Alternative formulation of relativistic quantum mechanics

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Abstract: When determining the coefficients α_i and β of the Dirac equation (which is a relativistic wave equation), Dirac assumed that the equation satisfies the Klein–Gordon equation. The Klein–Gordon equation is an equation that quantizes Einstein's relationship $E^2 = c^2p^2 + E_0^2$. Therefore, this paper derives an equation similar to the Klein–Gordon equation by quantizing the relationship $E_{\mathrm{re},n}^2 + c^2p_n^2 = E_0^2$ between energy and momentum of the electron in a hydrogen atom derived by the author. By looking into the Dirac equation, it is predicted that there is a relativistic wave equation, which satisfies that equation, and its coefficients are determined. With the Dirac equation, it was necessary to insert a term for potential energy into the equation when describing the state of the electron in a hydrogen atom. However, in this paper, a potential energy term was not introduced into the relativistic wave equation. Instead, potential energy was incorporated into the equation by changing the coefficient α_i of the Dirac equation. It may be natural to regard the equation derived in this paper and the Dirac equation as physically equivalent. However, if one of the two equations is superior, this paper predicts it will be the relativistic wave equation derived by the author. © *2011 Physics Essays Publication*. [DOI: 10.4006/1.3659280]

Résumé: Lorsqu'on établit les coefficients α_i et β de l'équation de Dirac, qui est une équation d'onde relativiste, Dirac supposa que cette équation satisfaisait l'équation de Klein-Gordon. L'équation de Klein-Gordon est une version quantifiée de la relation d'Einstein $E^2 = c^2p^2 + E_0^2$. Dans cet article, l'auteur est lui aussi arrivé à une équation analogue à celle de Klein Gordon en effectuant une quantification de la relation énergie-impulsion $E_{\mathrm{re},n}^2 + c^2p_n^2 = E_0^2$ pour l'électron d'un atome d'hydrogène. En examinant l'équation de Dirac, on prédit qu'il y a une équation d'onde relativiste qui satisfait celle équation, et les coefficients sont ensuite déterminés. Lorsque l'on cherche à décrire l'état d'un électron dans un atome d'hydrogène avec l'équation de Dirac, il est nécessaire d'introduire un terme d'énergie potentielle dans l'équation. Cependant, dans notre article, le terme d'énergie potentielle n'a pas été inséré dans l'équation, mais introduit en changeant le coefficient α_i de l'équation de Dirac. Il est tout à fait naturel de considérer que l'équation dérivée dans cet article et l'équation de Dirac son physiquement équivalentes. Néanmoins, si une notion de supériorité devait exister entre les deux équations, l'auteur prévoit que l'équation d'onde relativiste qu'il a établi surpasse celle de Dirac.

Key words: Einstein's Energy-Momentum Relationship; Special Theory of Relativity; Relativistic Energy; Hydrogen Atom; Relativistic Quantum Mechanics; Dirac Relativistic Wave Equation; Klein–Gordon Equation; Alternative Formulation.

I. INTRODUCTION

One of the most important relationships in the special theory of relativity (STR) is as follows:

$$E^2 = c^2p^2 + E_0^2. \tag{1}$$

Here, E is the relativistic energy of an object or a particle, and E_0 is the rest mass energy.

Currently, Einstein's relationship (1) is used to describe the energy and momentum of particles in free space, but for explaining the behavior of bound electrons inside atoms, opinion has shifted to quantum mechanics as represented by equations such as the Dirac equation.

However, in another paper, while agreeing on the importance of the Dirac equation, from a perspective of symmetry, the author poses the following questions: Would an equation similar to Einstein's relationship, which holds true in free space, also hold true in a hydrogen atom? If such an equation were to hold true, what would it look like?

Then, the author derives the following relationship for a bound electron in a hydrogen atom:[1]

$$E_{\mathrm{re},n}^2 + c^2p_n^2 = E_0^2, \quad E_0 = m_{\mathrm{e}}c^2. \tag{2}$$

Here, $E_{\mathrm{re},n}$ is the relativistic energy of a bound electron in a hydrogen atom.

