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THE DIRAC EQUATION FOR MANY-ELECTRON SYSTEMS

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1. INTRODUCTION

THE well-known relativistic wave equation for an electron[1] was derived by Dirac by factorising a second order equation into two linear equations. It is the object of the present note to point out that the Dirac equation is simply the eigenvalue equation of the magnitude of the momentum four-vector, and that one can derive it by expressing the magnitude of the momentum vector in terms of its four components.

The above idea enables one to generalise the Dirac equation and obtain a relativistic equation for systems containing several electrons. In Section 3, we have given the wave equation (Equation 16) for a system composed of several particles and this is very similar in form to the Dirac equation. Relativistic wave equations for a system of two electrons have previously been given by Eddington,[2] Gaunt[3] and Breit[5] of which the one given by Breit is the most satisfactory. By replacing the velocities $\mathbf{v}^{\mathrm{I}}$ and $\mathbf{v}^{\mathrm{II}}$ of the electrons by the spin matrices $-c\alpha^{\mathrm{I}}$ and $-c\alpha^{\mathrm{II}}$ in a Hamiltonian given by Darwin,[4] Breit was able to obtain an approximate wave equation for two-electron systems. It is shown in Section 4, that Equation (16) leads to the Breit equation when it is represented in the product space of the two electrons.

2. THE MOMENTUM FOUR-VECTOR

Before proceeding further, we first state a result which was first proved by Weyl[6] for a vector in a n-dimensional space and which we shall apply presently.

(*a*) *Lemma.*—Let $(x_1, x_2, \cdots, x_n)$ be the co-ordinates of a vector $\vec{r}$ in an Eucledian space with reference to a system of orthogonal axes, and let $r = (x_1{}^2 + x_2{}^2 + \cdots + x_n{}^2)^{\frac{1}{2}}$ denote the 'magnitude' or 'length' of the vector r. Then

$$r = \sum_{\mu=1}^{n} (\gamma_\mu x_\mu), \tag{1}$$

where the γ_μ's are elements of an abstract algebra satisfying the relations $(\gamma_\mu \gamma_\nu + \gamma_\nu \gamma_\mu) = 2\delta_{\mu\nu}$.

The γ's can be expressed as matrices and for the case $n = 4$, they are the Dirac matrices.

(*b*) *The Dirac Equation.*—Let x_1, x_2, x_3 and x_4 $(= ict)$ be the co-ordinates of a world point, and similarly let p_1, p_2, p_3 and p_4 $(= i\mathrm{E}/c)$ denote the components of the momentum four-vector. Besides x_4 and p_4, we shall also use the symbols x_0 and p_0 given by $x_4 = ix_0$ and $p_4 = ip_0$. Expressed as operators we have then $p_4 = -i\hbar\partial/\partial x_4$ and $p_0 = i\hbar\partial/\partial x_0$.

Now the momentum four-vector $\vec{\mathrm{P}}$ is a vector with constant magnitude im_0c where m_0 is the rest mass of the particle. Apply now the result (1) to the vector $\vec{\mathrm{P}} = (p_1, p_2, p_3, p_4)$. We then get

$$\sum_{i=1}^{4} \gamma_i p_i = im_0c. \tag{2}$$

If $|\psi\rangle$ is an eigenstate of the momentum four-vector, we get from (2) the equation of an electron as

$$\left(i\gamma_4 p_0 + \sum_{i=1}^{3} \gamma_i p_i - im_0c\right) |\psi\rangle = 0. \tag{3}$$

For the γ's we now choose the following representations:—

$$\gamma_4 = \begin{pmatrix} -\mathrm{I} & 0 \\ 0 & \mathrm{I} \end{pmatrix}; \quad \gamma_1 = \begin{pmatrix} 0 & -i\sigma_1 \\ i\sigma_1 & 0 \end{pmatrix}; \quad \gamma_2 = \begin{pmatrix} & -i\sigma_2 \\ i\sigma_2 & 0 \end{pmatrix};$$

$$\gamma_3 = \begin{pmatrix} 0 & -i\sigma_3 \\ i\sigma_3 & 0 \end{pmatrix}$$

where I, σ_1, σ_2 and σ_3 denote respectively the unit matrix in two dimensions and the three Pauli matrices.

