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THE EQUIVALENCE OF CLASSICAL MECHANICS AND DIRAC THEORY IN SPIN–ORBIT INTERACTION ENERGY OF HYDROGEN ATOM

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Abstract

Some of the microscopic phenomena at atomic-nuclear level can be better understood with the help of famous Dirac Theory of Relativistic Quantum Mechanics. But for many of the research scholar levels, particularly in the research fields the transition from classical to relativistic quantum mechanics is abstract in understanding. This paper is an attempt to show how the two approaches lead to the same results and how beautifully explain the energy quantization at atomic level. The origin of the internal magnetic field experienced by an electron moving in a one electron atom is easy to understand if we consider the motion of the nucleus from the point of view of the electron. In a frame of reference fixed on the electron, the charged nucleus moves around the electron and the electron is in effect, located inside a current loop which produces the magnetic field. The author asserts with mathematical logic and relevant equations how the two treatments converge beautifully to one point in bringing the expression of quantized energy of the electron. We consider a semi-classical model to describe the origin of the spin-orbit interaction in a simple system such as the hydrogen atom.. The correct ½ factor for the spin-orbit coupling energy is thus derived without the need to invoke the well-known Thomas precession in the rest-frame of the electron. This result is in quality agreement with the solution of the Dirac-Coulomb equation for hydrogen atom.

INTRODUCTION

A calculation of the interaction energy due to the addition of an electron spin to the atom model has been made on the quantum mechanics by Pauli, Darwin, Dirac, Gordon and others. By use of the vector model a semi classical calculation of the interaction energy may also be made which leads to the same result. In 1925 Uhlenbeck and Goudsmith introduce the idea of electron spin and showed that if the electron had a g-factor of 2, the anomalous Zeeman effect could be explained as well as the existence of multiple splitting .The Thomas precession, as it is called, also give a qualitatively explanation for a spin – orbit interaction in atomic nuclei. The discrepancy was removed by Thomas in 1926 by applying a classical relativistic approach. He pointed out that successive Lorentz transformations with the collinear relative velocities entail and additional spatial rotation of the coordinate axes of the reference frames involved. In this way we showed that the doublet separation due to spin orbit coupling is half the value derived by Uhlenbeck and Goudsmit. Later the problem of spin orbit interaction was solved by the relativistic quantum electron theory of Dirac. Nevertheless it is comforting that this effect has a classical explanation especially because the account of Thomas precession in the spin orbit coupling of the hydrogen atom is often considered a confirmation of special relativity. This result is in qualitative agreement with the solution of the Dirac-Coulomb equation for hydrogen like atoms, for which the radial part of the wave function depends on the spin projection.

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Hestenes has shown that the quantum behavior has direct effect in intrinsic spin. He and his associates observed that both the uncertainty relation and intrinsic spin, for some explanation, depends upon the Planck's constant and the magnitude of the spins itself participating in the dynamics can explain the irradiative states through resonance phenomena. L. Thomas in his land mark paper which is published in 1927, has considered the similar atomic model which is used here as a part of his application of the Thomas precession for explaining the anomalous factor for one-half Zeeman effect. He could not explain the hidden momentum of magnetic dipole in the electric field. Thomas concluded that total secular mechanical angular momentum is a constant of the motion for circular and elliptical orbit.

THEORY

The origin of the internal magnetic field experienced by an electron moving in a one electron atom is easy to understand if we consider the motion of the nucleus from the point of view of the electron. In a frame of reference fixed on the electron, the charged nucleus moves around the electron and the electron is in effect, located inside a current loop which produces the magnetic field on the electron (according to Ampere's law) is given by $\vec{B} = \frac{\mu_0}{4\pi} \frac{\vec{J} \times \vec{r}}{r^3}$

$$= \frac{\mu_0\, ze}{4\pi} \quad \frac{\vec{v} \times \vec{r}}{r^3} \tag{1}$$

Where $\vec{J}$ is the current element and is given by $\vec{J} = -\,z\,e\,\vec{v}$. Z is the charge of the nuclear, e is the charge on the electron and $\vec{v}$ is the velocity of the electron

Now the electric field E acting on the electron, according to coulomb's law, is given by

$$\vec{E} = \frac{ze}{4\pi\varepsilon_0} \; \frac{\vec{r}}{r^3}$$

$$\text{or,} \qquad z\,e = \quad 4\pi\varepsilon_0 \, \frac{\vec{r}}{r^3} \;\; \vec{E} \tag{2}$$

Using equation (2) in equation (1), we get

$$\vec{B} = -\,\mu_0 \varepsilon_0\, \vec{v} \times \vec{E}$$

Where μ_0 is the permeability and ε_0 is the permittivity of the medium

But the velocity of the plane electromagnetic wave in vacuum is C= $\frac{1}{\sqrt{\mu_0 \varepsilon_0}}$, then we have,

$$\vec{B} = -\,\frac{1}{C^2}\, \vec{v} \times \vec{E} \tag{3}$$

This is the magnetic field, experienced by electron due to the charged nucleus.