In addition, $E_{\mathrm{re},n}$ was defined classically as follows:[2]

$$E_{\mathrm{re},n} = E_0 + K_n + V(r_n) \tag{3a}$$

$$= E_0 + V(r_n)/2 \tag{3b}$$

$$= E_0 + E_n, \quad n = 1, 2, \ldots, \quad E_n < 0. \tag{3c}$$

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When describing the motion of a bound electron in a hydrogen atom, a term must be included in that equation for the potential energy.

Potential energy is not incorporated into Eq. (2) in a form which is visible to the eye. However, a quantity corresponding to $V(r_n)$ is incorporated from the beginning into $E_{\mathrm{re},n}$ due to the definition of Eq. (3a).

When establishing the coefficient for the Dirac equation, a relativistic wave equation, Dirac assumed that this equation satisfied the Klein–Gordon equation. However, the Klein–Gordon equation is a quantized equation of Einstein's relationship.

Thus, we attempt to derive an equation similar to the Klein–Gordon equation by quantizing Eq. (2) derived by the author. Then, the relativistic wave equation satisfying that equation is predicted, and its coefficients are determined.

II. CONFIRMING THE DIRAC RELATIVISTIC WAVE EQUATION AND ITS COEFFICIENTS

In preparation for the discussion in the next section, this section confirms the Dirac relativistic wave equation and its coefficients by referring to a quantum mechanics textbook.

The fact that when we perform quantization for Eq. (1), we obtain the following Klein–Gordon equation is evident:

$$-\hbar^2\frac{\partial^2}{\partial t^2}\psi=-\hbar^2c^2\left(\frac{\partial^2}{\partial x_1^2}+\frac{\partial^2}{\partial x_2^2}+\frac{\partial^2}{\partial x_3^2}\right)\psi+m^2c^4\psi. \quad (4)$$

This equation described the wave function in relativistic terms, but this interpretation was inconsistent with the interpretation according to the more commonly used Schrödinger equation.

Dirac approached the problem of finding a relativistic wave equation by starting from the Hamiltonian form is as follows:[3]

$$i\hbar\frac{\partial}{\partial t}\psi(\mathbf{r},t)=H\psi(\mathbf{r},t). \quad (5)$$

The simplest Hamiltonian that is linear in the momentum and mass term is as follows:

$$H=c\alpha\cdot\mathbf{p}+\beta mc^2. \quad (6)$$

By substituting this into Eq. (5), we obtain

$$(E-c\alpha\cdot\mathbf{p}-\beta mc^2)\psi=0. \quad (7)$$

We also substitute E and $\mathbf{p}$ in Eq. (7)

$$E\to i\hbar\frac{\partial}{\partial t},\quad \mathbf{p}\to -i\hbar\nabla. \quad (8)$$

The result is the following quantized expression:

$$\left(i\hbar\frac{\partial}{\partial t}+i\hbar c\alpha\cdot\nabla-\beta mc^2\right)\psi=0. \quad (9)$$

Dirac surmised that a correct equation to resolve this shortcoming must take the following form:[4]

$$i\hbar\frac{\partial}{\partial t}\psi=\left[-i\hbar c\left(\alpha_1\frac{\partial}{\partial x_1}+\alpha_2\frac{\partial}{\partial x_2}+\alpha_3\frac{\partial}{\partial x_3}\right)+\beta mc^2\right]\psi. \quad (10)$$

This is a rewritten form of Eq. (9).

Then, because this equation must satisfy the Klein–-Gordon equation, Dirac thought that all that was left was to determine the unknown coefficients α_i and β.