Multiplying (3) to the left by $-i\gamma_4^{-1}$, we get

$$\left(p_0 + \sum_{i=1}^{3} \alpha_i p_i + \beta m_0 c\right) |\psi\rangle = 0 \tag{4}$$

which is the Dirac equation in its conventional form.

When the electron is moving in a field, the components of the momentum four-vector are given by $(p_i + e/c\,\mathrm{A}_i)$ $(i = 0, 1, 2, 3)$ where A_0, A_1, A_2, A_3

are the scalar and vector potentials of the field. From the relations $\sum_{i=1}^{4} (p_i + e/c\, A_i)^2 = - m_0^2 c^2$, we see that the magnitude of the momentum four-vector is equal to $i m_0 c$ in this case also. Thus by replacing p_i by $(p_i + e/c\, A_i)$ in (4), we get the equation for an electron moving in field as

$$\left\{\left(p_0 + \frac{e}{c} A_0\right) + \sum_{i=1}^{3} a_i \left(p_i + \frac{e}{c} A_i\right) + \beta m_0 c\right\} | \psi \rangle = 0. \qquad (5)$$

The left-hand side of (2) is similar in form to the expression of the length of a vector in terms of its direction cosines. The γ's can thus be regarded as the representations in a matrix algebra of the direction cosines of the momentum four-vector. We have thus

$$\gamma_i = \frac{p_i}{|\vec{P}|} \qquad \text{or} \qquad i\gamma_i = u_i, \qquad (6)$$

where u_i $(i = 1, 2, 3, 4)$ are the components of the velocity four-vector. The matrices $i\gamma_i$ thus represent the components of the velocity four-vector. Since

$$a_i = - i\, (\gamma_4)^{-1}\, \gamma_i \;\; (i = 1, 2, 3),$$

we have

$$a_i = - \frac{i p_i}{p_4} = - \frac{\dot{x}_i}{c}$$

or

$$\dot{x}_i = - c a_i. \qquad (7)$$

Similarly

$$\beta = - \sqrt{1 - \frac{v^2}{c^2}}. \qquad (8)$$

We thus get the well-known expressions for the components of the velocity of the particle without calculating the commutation relations of x_1, x_2 and x_3 with the Hamiltonian.

In finding out the dynamical variables that are the classical analogues of products (or quotients) of matrices, care should be taken to verify that only the algebraical rules that are common to both the matrix and the ordinary algebras are used. We have derived (4) by multiplying (2) by $- i\gamma_4^{-1}$ making use of the relation $(\gamma_4)^{-1}\, \gamma_4 = 1$ which is common to both algebras, though one could equally well derive (4) by multiplying (2) by $-i\gamma_4$. The classical analogue of α_i is thus $-i(\gamma_4)^{-1}\gamma_i$ and not $-i\gamma_4\gamma_i$.

3. SYSTEM OF MANY ELECTRONS

We have seen that the Dirac equation can be derived by expressing the magnitude of the four-vector $\vec{P} + e/c\,\vec{A}$ in terms of its components. Now

$$\left(P_i + \frac{e}{c}A_i\right) = m_0 c u_i \qquad (i = 1, 2, 3, 4)$$

$$= \frac{m_0 \dot{x}_i}{\sqrt{1 - \frac{v^2}{c^2}}}, \tag{9}$$

where u_1, u_2, u_3, u_4 are the components of the velocity four-vector. natural way to generalise the Dirac equation for a system of particles would be to consider a four-vector whose components are respectively $\Sigma\, m_0 c u_i$ $(i = 1, 2, 3, 4, \text{ or } 0)$ where the sum is to be taken over all the particles of the system. We shall denote the components of this vector by $(P_0 + e/c\, A_0)$, $(P_1 + e/c\, A_1)$, $(P_2 + e/c\, A_2)$ and $(P_3 + e/c\, A_3)$.

