PONTIFICIA
ACADEMIA
SCIENTIARVM

ACTA
Vol. XII - N. 23
pag. 259-278

QUATERNIONS AND QUANTUM MECHANICS (*)

ARTHUR W. CONWAY
Pontifical Academician

SVMMARIVM. — Quaterniones certam habent cum spatio relationem; per eos fit ut quindecim Eddingtonianae matrices directe exprimi ita possint ut earum proprietates perspicue pateant; per ipsos etiam facile fit significare et describere concomitantes aequationis Diracensis.

Auctor inspicit quaternionem ut vectorem in quattuor mensurarum spatio; et eius perpendit rotationem, transitum in spatium hyperbolicum, transformationem seu mutationem spiralem, et nonnullos in rebus physicis usus, ut est vector Poyntingensis in campo Maxwell.

INTRODUCTION

During the second half of the last century the use of quaternions in Mathematical Physics was the subject of much controversy. Strongly defended by Tait the claims of vector algebra were put forward by Heaviside, Gibbs and others. Heaviside freely stated that quaternions could only have been invented by a genius and that vector algebra could be found out by anyone who observed the various combinations of quantities which continually recur but yet he pronounced quaternions as a « positive evil of no inconsiderable magnitude », a statement which has been repeated up to the present day by various mathematical commentators. – Heaviside was in fact largely right for the time and the state of science. The advent of relativity brought

(*) Nota presentata nella Tornata ordinaria dell'8 febbraio 1948.

under consideration that time which was a parameter now took its place as a coordinate and obviously quaternions or 4-vector algebra would seem to be indicated. In Quantum Mechanics, largely founded on HAMILTON's dynamical theories, it would be fitting that HAMILTON's other great discovery would be a suitable mode of mathematical expression. The quaternion treatment has certain differences or advantages over matrices.

Quaternions are more flexible and can be manipulated in many ways. The imaginary i is in plain sight and there is no difficulty in knowing what is real and what is imaginary (incidentally it is not necessary even to use the term HERMITIAN). No difficulty arises as to what quantities commute and what anti-commute. The only rules necessary to know are those of the fundamental units.

In the present paper the relativistic electron equation of DIRAC is considered. It is defined by two perpendicular unit-vectors and at the end of a calculation of (say) a wave-function its dependence its on these vectors is in full right. At the least quaternions gives a different view-point from matrices.

CONTENTS

I. — GENERAL FORMULAE

Denoting a quaternion $q_r (r=1,2...)$ by $w_r+\alpha x_r+\beta y_r+\gamma z_r$ where α, β, γ are the usual quaternion vectors ($\alpha^2=\beta^2=\gamma^2=-1$; $\beta\gamma=-\gamma\beta=\alpha$ etc.). The quaternion conjugate denoted by $\bar{q}_r$ is given by

$$\bar{q}_r = w_r - \alpha x_r - \beta y_r - \gamma z_r$$

and the modulus of the quaternion $|q_r|$ is given by

$$q_r \bar{q}_r = |q_r|^2 = w_r^2 + x_r^2 + y_r^2 + z_r^2 \ .$$

It is to be noted that if $q_r = \bar{q}_r$ the quaternion is a scalar and that if $q_r = -\bar{q}_r$ it is a vector. Two formulae are of great use

$$S q_1 q_2 \dots q_{n-1} q_n = S q_n q_1 q_2 \dots q_{n-1}$$

$$\overline{(q_1 q_2 \dots q_{n-1} q_n)} = \bar{q}_n \bar{q}_{n-1} \dots \bar{q}_2 \bar{q}_1 \ ,$$

we have

$$S q_r \bar{q}_s = w_r w_s + x_r x_s + y_r y_s + z_r z_s \ .$$

Consider the transformation

$$q'_r = a q_r b$$

$$q'_s = a q_s b$$

where a and b are *versors* i. e. $|a| = |b| = 1$.

Then

$$S q'_r \bar{q}'_s = S a q_s b \bar{b} \bar{q}_s \bar{a}$$

$$= S \bar{a} a q_r q_s = S q_r \bar{q}_s$$

and in particular

$$|q'_r|^2 = S q'_r \bar{q}'_r = |q_r|^2 \ .$$

This can be immediately interpreted as 4-space.

