq. (20).

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