The electron and its spin magnetic dipole moment can assume different orientations in the internal magnetic field of the atoms and its potential energy is different for each of these orientations. The oriental potential energy (ΔE) of the magnetic dipole moment ($\vec{\mu_s}$) due to spin of an electron in this magnetic field is given by

$$\Delta E = -\,\vec{\mu}_s \cdot \vec{B} \tag{4}$$

But as, $$\vec{\mu_s} = -\,\frac{g_s\, \mu_B}{\hbar} \cdot \vec{S}$$

Where μ_B = the Bohr magneton.

Thus the oriental potential energy due to the magnetic dipole moment in terms of the electron's spin angular momentum $\vec{S}$ is given by

$$\Delta E = \frac{g_s\, \mu_B}{\hbar}\, \vec{S}\cdot\vec{B} \tag{5}$$

Where g_s is called the spin g-factor.

This energy has been evaluated in a frame of reference in which the electron is at rest but we are also interested to measure this energy in the normal frame of reference in which the nucleus is at rest. Due to an effect of the relativistic transformation of velocities, called the Thomas precession, the transformation back to the nucleus rest frame and resulting in a reduction of the oriental potential energy by a factor of 2. Thus the spin- orbit interaction energy is given by

$$\Delta E_{S.O} = \frac{1}{2}\, \frac{g_s\, \mu_B}{\hbar}\, \vec{S}\cdot\vec{B} \tag{6}$$

The transformation leading to the factor of 2 is interesting but it is complicated, so we shall not carry it out here. It is feeling convenient to express equation (6) in terms of the scalar product of the spin and orbital angular momentum vectors.

The force acting on the electron due to the electric field is given by

$$\vec{F} = -\, e\vec{E} \tag{7}$$

Where $\vec{E}$ be the electric field and $-e$ be the charge on the electron. We also use the relation between the force and the potential energy as given by

$$\vec{F} = -\,\frac{dv(r)}{dr}\,\frac{\vec{r}}{r} \tag{8}$$

Where $\frac{\vec{r}}{r}$ is a unit vector which gives the direction of $\vec{F}$ in the radial direction. With this substitution, equation (7) becomes,

$$-\, e\vec{E} = -\,\frac{dv(r)}{dr}\,\frac{\vec{r}}{r}$$

Or, $$\vec{E} = \frac{1}{e}\,\frac{dv(r)}{dr}\,\frac{\vec{r}}{r} \tag{9}$$

With the substitution of equation (9) in equation (3), we get,

$$\vec{B} = \frac{1}{ec^2}\,\frac{1}{r}\,\frac{dv(r)}{dr}\,\vec{v}\times\vec{r} \tag{10}$$

The orbital angular momentum ($\vec{L}$)is given by

$$\vec{L} = \vec{r}\times m\vec{v} = -\, m\vec{v}\times\vec{r}$$

With this substitution equation (10) becomes

$$\vec{B} = \frac{1}{mec^2}\,\frac{1}{r}\,\frac{dv(r)}{dr}\,\vec{L} \tag{11}$$

Using equation (11) in equation (6) we get,

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$$\Delta E_{S.O} = \frac{1}{2}\frac{1}{mec^2}\ \frac{1}{r}\frac{g_s\ \mu_B}{\hbar}\frac{dv(r)}{dr}\ \vec{S}\cdot\vec{L} \tag{12}$$

Evaluating g_s and μ_B , we obtain

$$\Delta E_{S.O} = \frac{1}{2}\frac{1}{m^2c^2}\ \frac{1}{r}\ \frac{dv(r)}{dr}\ \vec{S}\cdot\vec{L} \tag{13}$$

This equation was first derived by Thomas in 1926 using the combination of Bohr model, Schrodinger quantum mechanics and relativistic kinematics. However it is in complete agreement with the results of the relativistic quantum mechanics of Dirac. It can be expressed in terms of L, S and J, we can first write

$$\vec{J} = \vec{L} + \vec{S}$$

Taking the scalar product of this equality times itself and employing the fact that,

$$\vec{S}\cdot\vec{L} = \vec{L}\cdot\vec{S}$$

$$\vec{J}\cdot\vec{J} = \vec{L}\cdot\vec{L} + \vec{S}\cdot\vec{S} + 2\,\vec{S}\cdot\vec{L}$$

$$\vec{S}\cdot\vec{L} = \tfrac{1}{2}(\vec{J}\cdot\vec{J} - \vec{L}\cdot\vec{L} - \vec{S}\cdot\vec{S})$$

or, $$\vec{S}\cdot\vec{L} = \tfrac{1}{2}\ (\vec{J}^2 - \vec{L}^2 - \vec{S}^2)$$

In a quantum state associated with the quantum numbers L, S, and J, each term on the R.H.S has a fixed value and $\vec{S}\cdot\vec{L}$ has the fixed value

$$\vec{S}\cdot\vec{L} = \tfrac{\hbar}{2}\,[\vec{J}(\vec{J}+1) - \vec{L}(\vec{L}+1) - \vec{S}(\vec{S}+1)]$$