If $(w_r x_r y_r z_r)$ and $(w_s x_s y_s z_s)$ represent two points in 4-space then the operation $a(\ )b$ preserves lengths and angles and is the general rotation in four dimensions.

A particular case is the conical rotation $r(\ )r^{-1}$ e. g. if $r = \cos\theta + \eta \sin\theta$ this rotation turns all vectors around the axis η through an angle 2θ. We can always solve the equation $a = cr$, $b = r^{-1}c$, $c^2 = ab$ and hence

$$c = \frac{1 + ab}{|1 + ab|} \quad \text{and} \quad r = \frac{a + \bar{b}}{|1 + ab|} \ .$$

So that the operation $a(\ )b$ can be made up a conical rotation $r(\ )r^{-1}$ followed by an operation $c(\ )c$.

So far the quaternions have been all real but we shall have to deal with quaternions with the scalar part imaginary and the vector part real thus

$$q = it + \alpha x + \beta y + \gamma z$$

and more generally

$$\psi = \psi' + i\psi''$$

where $\psi = \psi_1 \alpha + \psi_2 \beta + \psi_3 \gamma + \psi_4$ etc.

We now introduce the sign $(\ )^*$ which is to mean the complex conjugate of the quaternion conjugate.

Then

$$q^* = -it - \alpha x - \beta y - \gamma z = -q$$

which of course only holds for quaternions of this particular type.

More generally

$$\psi^* = \bar{\psi}' - i\bar{\psi}''$$

so that

$$\psi^* \psi = \psi' \bar{\psi}' + \psi'' \bar{\psi}'' + i(\bar{\psi}' \psi'' - \bar{\psi}'' \psi')$$

$$= |\psi'|^2 + |\psi''|^2 + i\sigma$$

were σ is a vector, for $\bar{\sigma} = \bar{\psi}'' \psi' - \bar{\psi}' \psi'' = -\sigma$.

We may also note the formula

$$(\psi \varphi \ldots \chi)^* = \chi^* \ldots \varphi^* \psi^* .$$

Returning now to the quaternion

$$q = it + \alpha x + \beta y + \gamma z$$

and the transformation

$$aqb = q' = it' + \alpha x' + \beta y' + \gamma z'$$

we see that a and b must be restricted for

$$b^* q^* a^* = q^{*\prime} \qquad \text{or} \qquad b^* q\, a^* = q'$$

and we can show that we must have

$$b^* = a \,; \quad a^* = b \,.$$

If ψ is any quaternion the equation

$$\psi = \psi^* \quad \text{gives} \quad \psi' = \bar{\psi}' \,; \; \psi'' = -\bar{\psi}''$$

so that the scalar part is real and the vector part imaginary and since $ab = b^* a^* = (ab)^*$, ab has the scalar part real and the vector part imaginary and so we easily see that

$$c = \frac{1 + ab}{|1 + ab|}$$

can be writen $c = l - i m \varepsilon$ where ε is *a* unit vector and since $c\bar{c} = 1$ we get $(l - i m \varepsilon)(l + i m \varepsilon) = 1$ or $l^2 - m^2 = 1$.

We can also see that if $\bar{\psi} = \psi^*$, ψ is a real quaternion and from this it is easy to infer that $r = \dfrac{a + \bar{b}}{|1 + ab|}$ is a real quaternion and so the most general form of $a(\;)b$ which will transform a quaternion with scalar imaginary vector real into one of the some type is of the form

$$(l - i m \varepsilon)(\cos\theta + \eta \sin\theta)(\qquad)(\cos\theta - \eta \sin\theta)(l - i m \varepsilon) \,.$$

This is the general LORENTZ transformation and for simplicity we can put $r = \cos\theta + \eta \sin\theta = 1$ and deal with

$$(l - i m \varepsilon)(\qquad)(l - i m \varepsilon) \,.$$

Denoting $\alpha \dfrac{\partial}{\partial x} + \beta \dfrac{\partial}{\partial y} + \gamma \dfrac{\partial}{\partial z}$ by the usual ∇ we have

$$-d = -dt \frac{\partial}{\partial t} - dx \frac{\partial}{\partial x} - dy \frac{\partial}{\partial y} - dz \frac{\partial}{\partial z}$$

$$= \mathrm{S}\left(\nabla + i \frac{\partial}{\partial t}\right)(i\,dt + d\rho) \,.$$

Since $-d$ is an invariant, if $idt + d\rho$ is transformed by $a(\;)b$ then $\nabla + i \dfrac{\partial}{\partial t}$ is transformated by $\bar{b}(\;)\bar{a}$ or $(l + i m \varepsilon)(\;)(l + i m \varepsilon)$.

