

THE DIRAC EQUATION FOR MANY-ELECTRON SYSTEMS

BY K. S. VISWANATHAN, F.A.Sc.

(Memoir No. 122 of the Raman Research Institute, Bangalore-6)

Received June 11, 1960

1. INTRODUCTION

THE well-known relativistic wave equation for an electron¹ 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 Gaunt³ and Breit⁵ of which the one given by Breit is the most satisfactory. By replacing the velocities v^I and v^{II} of the electrons by the spin matrices $-ca^I$ and $-ca^{II}$ 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 Weyl⁶ for a vector in a n -dimensional space and which we shall apply presently.

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

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

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 $p_4 (= iE/c)$ 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{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 $\vec{P} = (p_1, p_2, p_3, p_4)$. We then get

$$\sum_{i=1}^4 \gamma_i p_i = im_0c. \quad (2)$$

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

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

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

$$\begin{aligned} \gamma_4 &= \begin{pmatrix} -I & 0 \\ 0 & I \end{pmatrix}; \quad \gamma_1 = \begin{pmatrix} 0 & -i\sigma_1 \\ i\sigma_1 & 0 \end{pmatrix}; \quad \gamma_2 = \begin{pmatrix} 0 & -i\sigma_2 \\ i\sigma_2 & 0 \end{pmatrix}; \\ \gamma_3 &= \begin{pmatrix} 0 & -i\sigma_3 \\ i\sigma_3 & 0 \end{pmatrix} \end{aligned}$$

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

$$\left(p_0 + \sum_{i=1}^3 a_i p_i + \beta m_0c \right) |\psi\rangle = 0 \quad (4)$$

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 $(p_i + e/c A_i)$ ($i = 0, 1, 2, 3$) 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 $im_0 c$ 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

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

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

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

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

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

we have

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

or

$$\dot{x}_i = -ca_i. \quad (7)$$

Similarly

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

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

$$\begin{aligned} \left(P_i + \frac{e}{c}A_i\right) &= m_0cu_i \quad (i = 1, 2, 3, 4) \\ &= \frac{m_0\dot{x}_i}{\sqrt{1 - \frac{v^2}{c^2}}}, \end{aligned} \quad (9)$$

where u_1, u_2, u_3, u_4 are the components of the velocity four-vector. A natural way to generalise the Dirac equation for a system of particles would be to consider a four-vector whose components are respectively Σm_0cu_i ($i = 1, 2, 3, 4$, 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 $(P_0 + e/cA_0)$, $(P_1 + e/cA_1)$, $(P_2 + e/cA_2)$ and $(P_3 + e/cA_3)$.

Now in the special theory of relativity the components of the total momentum are given by⁷

$$P_i = -\frac{i}{c} \int T_{ik} dS_k + \Sigma m_0cu_i, \quad (10)$$

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

$$\int \frac{\mathbf{S}}{c^2} dV + \Sigma \mathbf{p} \quad (10 a)$$

and for the energy

$$\int W dV + \Sigma \mathcal{E}, \quad (10 b)$$

where

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

is the Poynting vector and

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

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

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

where

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

Thus

$$\begin{aligned} - P'^2 = & - c^2 \left(\sum m_i^2 + 2 \sum_{\substack{i,j \\ i < j}} m_i m_j \right) \\ & + \left(\sum_i m_i^2 v_i^2 + 2 \sum_{\substack{i,j \\ i < j}} m_i m_j v_i \cdot v_j \right) \end{aligned}$$

or

$$P'^2 = \sum m_i^2 c^2 \left(1 - \frac{v_i^2}{c^2} \right) + 2 \sum m_i m_j c^2 \left(1 - \frac{v_i \cdot v_j}{c^2} \right). \quad (12)$$

Now

$$\begin{aligned} & m_i m_j c^2 \left(1 - \frac{v_i \cdot v_j}{c^2} \right) \\ &= \frac{m_{0i} m_{0j} c^2}{\sqrt{\left(1 - \frac{v_i^2}{c^2} \right) \left(1 - \frac{v_j^2}{c^2} \right)}} \left(1 - \frac{v_i \cdot v_j}{c^2} \right) \\ &\sim m_{0i} m_{0j} c^2 \left(1 + \frac{v_{ij}^2}{2c^2} \right), \end{aligned} \quad (13)$$

where

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

Substituting (13) in (12), we get

$$\begin{aligned} P'^2 &\sim \Sigma m_{0i}^2 c^2 + 2 \Sigma m_{0i} m_{0j} c^2 \left(1 + \frac{v_{ij}^2}{c^2}\right) \\ &= (\Sigma m_{0i} c)^2 + \Sigma m_{0i} m_{0j} v_{ij}^2. \end{aligned}$$

Thus a second approximation for P' is given by

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

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

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

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 a_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