Dirac obtained the following for coefficients α_i and β:

$$\alpha_1=\begin{bmatrix}0&0&0&1\\0&0&1&0\\0&1&0&0\\1&0&0&0\end{bmatrix}\quad \alpha_2=\begin{bmatrix}0&0&0&-i\\0&0&i&0\\0&-i&0&0\\i&0&0&0\end{bmatrix}$$
$$\alpha_3=\begin{bmatrix}0&0&1&0\\0&0&0&-1\\1&0&0&0\\0&-1&0&0\end{bmatrix}\quad \beta=\begin{bmatrix}1&0&0&0\\0&1&0&0\\0&0&-1&0\\0&0&0&-1\end{bmatrix}. \quad (11)$$

This coefficient was derived from the following conditions:

$$\left.\begin{aligned}&\alpha_i^2=1\\&\alpha_i\alpha_j+\alpha_j\alpha_i=0\\&\alpha_i\beta+\beta\alpha_i=0\\&\beta^2=1\end{aligned}\right\},\quad i,j=1,2,3(i\neq j). \quad (12)$$

Terms that involve the electromagnetic potentials can be added to Eq. (9) in a relativistic way by making the usual replacements as follows, where the particle described by the equation has electric charge e

$$c\mathbf{p}\to c\mathbf{p}-e\mathbf{A},\ E\to E-e\varphi. \quad (13)$$

Here, E and $\mathbf{p}$ represent the operators of Eq. (8).

In special cases like a central field (in which $\mathbf{A}=0$ and φ are spherically symmetric), because $\mathbf{A}(\mathbf{r},t)=0$, $\varphi(\mathbf{r},t)=\varphi(r)$, this enables us to obtain

$$i\hbar\frac{\partial\psi}{\partial t}=H\psi,$$

$$H=c\alpha\cdot\mathbf{p}+\beta mc^2+V. \quad (14)$$

where $V=e\varphi$.

Represented in the same style as Eq. (9), we obtain

$$\left(i\hbar\frac{\partial}{\partial t}+i\hbar c\alpha\cdot\nabla-\beta mc^2-V\right)\psi=0. \quad (15)$$

The energies of a hydrogen atom derived from Eqs. (2) and (15) are compared (see Appendix).

III. NEW RELATIONAL EXPRESSION QUANTIZATION

In this section, we shall attempt to quantize the newly obtained relationship (2).

Now, when we perform quantization on Eq. (2), we obtain the following:

$$-\hbar^2\frac{\partial^2}{\partial t^2}\psi=\hbar^2c^2\left(\frac{\partial^2}{\partial x_1^2}+\frac{\partial^2}{\partial x_2^2}+\frac{\partial^2}{\partial x_3^2}\right)\psi+m_e^2c^4\psi. \quad (16)$$

This equation corresponds to the Klein–Gordon Equation (4) obtained by quantizing Eq. (1). This paper predicts the relativistic wave equation, which takes the place of the Dirac equation, and its coefficients are determined so that the wave equation satisfies Eq. (16).

To do so, in order to differentiate from the existing Dirac Equation (10), we assume that the expression derived in this paper has the coefficients α_i' and β

$$i\hbar\frac{\partial}{\partial t}\psi=\left[-i\hbar c\left(\alpha_1'\frac{\partial}{\partial x_1}+\alpha_2'\frac{\partial}{\partial x_2}+\alpha_3'\frac{\partial}{\partial x_3}\right)+\beta' m_e c^2\right]\psi. \quad (17)$$

Equation (10) was obtained by rewriting Eq. (9), but Eq. (17) was obtained by rewriting the following equation:

$$\left(i\hbar\frac{\partial}{\partial t}+i\hbar c\alpha'\cdot\nabla-\beta' m_e c^2\right)\psi=0. \quad (18)$$

Extracting only the operator from Eq. (17), and making an equation by squaring both sides, we obtain

$$\begin{aligned}-\hbar^2\frac{\partial^2}{\partial t^2}\psi=\Bigg[&-\hbar^2c^2\left(\alpha_1'\frac{\partial}{\partial x_1}+\alpha_2'\frac{\partial}{\partial x_2}+\alpha_3'\frac{\partial}{\partial x_3}\right)^2\\&-i\hbar c\left(\alpha_1'\frac{\partial}{\partial x_1}+\alpha_2'\frac{\partial}{\partial x_2}+\alpha_3'\frac{\partial}{\partial x_3}\right)\beta' m_e c^2\\&-\beta' m_e c^2 i\hbar c\left(\alpha_1'\frac{\partial}{\partial x_1}+\alpha_2'\frac{\partial}{\partial x_2}+\alpha_3'\frac{\partial}{\partial x_3}\right)\\&+\beta'^2 m_e^2c^4\Bigg]\psi. \end{aligned} \quad (19)$$

Since the left side of this equation is the same as the Klein-–Gordon equation and Eq. (16), the right side should finally be the same as the right side of Eq. (16).