Now in the special theory of relativity the components of the total momentum are given by[7]

$$P_i = -\frac{i}{c}\int T_{ik}\,dS_k + \Sigma\, m_0 c u_i, \tag{10}$$

where T_{ik}.. are the components of the energy-momentum tensor. In three-dimensional form, we can write for the total momentum of field *plus* charges

$$\int \frac{S}{c^2}\,dV + \Sigma\, p \tag{10 a}$$

and for the energy

$$\int W\,dV + \Sigma\, \mathcal{E}, \tag{10 b}$$

where

$$S = \frac{c}{4\pi}\,E \times H$$

is the Poynting vector and

$$W = \frac{1}{8\pi}(E^2 + H^2)$$

is the density of the field energy. For a system of charges, the electrostatic energy (U), apart from the self-energy terms, is equal to

$$U = \int W dV = \sum \frac{e_A e_B}{r_{AB}} .$$

We thus see that the quantities

$$-\frac{e}{c}(A_0, A_1, A_2, A_3)$$

stand respectively for the energy-momentum of the field.

Let us denote the magnitude of $\vec{P} + e/c\,\vec{A}$ by iP'. P' is equal to $\sum_i m_{0i}c$ only as a first approximation. We have in fact

$$-P'^2 = -c^2\left(\sum_i m_i\right)^2 + \sum_{k=1}^{3}\left(\sum_{i=1}^{n} m_i\dot{x}_{ik}\right)^2, \tag{11}$$

where

$$m_i = \frac{m_{0i}}{\sqrt{1-\frac{v_i^2}{c^2}}} .$$

Thus

$$-P'^2 = -c^2\left(\Sigma m_i^2 + 2\sum_{\substack{i,j\\ i<j}} m_i m_j\right) + \left(\sum_i m_i^2 v_i^2 + 2\sum_{\substack{i,j\\ i<j}} m_i m_j \mathbf{v}_i\cdot\mathbf{v}_j\right)$$

or

$$P'^2 = \Sigma m_i^2 c^2\left(1-\frac{v_i^2}{c^2}\right) + 2\Sigma m_i m_j c^2\left(1-\frac{\mathbf{v}_i\cdot\mathbf{v}_j}{c^2}\right). \tag{12}$$

Now

$$m_i m_j c^2\left(1-\frac{\mathbf{v}_i\cdot\mathbf{v}_j}{c^2}\right) = \frac{m_{0i}m_{0j}c^2}{\sqrt{\left(1-\frac{v_i^2}{c^2}\right)\left(1-\frac{v_j^2}{c^2}\right)}}\left(1-\frac{\mathbf{v}_i\cdot\mathbf{v}_j}{c^2}\right)$$

$$\sim m_{0i}m_{0j}c^2\left(1+\frac{v_{ij}^2}{2c^2}\right), \tag{13}$$

where

$$v_{ij} = (v_i - v_j). \tag{14}$$

Substituting (13) in (12), we get

$$P'^2 \sim \Sigma m_{0i}{}^2 c^2 + 2\,\Sigma m_{0i} m_{0j} c^2 \left(1 + \frac{v_{ij}{}^2}{c^2}\right)$$

$$= (\Sigma m_{0i} c)^2 + \Sigma m_{0i} m_{0j} v_{ij}{}^2.$$

Thus a second approximation for P′ is given by

$$P' \sim \sum_{i=1}^{n} m_{0i} c + \tfrac{1}{2} \frac{\sum_{ij} m_{0i} m_{0j} v_{ij}{}^2}{\sum_{i} m_{0i} c}. \tag{15}$$

Applying now the results of Section 1 to the vector $P + e/c\, A$, we get the equation for the system of electrons as

$$\left\{\left(P_0 + \frac{e}{c} A_0\right) + \sum_{k=1}^{3} \alpha_k \left(P_k + \frac{e}{c} A_k\right) + \beta P'\right\} | \psi \rangle = 0. \tag{16}$$

4. Representation in the Product Space and the Breit Equation

Equation (16) describes the system as a whole and can be considered to be the equation of motion for the centre of inertia of the system. Since we are operating in a four-dimensional space, the matrices α_k and β are all four-dimensional. They refer to the entire-system of electrons and do not contain any labels of the individual particles. In practice, however, one needs equations that bring in explicitly the positions and spins of the individual electrons of the system. We shall see presently that Equation (16) can be transformed into one that contains explicit reference to the spins of the electrons if it is represented in the *product space* of the electrons.