From

[1] $$\nabla' + i\frac{\partial}{\partial t'} = (l + im\,\varepsilon)\left(\nabla + i\frac{\partial}{\partial t}\right)(l + im\varepsilon)$$

we get

$$\nabla' = l^2\nabla - m^2\,\varepsilon\nabla\varepsilon + 2\,l\,m\,\varepsilon\,\frac{\partial}{\partial t}$$

$$\frac{\partial}{\partial t'} = (l^2 + m^2)\frac{\partial}{\partial t} - lm\,(\nabla\varepsilon + \varepsilon\nabla)\ .$$

One of the earliest applications to electromagnetic theory is to the MAXWELL field equations for **E**, **H**, which can all be comprised in

$$\left(\nabla + i\frac{\partial}{\partial t}\right)(\mathbf{H} + i\mathbf{E}) = 0$$

i. e.

$$\frac{\partial \mathbf{E}}{\partial t} = \mathrm{V}\nabla\mathbf{H}\ ; \qquad \mathrm{S}\nabla\mathbf{H} = 0$$

$$\frac{\partial \mathbf{H}}{\partial t} = -\,\mathrm{V}\nabla\mathbf{E}\ ; \qquad \mathrm{S}\nabla\mathbf{E} = 0$$

And for the 4-potential A_0, $\mathbf{A}$

$$\left(\nabla + i\frac{\partial}{\partial t}\right)(A_0 - i\mathbf{A}) = -\,\mathbf{E} - i\mathbf{H}\ ,$$

$$\nabla A_0 + \frac{\partial \mathbf{A}}{\partial t} = -\,\mathbf{E}\ ; \qquad \overline{\mathrm{V}}\nabla\mathbf{A} = \mathbf{H}\ ; \qquad \mathrm{S}\nabla\mathbf{A} - \frac{\partial A_0}{\partial t} = 0$$

From equation [1] we see that since

$$\triangle' + i\frac{\partial}{\partial t'} = \bar{b}\left(\nabla + i\frac{\partial}{\partial t}\right)\bar{a}$$

then

$$\mathbf{H}' + i\mathbf{E}' = a(\mathbf{H} + i\mathbf{E})\,\bar{b}$$

or

$$= (l - im\,\varepsilon)(\mathbf{H} + i\mathbf{E})(l + im\varepsilon)$$

From which

$$\mathbf{H}' = l^2\mathbf{H} + m^2\varepsilon\mathbf{H}\varepsilon - lm(\mathbf{E}\varepsilon - \varepsilon\mathbf{E})$$

$$\mathbf{E}' = lm(\mathbf{H}\,\varepsilon - \varepsilon\,\mathbf{H}) + l^2\,\mathbf{E} + m^2\varepsilon\,\mathbf{E}\,\varepsilon\ .$$

II. — THE LINEAR FUNCTION.

The matrix (ψ_r) when operated on by the matrix (f_{sr}) is the single-row matrix $f_{sr}\psi_r$.

In quaternions this is denoted by $f(\psi)$ or $f\varphi$. There are many explicit forms for $f\psi$ such as $\sum r\psi s$ where the r's and the s's are quaternions. The transpose of f denoted by f_T is given by $\sum s\psi r$ or the equation

$$S\varphi f\psi = S\psi f_T\varphi$$

we see at once $f^*(\ \ ) = \sum s^*(\ \ )r^*$.

A function which makes $f^* = f_T$ is *Hermitian.*

The equation

$$f\psi = x\psi$$

has in general four values of x, the latent roots or eigenvalues.

The functions $\alpha(\ \ )\beta$, $\gamma(\ \ )i$ are examples of Hermitian linear operators or linear functions. It will be noted that these functions are such that $f^2 = 1$ so that the four roots are equal in pairs.

