Relativistic Pauli equation

AYMAN H. ALTORRA

Department of Physics, University of Aleppo, Aleppo, Syria

ABSTRACT. We derived relativistic Pauli equation depending on modified Dirac Hamiltonian and without using any kind of approximation. This equation affords relativistic entity to the electron magnetic moments, that enabled us to obtain straightforward formulation to relativistic Zeeman effect (ZE) which elucidates the very physical essence of the ZE.

1 Introduction

To solve the problem of negative probability density related to the Klein-Gordon equation Dirac had introduced Hamiltonian to obtain relativistic wave equation that is linear in the derivatives for both space and time. The Dirac Hamiltonian for free electron is written as following [1]

$$\hat{H} = c\,\boldsymbol{\alpha}\cdot\mathbf{p} + m_0 c^2 \beta \ , \tag{1}$$

where c is the speed of light, m_0 is the rest mass of electron, $\mathbf{p}$ is the electron momentum and α and β are the Dirac matrices.

Serious problem known as "Zitterbewegung" had emerged after the publication of the Dirac equation that is the expected value of the electron velocity always equals the speed of light, a result which contradicts the special relativity theory. For example, the electron velocity component on the OX axis when calculated from the Poisson bracket using the Dirac Hamiltonian gives the following result [1, 2]

$$\dot{x} = [x, \hat{H}] = \frac{\partial \hat{H}}{\partial \mathrm{p}_x} = c\,\alpha_1 \,. \tag{2}$$

It is clear from Eq.(2) that the expected value of $\dot{x}$ will be either $+c$ or $-c$.

E. G. Bakhoum [2] offered an attempt to solve this problem when he proposed a modification in the mass-energy equivalence principle using the relativistic energy formula $m\,\mathrm{v}^2$, where m is relativistic mass of a particle and v is its velocity. This energy formula also reconciles the de Broglie wave theory with the relativity theory without the well-known disagreement [2, 3].

An essential result of the Dirac equation was presenting theoretical derivation to the electron spin and its magnetic moment. However, a problem is that this description is not relativistic although the Dirac equation is relativistic equation, since the electron spin and its magnetic moment are described through non-relativistic Pauli equation that is obtained as non-relativistic approximation to the Dirac equation [1].

In this paper, we derive relativistic Pauli equation using modified Dirac Hamiltonian that we obtain depending on the relativistic energy relation $H = m\,\mathrm{v}^2$. This relativistic Pauli equation has very important consequences, as it affords relativistic description to the electron spin and its magnetic moments. For instance, it gives an original formulation to relativistic Zeeman effect (ZE) which elucidates the very physical essence of the ZE.

2 Derivation of relativistic Pauli equation

We derive at first modified Dirac Hamiltonian for free electron, and we start by squaring the relation of relativistic mass $m = m_0 (1 - \mathrm{v}^2/c^2)^{-1/2}$, and multiplying both sides of the resulting equation with $\mathrm{v}^2 c^2$, so we obtain

$$m^2 \mathrm{v}^2 c^2 - m^2 \mathrm{v}^4 = m_0^2 \mathrm{v}^2 c^2 \,. \tag{3}$$

We use the relation $H = m\,\mathrm{v}^2$ in Eq.(3), and after some algebra we find

$$H^2 = c^2\mathbf{p}^2 - m_0^2 c^2 \mathrm{v}^2 = c^2\mathbf{p}^2\left(1-(m_0/m)^2\right) = \mathrm{v}^2\mathbf{p}^2 \; . \tag{4}$$

Depending on Eq.(4) and implementing the method of Dirac in writing the Hamiltonian as linear combination of momentum components, we introduce modified Dirac Hamiltonian for free electron as following

$$m\,\mathrm{v}^2 I = \hat{H} = \mathrm{v}\,\boldsymbol{\sigma}\cdot\mathbf{p} \;, \tag{5}$$

where I is the identity matrix and the vector σ consists of the Pauli spin matrices that satisfy anti-commutation relations similar to those satisfied by the Dirac matrices [1].

The cause of the Zitterbewegung problem is the existence of the speed of light in the term $c\,\boldsymbol{\alpha}\cdot\mathbf{p}$ in Dirac's Hamiltonian. If we use the modified Dirac Hamiltonian $\hat{H} = \mathrm{v}\,\boldsymbol{\sigma}\cdot\mathbf{p}$ in Eq.(2) we find that the expected value of the electron velocity will be either $+\mathrm{v}$ or $-\mathrm{v}$, which is the same result obtained by Bakhoum [2] that eliminates the Zitterbewegung problem.