Since the γ's represent the direction cosines of the momentum four-vector, their classical analogues are given by

$$\gamma_k = \frac{\sum_{i=1}^{n} m_i \dot{x}_{ik}}{iP'} \qquad (k = 1, 2, 3)$$

and

$$\gamma_4 = \frac{(\Sigma\, i m_i c)}{iP'}. \tag{17 a}$$

Thus we have

$$a_k = -\,i\,(\gamma_4)^{-1}\,\gamma_k = -\,\frac{\Sigma\, m_i \dot{x}_{ik}}{c\,\Sigma\, m_i}$$

and

$$\beta P' = -\,\frac{P'^2}{c\,\Sigma\, m_i}\,. \qquad (17\,b)$$

Thus we have

$$\sum_{k=1}^{3} a_k \left(P_k + \frac{e}{c} A_k\right) + \beta P'$$

$$= \frac{\left\{-\sum\limits_{k=1}^{3}\left(\sum\limits_{i} m_i \dot{x}_{ik}\right)^2 - P'^2\right\}}{c \sum\limits_{i} m_i}$$

$$= -\sum m_i c = -\,c \sum_i \frac{m_{0i}}{\sqrt{\left(1 - \frac{v_i^2}{c^2}\right)}}$$

$$= -\sum_{i=1}^{n} m_{0i} c \sqrt{1 - \frac{v_i^2}{c^2}} - \frac{1}{c} \sum_{i=1}^{n} m_i v_i^2 \qquad (18)$$

correct to terms of the order of v_i^4/c^3.

Alternatively, one can get (18) without using the idea of direction cosines at all. From (16) we have

$$\left\{\sum_{k=1}^{3} a_k \left(P_k + \frac{e}{c} A_k\right) + \beta P'\right\} |\,\psi\,\rangle = -\left(P_0 + \frac{e}{c} A_0\right) |\,\psi\,\rangle$$

and by definition,

$$-\left(P_0 + \frac{e}{c} A_0\right) = -\sum_i m_i c;$$

this leads now to the right-hand of (18).

For an electron moving in a field, we have

$$m\mathbf{v} = \mathbf{P} + \frac{e}{c}\mathbf{A}$$

where **P** is the momentum conjugate to the position of the particle and **A** is the vector potential of the field. Thus we have

$$\sum m_i v_i^2 = \sum \mathbf{v}_i \cdot \left(\mathbf{P}^i + \frac{e}{c}\mathbf{A}^i\right). \tag{19}$$

The term $e/c\,\Sigma\,\mathbf{v}_i \cdot \mathbf{A}^i$ gives the interaction energy of the charges with the magnetic field produced by the motion of the electrons.

Now the potentials arising from the motion of a charge e have been worked out in Landau and Lifshitz[7] and these are given by

$$\phi' = \frac{e}{r}; \quad \mathbf{A}' = e\,\frac{[\mathbf{v} + (\mathbf{v}\cdot\boldsymbol{n})\,\boldsymbol{n}]}{2cr}, \tag{20 a}$$

where r is the distance of the charge from the field point and $\boldsymbol{n} = \boldsymbol{r}/r$. When there are several charges we must sum over all the charges. Thus the potentials acting at the position of charge 1 due to the motions of charges 2, 3, $\cdots$, n are given by

$$\phi' = \sum_{j=2}^{n} \frac{e}{r_{1j}}$$

and

$$\mathbf{A}' = e \sum_{j=2}^{n} \frac{[\mathbf{v}_j + (\mathbf{v}_j \cdot \boldsymbol{n}_{1j})\,\boldsymbol{n}_{1j}]}{2cr_{1j}}. \tag{20 b}$$

Let us suppose that our system consists of n electrons moving in a static electric field V $(\boldsymbol{r})$ (the field of the nuclei). We can write the potential energy of the system as

$$\mathrm{U} = -\,e\Phi = -\,e\sum_{i=1}^{n}\phi_i$$

where

$$\phi_i = \mathrm{V}(\boldsymbol{r}_i) - \frac{1}{2}\sum_j{}' \frac{e}{r_{ij}}.$$