Next, expanding the right side of Eq. (19), we obtain the following:

$$\begin{aligned}-\hbar^2\frac{\partial^2}{\partial t^2}\psi=\Bigg[&-\hbar^2c^2\left(\alpha_1'^2\frac{\partial^2}{\partial x_1^2}+\alpha_2'^2\frac{\partial^2}{\partial x_2^2}+\alpha_3'^2\frac{\partial^2}{\partial x_3^2}\right)\\&-\hbar^2c^2\left(\alpha_1'\alpha_2'+\alpha_2'\alpha_1'\right)\frac{\partial}{\partial x_1}\frac{\partial}{\partial x_2}\\&-\hbar^2c^2\left(\alpha_2'\alpha_3'+\alpha_3'\alpha_2'\right)\frac{\partial}{\partial x_2}\frac{\partial}{\partial x_3}\\&-\hbar^2c^2\left(\alpha_3'\alpha_1'+\alpha_1'\alpha_3'\right)\frac{\partial}{\partial x_3}\frac{\partial}{\partial x_1}\\&-i\hbar m_e c^3\left(\alpha_1'\beta'+\beta'\alpha_1'\right)\frac{\partial}{\partial x_1}\\&-i\hbar m_e c^3\left(\alpha_2'\beta'+\beta'\alpha_2'\right)\frac{\partial}{\partial x_2}\\&-i\hbar m_e c^3\left(\alpha_3'\beta'+\beta'\alpha_3'\right)\frac{\partial}{\partial x_3}+\beta'^2m_e^2c^4\Bigg]\psi. \end{aligned} \quad (20)$$

In order to make Eqs. (16) and (20) the same, the coefficients α_i' and β' must be a 4×4 matrix satisfying the following conditions:

$$\left.\begin{aligned}&\alpha_i'^2=-1\\&\alpha_i'\alpha'_j+\alpha'_j\alpha_i'=0\\&\alpha_i'\beta'+\beta'\alpha_i'=0\\&\beta'^2=1\end{aligned}\right\},\quad i,j=1,2,3(i\neq j). \quad (21)$$

The solution which satisfies these conditions and is a clean combination is as follows:

$$\alpha_1'=\begin{bmatrix}0&0&0&1\\0&0&-1&0\\0&1&0&0\\-1&0&0&0\end{bmatrix}\quad \alpha_2'=\begin{bmatrix}0&0&0&i\\0&0&i&0\\0&i&0&0\\i&0&0&0\end{bmatrix}$$

$$\alpha_3'=\begin{bmatrix}0&0&1&0\\0&0&0&1\\-1&0&0&0\\0&-1&0&0\end{bmatrix}\quad \beta'=\begin{bmatrix}1&0&0&0\\0&1&0&0\\0&0&-1&0\\0&0&0&-1\end{bmatrix}. \quad (22)$$

We have thus confirmed that $\beta=\beta'$.

Therefore, Eq. (18) becomes as follows:

$$\left(i\hbar\frac{\partial}{\partial t}+i\hbar c\alpha'\cdot\nabla-\beta m_e c^2\right)\psi=0. \quad (23)$$

Equation (15) was obtained by inserting a term V into the Hamiltonian in Eq. (9). On the other hand, Eq. (23) was obtained by changing the coefficient in Eq. (9) from α_i (11) to α_i' (22). The change in this coefficient corresponds to incorporating potential energy into the Hamiltonian in Eq. (9).