Thus,

$$\Delta E_{S.O} = \frac{\hbar^2}{4}\frac{1}{m^2c^2}\ [\vec{J}(\vec{J}+1) - \vec{L}(\vec{L}+1) - \vec{S}(\vec{S}+1)]\ \frac{1}{r}\frac{dv(r)}{dr} \tag{14}$$

It should be evident that the spin-orbit energy for the state is the expectation value of the quantity i.e. the energy arising from the spin-orbit interaction is

$$\overline{\Delta E_{S.O}} = \frac{\hbar^2}{4}\frac{1}{m^2c^2}\ [\vec{J}(\vec{J}+1) - \vec{L}(\vec{L}+1) - \vec{S}(\vec{S}+1)]\ \overline{\frac{1}{r}\frac{dv(r)}{dr}} \tag{15}$$

Where the expectation value of $\overline{\frac{1}{r}\frac{dv(r)}{dr}}$ is calculated by using the potential function V(r) for the system and we have,

$$\overline{\frac{1}{r}\ \frac{dv(r)}{dr}} = \frac{1}{r}\frac{e^2}{4\pi\varepsilon_0 r^2}$$

With this substitution the above equation becomes

$$\overline{\Delta E_{S.O}} = \frac{\hbar^2}{4}\frac{1}{m^2c^2}\ [\vec{J}(\vec{J}+1) - \vec{L}(\vec{L}+1) - \vec{S}(\vec{S}+1)]\frac{1}{r}\frac{e^2}{4\pi\varepsilon_0 r^2} \tag{16}$$

It is found that the energy is shifted up if $\vec{L}$ is approximately parallel to $\vec{S}$ and it is shifted down if $\vec{L}$ is approximately anti-parallel to $\vec{S}$. A complete treatment of all the effects of relativity on the energy levels of hydrogen atom can be given only in terms of the Dirac relativistic field theory. Therefore the result of Dirac's completely relativistic treatment of the hydrogen atom energy levels is in complete agreement with the classical mechanics which predict that the energies are

$$E_{s.o} = -\frac{\mu e^4}{(4\pi\varepsilon_0)^2 2\hbar^2 n^2}\left[1+\frac{\alpha^2}{n}\left(\frac{1}{J+\frac{1}{2}}-\frac{3}{4n}\right)\right] \tag{17}$$

Where μ is the reduced mass of the electron, $\mu = \frac{mM}{m+M}$ and $\alpha = \frac{e^2}{4\pi\varepsilon_0 \hbar c}$.

CONCLUSION

We have summarized the approaches to the classical derivation of the spin – orbit coupling in hydrogen atom suggested by Thomas and Frenkel and showed that both approaches symmetrically ignore the additional force acting between the electrons and nucleus due to the relativistic polarization of the orbiting electron. This result agrees qualitatively with the solution of the Dirac-Coulomb equation, where the position of the maximum of the radial part of electron's wave function differ from each other for different values of the quantum number j and the relative variation of the position of the maximum has the same order of magnitude $(Z\alpha)^2$, in the semi classical expression.

In this paper I have tried to calculate only the kinetic energy, potential energy, and spin-orbit interaction energy between the nucleus electric field and magnetic moment of electron in the rest frame of the nucleus with a condition that the orbit of the electron must has a constant radius in the flip-transition and the correct 1/2 factor has also been derived without use of Thomas precession. The spin-orbit interaction energy is calculated in the both cases either in rest frame of the electron or rest frame of the nucleus has near about the same result.

In conclusion, Bohr's model of the hydrogen atom can be extended to account for the observed spin-orbit interaction with the stipulation that, during a spin-flip transition, the orbital radius r remains constant. In other words, if there is a desire to extend Bohr's model to accommodate the spin of the electron, then experimental observations mandate robust orbits during spin-flip transitions. This is tantamount to admitting that Bohr's model is of limited value, and that one should really rely on Dirac's equation for the physical meaning of spin, for the mechanism that gives rise to g = 2, for Zeeman splitting, for relativistic corrections to Schrödinger's equation, for Darwin's term, and for the correct ½ factor in the spin-orbit coupling energy. Bohr's model is a poor man's way of understanding the hydrogen atom. If one desires to extend Bohr's model to account for the spin-orbit interaction, then one must introduce the adhoc assumption that the orbit radius r is invariant during a spin-flip transition. While a strong physical justification in support of this assumption does not seem to exist, it at least provides a possibility argument for the observed ½ factor.

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