The factor $\frac{1}{2}$ in the above expression for ϕ_i is introduced to take care that the interaction energy between two electrons is not counted twice. The energy is thus expressible as the sum of n different terms, each term standing for the energy density of a particle. Consider now ϕ_1. We have

$$\phi_1 = V(r_1) - \frac{1}{2} \sum_j{}' \frac{e}{r_{1j}};$$

this can be interpreted as the potential at the field point of electron 1 due to the static field $V(r)$ and the fields of $(n-1)$ moving charges, each having a charge of $-e/2$. Thus the vector potential A^1 that arises as a consequence of the motion of electrons $2, 3, \ldots, n$ can be obtained by multiplying (20 *b*) by $-\frac{1}{2}$. We have

$$\phi_1 = V(r_1) - \frac{1}{2} \sum_j{}' \frac{e}{r_{1j}};$$

$$A^1 = -e \sum_j \frac{[v_j + (v_j \cdot n_{1j})\, n_{1j}]}{4cr_{1j}}. \tag{21}$$

In general we have

$$A^i = -e \sum_j \frac{[v_j + (v_j \cdot n_{ij})\, n_{ij}]}{4cr_{ij}}.$$

Substituting (21) in (19) we get

$$\sum_{i=1}^{n} m_i v_i^2 = \sum_{i=1}^{n} v_i \cdot P^i - \frac{e^2}{2c^2} \sum_{\substack{ij \\ i<j}} \frac{[v_i \cdot v_j + (v_i \cdot n_{ij})(v_j \cdot n_{ij})]}{r_{ij}}. \tag{22}$$

Substituting (22) in (18) we get

$$\sum_{k=1}^{3} a_k \left(P_k + \frac{e}{c} A_k\right) + \beta P' = -\sum_i m_{0i} c \sqrt{1 - \frac{v_i^2}{c^2}} - \frac{1}{c} \sum v_i \cdot P^i + \frac{e^2}{2c^3} \sum_{ij} \left[\frac{v_i \cdot v_j}{r_{ij}} + \frac{(v_i \cdot r_{ij})(v_i \cdot r_{ij})}{r_{ij}^3}\right]. \tag{23}$$

We have seen that the velocity of the electron is related to the spin matrices by means of the relations

$$v = -ca$$

and

$$\beta = -\sqrt{1-\frac{v^2}{c^2}}.$$

Let us therefore introduce a set of matrices α^i and β^i by means of the relations

$$v_i = -c\alpha^i$$

and

$$\beta^i = -\sqrt{1-\frac{v_i^2}{c^2}}. \tag{24}$$

A representation for the matrices α^i and β in the product space of the electrons can be obtained by adopting the following rule[8]: If two physical systems *a* and *b* are compounded to form a total system *c*, then the system space H of *c* is R×G where R is the system space of *a* and G of *b*. In the system *c* obtained by composition, a Hermitean form $A\times I_2$ is associated with a quantity α of a and $I_1\times B$ with β of *b* where A and B are the forms associated with α, β in R, G respectively, and I_1 and I_2 are the unit forms in R and G.

In the product space, therefore, the matrices α^i and β are given by

$$\alpha^i = I\times I\times I\ldots\times\alpha\times I\ldots\times I$$

and

$$\beta^i = I\times I\times I\ldots\times\beta\times I\ldots\times I. \tag{25}$$

In the above, the product contains n terms, and α and β occur in the i-th place; further the $\times$ denotes direct product multiplication. Substituting (25), (24) and (23) in (16), we get the equation for the system as

$$\left\{\left(P_0+\frac{e}{c}A_0\right)+\sum_{i=1}^{n}\sum_{k=1}^{3}\alpha_k{}^iP_k{}^i+m_0c\left(\sum_{i=1}^{n}\beta^i\right)\right.$$
$$\left.+\frac{e^2}{2c}\left[\sum_{\substack{ij\\ i<j}}\frac{\alpha^i\cdot\alpha^j}{r_{ij}}+\sum_{\substack{ij\\ i<j}}\frac{(\alpha^i\cdot r_{ij})(\alpha^j\cdot r_{ij})}{r_{ij}{}^3}\right]\right\}\psi=0. \tag{26}$$

For the case $n=2$, the above equation reduces to the well-known Breit equation.

Summary

It is shown that the Dirac equation for an electron moving in a field can be derived by expressing the magnitude of the momentum four-vector in terms of its components. By considering a four-vector whose components denote the total momentum and energy of the particles, a relativistic equation for a system of several electrons has been derived. A representation of this equation has been made in the product space of the electrons and it is shown that for the special case of a system containing two electrons, it leads to the well-known Breit equation.

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