IV. CONCLUSION

The Dirac relativistic wave equation, which describes the energy of a hydrogen atom, is given as

$$\left(i\hbar\frac{\partial}{\partial t}+i\hbar c\alpha\cdot\nabla-\beta mc^2-V\right)\psi=0. \quad (24)$$

where

$$\alpha_1=\begin{bmatrix}0&0&0&1\\0&0&1&0\\0&1&0&0\\1&0&0&0\end{bmatrix}\quad \alpha_2=\begin{bmatrix}0&0&0&-i\\0&0&i&0\\0&-i&0&0\\i&0&0&0\end{bmatrix}$$

$$\alpha_3=\begin{bmatrix}0&0&1&0\\0&0&0&-1\\1&0&0&0\\0&-1&0&0\end{bmatrix}\quad \beta=\begin{bmatrix}1&0&0&0\\0&1&0&0\\0&0&-1&0\\0&0&0&-1\end{bmatrix}. \quad (25)$$

Here, rather than changing the Dirac Equation (9) coefficient that is true in free space, the problem is solved by adding the term $-V$ to the Hamiltonian.

In this paper, however, we have shown that the energy of a hydrogen atom can be described by the following equation as well:

$$\left(i\hbar\frac{\partial}{\partial t} + i\hbar c\alpha' \cdot \nabla - \beta m_e c^2\right)\psi = 0. \tag{26}$$

where

$$\alpha_1' = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{bmatrix} \quad \alpha_2' = \begin{bmatrix} 0 & 0 & 0 & i \\ 0 & 0 & i & 0 \\ 0 & i & 0 & 0 \\ i & 0 & 0 & 0 \end{bmatrix}$$

$$\alpha_3' = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{bmatrix} \quad \beta = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}. \tag{27}$$

Because the Dirac Equation (9) does not include potential energy, the term V has been newly added in Eq. (15). However, V is already included within $E_{\mathrm{re},n}$ in Eq. (2).

Therefore, there is no need to add again the term V to Eq. (17), which satisfies Eq. (16) derived by quantizing Eq. (2).

In this paper, the problem is solved not by adding $-V$ to the Dirac Equation (9) but by changing the coefficient from α_i to α_i'.

Incidentally, for methods of handling equations in quantum mechanics, there are the Schrödinger representation and the Heisenberg representation. The former of these calculate time change under a wave function (state), while the latter calculates using time-dependent operators, and the states are constant. Equation (23) of this paper and the existing Eq. (15) stand in contrast to each other like these two representations.

Taking this into account, it may be natural to regard Eqs. (23) and (15) as equivalent equations describing the state of the bound electron in a hydrogen atom. However, if one of the two equations is superior, this paper predicts that it will be Eq. (23) derived by the author.

The three reasons for this are as follows:

(1) The equation which served as the point of departure for deriving Eq. (15) was Eq. (1), but the equation which served as the point of departure for deriving Eq. (23) was Eq. (2). Starting from Eq. (2) is believed to be a valid approach for deriving an equation to describe the behavior of the bound electron inside an atom.

(2) Equation (23) is simpler than Eq. (15).

(3) The approximate value of the energy of the hydrogen atom can be derived much more simply from Eq. (2) than from the Dirac equation.[1]

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APPENDIX

In the textbook of Schiff, the following eigenvalue for the energy of a hydrogen atom was obtained by performing complex calculations based on Eq. (15):

$$E = m_e c^2\left[1 + \frac{\alpha^2}{(s+n')^2}\right]^{-1/2}, \quad n' = 0, 1, 2, \ldots. \tag{A1}$$

Additionally, the correct quantum number for Eq. (A1) is

$$s = \sqrt{k^2 - \alpha^2}, \quad n = n' + |k|. \tag{A2}$$

If we now substitute Eq. (A2) into Eq. (A1), and take the terms of order α^4, we obtain

$$E = m_e c^2\left[1 - \frac{\alpha^2}{2n^2} - \frac{\alpha^4}{2n^4}\left(\frac{n}{|k|} - \frac{3}{4}\right)\right]. \tag{A3}$$

n is the total quantum number, n' is the radial quantum number, and $|k|$ can take on positive integer values. Equation (A3) shows that the energy increases with increasing $|k|$.