The modified Dirac Hamiltonian for electron existing in vector potential A and Coulomb potential ϕ could be written as following

$$\hat{H} = \mathrm{v}\,\boldsymbol{\sigma}\cdot(\mathbf{p} - \tfrac{e}{c}\mathbf{A}) - e\phi \; . \tag{6}$$

From Eq.(6) we get

$$\hat{H} + e\phi = \mathrm{v}\,\boldsymbol{\sigma}\cdot(\mathbf{p} - \tfrac{e}{c}\mathbf{A}) . \tag{6a}$$

Squaring Eq.(6a) and dividing it on ($m\,\mathrm{v}^2 + e\phi$) gives

$$\frac{(\hat{H}+e\phi)^2}{m\,\mathrm{v}^2 + e\phi} = \frac{\mathrm{v}^2}{m\,\mathrm{v}^2 + e\phi}\left(\boldsymbol{\sigma}\cdot(\mathbf{p} - \tfrac{e}{c}\mathbf{A})\right)^2 . \tag{6b}$$

By using the left equation of (5) in the l.h.s of Eq.(6b) we obtain

$$\frac{(m\,\mathrm{v}^2 + e\phi)(\hat{H}+e\phi)}{m\,\mathrm{v}^2 + e\phi} = \frac{\mathrm{v}^2}{m\,\mathrm{v}^2 + e\phi}\left(\boldsymbol{\sigma}\cdot(\mathbf{p} - \tfrac{e}{c}\mathbf{A})\right)^2 . \tag{6c}$$

We get from Eq.(6c)

$$\hat{H} = \frac{\mathrm{v}^2}{m\mathrm{v}^2 + e\phi}\Big(\boldsymbol{\sigma}\cdot(\mathbf{p} - \frac{e}{c}\mathbf{A})\Big)^2 - e\phi \ . \tag{7}$$

For electron in hydrogen-like ion the equality $e\phi = m\,\mathrm{v}^2$ is fulfilled [9]. Thus, using it in the denominator on the r.h.s. of Eq.(7) we get

$$\hat{H} = \frac{1}{2m}\Big(\boldsymbol{\sigma}\cdot(\mathbf{p} - \frac{e}{c}\mathbf{A})\Big)^2 - e\phi \ . \tag{8}$$

It is demonstrated in related textbooks [1] that the following equation holds

$$\Big(\boldsymbol{\sigma}\cdot(\mathbf{p} - \frac{e}{c}\mathbf{A})\Big)^2 = (\mathbf{p} - \frac{e}{c}\mathbf{A})^2 - \frac{e\hbar}{c}\boldsymbol{\sigma}\cdot\mathbf{B} \ . \tag{9}$$

Substituting Eq.(9) in Eq.(8), we obtain

$$\hat{H} = \frac{1}{2m}(\mathbf{p} - \frac{e}{c}\mathbf{A})^2 - \frac{e}{mc}\mathbf{S}\cdot\mathbf{B} - e\phi \ , \tag{10}$$

where S denotes the spin vector of the electron which relates to the vector σ through the known formula $\mathbf{S} = \frac{1}{2}\hbar\,\boldsymbol{\sigma}$.

We introduce the concept of relativistic spin magnetic moment of electron $-e\,\mathbf{S}/mc$ (since here we have relativistic mass *m*). So, the second term on the r.h.s. of Eq.(10) represents the interaction of the electron relativistic spin magnetic moment with the magnetic field B.

Replacing H with $i\hbar\,\partial/\partial t$ and $\mathbf{p}$ with $-i\hbar\nabla$ in Eq.(10), and operating with both sides of the resulting equation on the wave function $\psi(r,t)$, we get

$$i\hbar\frac{\partial}{\partial t}\psi(r,t) = \frac{1}{2m}(-i\hbar\nabla - \frac{e}{c}\mathbf{A})^2\psi(r,t) - \frac{e}{mc}\mathbf{S}\cdot\mathbf{B}\,\psi(r,t) - e\phi\,\psi(r,t), \tag{11}$$

where $\psi(r,t)$ is two-component spinor, which is a combination of two wave functions $\psi_{\uparrow}(r,t)$ and $\psi_{\downarrow}(r,t)$ that corresponds to two different states of the electron spin orientation.

A significant characteristic of Eq.(10) is that we did not use any approximation to obtain it. Therefore, it contains relativistic mass *m*, not the rest mass m_0. Hence, Eq.(11) is considered relativistic Pauli equation. We devote the next paragraph to a vital application of this equation that is original formulation to the relativistic ZE.

3 Novel description to the relativistic Zeeman effect

The ZE is attributed as a physical effect to the interaction of the orbital and spin magnetic moments of an electron in atom with a steady uniform magnetic field. The physical essence of the ZE appears explicitly in non-relativistic quantum mechanics treatment of The ZE [4, 5].