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

and

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

Thus we have

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

and

$$\beta P' = -\frac{P'^2}{c \sum m_i}. \quad (17 b)$$

Thus we have

$$\begin{aligned} & \sum_{k=1}^3 \alpha_k \left(P_k + \frac{e}{c} A_k \right) + \beta P' \\ &= \frac{\left\{ -\sum_{k=1}^3 \left(\sum_i m_i \dot{x}_{ik} \right)^2 - P'^2 \right\}}{c \sum_i m_i} \\ &= -\sum m_i c = -c \sum_i \frac{m_{0i}}{\sqrt{\left(1 - \frac{v_i^2}{c^2}\right)}} \\ &= -\sum_{i=1}^n m_{0i} c \sqrt{1 - \frac{v_i^2}{c^2}} - \frac{1}{c} \sum_{i=1}^n m_i v_i^2 \end{aligned} \quad (18)$$

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

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

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 \mathbf{P} is the momentum conjugate to the position of the particle and \mathbf{A} is the vector potential of the field. Thus we have

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

The term $e/c \sum v_i \cdot \mathbf{A}^i$ 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 Lifshitz⁷ and these are given by

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

where r is the distance of the charge from the field point and $\mathbf{n} = \mathbf{r}/r$. 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, \dots , n are given by

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

and

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

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

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

where

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

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, ..., n can be obtained by multiplying (20 b) by $-\frac{1}{2}$. We have

$$\begin{aligned} \phi_1 &= V(r_1) - \frac{1}{2} \sum_j' \frac{e}{r_{1j}}; \\ A^1 &= -e \sum_j \frac{[v_j + (v_j \cdot n_{1j}) n_{1j}]}{4cr_{1j}}. \end{aligned} \quad (21)$$

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

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

Substituting (22) in (18) we get

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

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

$$v = -c\alpha$$

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

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

A representation for the matrices α^i and β in the product space of the electrons can be obtained by adopting the following rule⁸: If two physical systems a and b are compounded to form a total system c , then the system space H of c is $R \times G$ 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

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

and

$$\beta^i = I \times I \times I \dots \times \beta \times I \dots \times I. \quad (25)$$

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

$$\left\{ \left(P_0 + \frac{e}{c} A_0 \right) + \sum_{i=1}^n \sum_{k=1}^3 a_k^i P_k^i + m_0 c \left(\sum_{i=1}^n \beta^i \right) + \frac{e^2}{2c} \left[\sum_{\substack{ij \\ i < j}} \frac{\alpha^i \cdot \alpha^j}{r_{ij}} + \sum_{\substack{ij \\ i < j}} \frac{(\alpha^i \cdot r_{ij})(\alpha^j \cdot r_{ij})}{r_{ij}^3} \right] \right\} \psi = 0. \quad (26)$$

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.

ACKNOWLEDGEMENT

The author's grateful thanks are due to Professor Sir C. V. Raman for his encouragement and kind interest in this work.

REFERENCES

1. Dirac, P. A. M. .. *Principles of Quantum Mechanics*, Third Edition, 1947, Chapter XI.
2. Eddington, A. S. .. *Proc. Roy. Soc.*, 1929, **122 A**, 358.
3. Gaunt, J. A. .. *Ibid.*, 1929, **122 A**, 513.
4. Darwin, C. G. .. *Phil. Mag.*, 1920, **39**, 537.
5. Breit, G. .. *Phy. Rev.*, 1929, **34**, 553; 1932, **39**, 616.
6. Weyl, H. .. *The Classical Groups*, Princeton, New Jersey, Princeton University Press, 1946. pp. 270-73.
7. Landau, L. and Lifshitz, E. .. *The Classical Theory of Fields*, Addison-Wesley Press, 1951, pp. 59, 86, 180-85.
8. Weyl, H. .. *The Theory of Groups and Quantum Mechanics*, Methuen & Co., Ltd., 1931, pp. 89-92.

3-9-60

ON THE SYSTEM AND ENGINEERING DESIGN OF THE GENERAL PURPOSE ELECTRONIC DIGITAL COMPUTER AT T.I.F.R.

BY R. NARASIMHAN

(*Tata Institute of Fundamental Research, Bombay*)

Received March 14, 1960

(Communicated by Dr. S. S. Dharmatti, F.A.Sc.)

1. INTRODUCTION

SINCE 1955, the Computer Section of the Tata Institute of Fundamental Research has been engaged in the development and construction of a large-scale electronic digital computer for doing scientific computations. As a preliminary to this, a pilot digital calculator was designed and completed in September 1956 and was kept in operation for about a year.¹ The design of the full-scale machine was started early in 1957 and its final assembly completed in February 1959. Unfortunately, owing to the lack of air-conditioning facilities, the work had to be suspended till almost the end of 1959. The actual testing was begun in mid-November 1959 with an auxiliary air-conditioning system and the computer was commissioned for routine work in the third week of February 1960. This paper describes briefly the main features of the system and engineering design of this digital computer. In a companion paper, some aspects of the circuitry will be dealt with.

The T.I.F.R. computer is a parallel, binary, asynchronous machine. It is controlled by a stored programme of single-address instructions and has a fast access ferrite-core memory consisting of 1,024 locations. The input to the computer is by means of a punched paper tape (5-hole commercial teletype tape) and the output can be either printed out directly or punched on a paper tape again.

Both in the system and engineering design, the principal emphasis has been on reliability of operation and ease in maintenance. With this in view, the logical circuit types have been kept to the minimum consistent with flexibility and the wired circuits were put through a rigid acceptance test to check their performance under extreme operating conditions. For rapid fault localization and servicing, a large part of the computer has been assembled