When $n/|k| = 1$ in Eq. (A3), the contents of the third term in parentheses on the right side equal $1/4$, so we can rewrite as

$$E_n = m_e c^2\left(1 - \frac{\alpha^2}{2n^2} - \frac{\alpha^4}{8n^4} - \cdots\right). \tag{A4}$$

Next, we shall derive the energy of a hydrogen atom from Eq. (2). First, we can rewrite Eq. (2) as

$$E_{\mathrm{re},n} = (m_e^2 c^4 - c^2 p_n^2)^{1/2} \tag{A5a}$$

$$= m_e c^2\left(1 - \frac{p_n^2}{m_e^2 c^2}\right)^{1/2}. \tag{A5b}$$

Incidentally, in Ref. 1, the author derived the following relation from Eq. (2) in this paper:

$$p_n^2 = \left(\frac{\alpha^2}{n^2} - \frac{\alpha^4}{4n^4}\right)(m_e c)^2. \tag{A6}$$

Also, because $\alpha^4 = (5.325 \times 10^{-5})\alpha^2$, if we now set $\alpha^4/4n^4 \approx 0$, Eq. (A6) can be written as

$$p_n \approx \frac{\alpha m_e c}{n} \tag{A7a}$$

$$= \left(\frac{1}{4\pi\varepsilon_0}\right)\frac{m_e e^2}{n\hbar}. \tag{A7b}$$

However, α here is the following fine structure constant:

$$\alpha = \frac{e^2}{4\pi\varepsilon_0 \hbar c}. \tag{A8}$$

Then, using the relationship from Eq. (A7a), an approximation, we obtain

$$E_{\mathrm{re},n} \approx m_{\mathrm{e}}c^2\left(1-\frac{\alpha^2}{n^2}\right)^{1/2}. \tag{A9}$$

Using the binomial theorem expansion here, we obtain

$$E_{\mathrm{re},n} \approx m_{\mathrm{e}}c^2\left(1-\frac{\alpha^2}{2n^2}-\frac{\alpha^4}{8n^4}-\cdots\right). \tag{A10}$$

The Dirac equation obtains the energy levels through complex calculations based on Eq. (15). However, we can easily obtain the energy levels by starting from Eq. (A5b), which has been derived in previous paper.

The following accurate value is obtained if the value of Eq. (A6) is substituted for p_n^2 in Eq. (A5b) without using the approximation in Eq. (A7a):

$$E_{\mathrm{re},n} = m_{\mathrm{e}}c^2\left(1-\frac{\alpha^2}{n^2}+\frac{\alpha^4}{4n^4}\right)^{1/2} \tag{A11a}$$

$$= m_{\mathrm{e}}c^2\left(1-\frac{\alpha^2}{2n^2}\right). \tag{A11b}$$

However, because Eq. (A11b) is not a quantized expression, the energy value of Eq. (A10) can only be obtained for the energy values of degenerative states.

If this energy is described with the energy E_n in classical quantum theory, then it becomes as follows.

$$\begin{aligned} E_n &= -\left(m_{\mathrm{e}}c^2 - E_{\mathrm{re},n}\right) = -\frac{\alpha^2 m_{\mathrm{e}}c^2}{2n^2} \\ &= -\frac{1}{2}\left(\frac{1}{4\pi\varepsilon_0}\right)^2 \frac{m_{\mathrm{e}}e^4}{\hbar^2}\cdot\frac{1}{n^2}. \end{aligned} \tag{A12}$$

It is ironic that E_n matches the accurate value, even though the energy of a hydrogen atom is found through approximation in classical quantum theory. This is due to the following reason.

In classical quantum theory, the following approximation is used first:

$$K_n \approx \frac{p_n^2}{2m_{\mathrm{e}}}. \tag{A13}$$

Next, the following value is obtained if Eq. (A7a), which is an approximate value, is substituted for p_n in this equation:

$$E_n = -K_n = -\frac{1}{2m_{\mathrm{e}}}\frac{\alpha^2 m_{\mathrm{e}}^2 c^2}{n^2} = -\frac{1}{2}\left(\frac{1}{4\pi\varepsilon_0}\right)^2 \frac{m_{\mathrm{e}}e^4}{\hbar^2}\cdot\frac{1}{n^2}. \tag{A14}$$

This value matches with Eq. (A12).

In the end, the solution eventually obtained by using two approximations in classical quantum theory matches the correct solution.

The task of deriving the energy of the hydrogen atom from Eq. (23) will be carried out in a separate paper.

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