The relativistic treatment of the ZE in some text-books [1] and literatures [6] make use of perturbation theory. For instance, the Hamiltonian for electron in hydrogen-like ion is written as $\hat{H} = \hat{H}_0 + \hat{H}'$, $\hat{H}_0$ being the Dirac Hamiltonian for electron with zero applied magnetic field, and H' is the perturbation attributed to the interaction with the magnetic field which has the form $\hat{H}' = -e(\boldsymbol{\alpha}\cdot\mathbf{A})$ [1, 6], where e is the electron charge, the vector $\boldsymbol{\alpha}$ consists of the Dirac α matrices and A is the vector potential. Besides the mathematical complexity of this approach [1], it does not reveal the very physical essence of the ZE. However, other textbooks [7] and literatures [8], use another approach by constructing Hamiltonian which contain terms that represent relativistic corrections added to terms that represent non-relativistic ZE.

In the study here we assume a spinless nucleus with infinite mass, and no radiative corrections. We consider the relativistic Pauli equation, Eq.(11), for hydrogen-like ion in steady magnetic filed, and we separate the variables in the wave function $\psi(r,t)$ which we can write as following

$$\psi(r,t) = \begin{pmatrix} \psi_{\uparrow}(r) \\ \psi_{\downarrow}(r) \end{pmatrix} e^{-iEt/\hbar} = \psi(r)\, e^{-iEt/\hbar}. \tag{12}$$

Consequently, Eq.(11) becomes

$$E\,\psi(r) = \frac{1}{2m}(-i\hbar\nabla - \frac{e}{c}\mathbf{A})^2\,\psi(r) - \frac{e}{mc}\mathbf{S}\cdot\mathbf{B}\,\psi(r) - \frac{Ze^2}{r}\psi(r). \quad (13)$$

The first term on the r.h.s. of Eq.(13) could be written as following

$$\frac{1}{2m}(-i\hbar\nabla - \frac{e}{c}\mathbf{A})^2 = -\frac{\hbar^2\Delta}{2m} + \frac{i\hbar e}{mc}\mathbf{A}\cdot\nabla + \frac{e^2}{2mc^2}\mathbf{A}^2. \quad (14)$$

For steady uniform magnetic filed we may take $\mathbf{A} = \mathbf{B}\times\mathbf{r}/2$, so we can write the second term on the r.h.s. of Eq.(14) as $(i\hbar e/mc)\mathbf{A}\cdot\nabla = (-e/2mc)\mathbf{L}\cdot\mathbf{B}$. Hence, this term represents the interaction of the electron relativistic orbital magnetic moment $-e\mathbf{L}/2mc$ with the magnetic field B.

If the magnitude of the magnetic filed is small, then the third term on the r.h.s. of Eq.(14) is negligible, and Eq.(13) becomes

$$E\,\psi(r) = -\frac{\hbar^2\Delta}{2m}\psi(r) - \frac{e}{2mc}(\mathbf{L} + 2\mathbf{S})\cdot\mathbf{B}\,\psi(r) - \frac{Ze^2}{r}\psi(r). \quad (15)$$

The second term on the r.h.s. of this equation represents formulation to relativistic ZE which obviously maintains the very physical essence of the ZE based on the definition of relativistic spin and orbital magnetic moments of electron that we afforded above, and we can use this term to obtain relativistic corrections to non-relativistic ZE.

4 Conclusion

The relativistic spin and orbital magnetic moments of electron that we introduced through the relativistic Pauli equation opens the door to further vital investigations in several disciplines of physics for new relativistic formulations to many physical effects that depends on both or one of these magnetic moments, and probably afford solutions to some unsolved problems in these disciplines of physics.

[1] References

[2] Strange. P., Relativistic Quantum Mechanics, Cambridge University Press, Cambridge (1998).

[3] Bakhoum E. G., Phys. Essays, **15**, 87, (2002).

[4] Hamdan N., Ann. Fond. L. de Broglie, **32**, 1, (2007).

[5] McGervey J. D., Quantum Mechanics, Academic Press Inc., London (1995).
[6] Gasiorowicz. S., Quantum Physics, John Wiley & Sons Inc., New York (1996).
[7] Moskovkin D. L. and Shabaev V. M., Phys. Rev. A, **73**, 52506, (2006).
[8] Grant I. P., Relativistic Quantum Theory of Atoms and Molecules, Springer, New York (2007).
[9] Anthony J. M. and Sebastian K. J., Phys. Rev. A, **49**, 192, (1994).
[10] Bakhoum E. G., Phys. Essays, **15**, 439, (2002).

(Manuscrit reçu le 10 juillet 2008)