We can easily see that from

$$\alpha\psi\beta = \psi \text{ we get } \psi = c'(\alpha - \beta) + c''(1 + \alpha\beta)$$

and from

$$\alpha\psi\beta = -\psi \text{ we get } \psi = c'''(\alpha + \beta) + c^{IV}(1 - \alpha\beta)$$

where c', c'', c''', c^{IV} are arbitrary scalars.

In the same way from

$$\gamma\psi i = \psi \text{ we get } \psi = c'(\alpha + i\beta) + c''(1 + \gamma i)$$

and from

$$\gamma\psi i = -\psi \text{ we get } \psi = c'''(\alpha - i\beta) + c^{IV}(1 - \gamma i).$$

If f and F are two functions such that $f^2 = F^2 = 1$ and $fF = -Ff$ then from

$$f\psi = \psi$$

we get

$$\mathrm{F} f \psi = \mathrm{F} \psi$$

or

$$f \mathrm{F} \psi = - \mathrm{F} \psi$$

so that $\mathrm{F}\psi$ is a solution corresponding to the negative eingevalue.

A type of function which we shall use is $f\psi = (k - ik_0 \alpha)\psi - \gamma\psi\omega$ where $|\omega| = p$. We require a solution of $f(\psi) = 0$ or $(k - ik_0\alpha)\psi = \gamma\psi\omega$. Taking the modulus of each side we get $k^2 - k^2_0 = p^2$ and no solution is possible unleses this is satisfied. We can easily verify that the complete solution is

$$\psi = (k\gamma - ik_0\beta - \omega)(\mathrm{A} + \mathrm{B}\,\omega)$$

in which A and B are arbitrary scalars (1).

Some properties of ∇ are useful.

We have

$$\mathrm{V}\rho\nabla = \alpha\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right) + \beta\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right) + \gamma\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial z}\right).$$

From which

[1] $$(\mathrm{V}\rho\nabla + 1)\nabla = -\nabla(\mathrm{V}\rho\nabla + 1)$$

$$\mathrm{V}\rho\nabla(\mathrm{V}\rho\nabla + 1) = -\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} - \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}$$

For instance if S_n is a surface harmonic of degree n

$$\mathrm{V}\rho\nabla(\mathrm{V}\rho\nabla + 1)\mathrm{S}_n = n(n+1)\mathrm{S}_n$$

or

[2] $$(\mathrm{V}\rho\nabla - n)(\mathrm{V}\rho\nabla + n + 1)\mathrm{S}_n = 0$$

[3] $$\nabla = -\frac{\rho^2}{r^2}\nabla = -\frac{\rho_1}{r}\rho\nabla = -\frac{\rho_1}{r}(\mathrm{S}\rho\nabla + \mathrm{V}\rho\nabla) = \frac{\rho_1}{r}\frac{d}{dr} - \frac{\rho_1}{r}\mathrm{V}\rho\nabla$$

[4] $$(\mathrm{V}\rho\nabla + 1)\rho_1 = -\rho_1(\mathrm{V}\rho\nabla + 1)$$

(1) For negative energy states, $k = -\sqrt{(p^2 + k_0^2)}$.

III. — DIRAC'S RELATIVISTIC EQUATION.

One form in which this may be written is

$$\frac{\partial\psi}{\partial t} = \alpha_1 \frac{\partial\psi}{\partial x} + \alpha_2 \frac{\partial\psi}{\partial y} + \alpha_3 \frac{\partial\psi}{\partial z} + i k_0 \alpha_4 \psi$$

in which ψ is a one-column matrix and $\alpha_1\ \alpha_2\ \alpha_3\ \alpha_4$ are 4×4 matrices. Here the velocity of light c is unity and $k_0 = \frac{m}{\hbar}$ where m is the mass of the electron. The four matrices are in order equivalent to

$$-\gamma(\ \ )\beta\ , \quad i\alpha(\ \ )\ , \quad -\gamma(\ \ )\alpha\ , \quad -\gamma(\ \ )\gamma$$

operating on the quaternion $\psi = \psi_1\alpha + \psi_2\beta + \psi_3\gamma + \psi_4$. We can get a symmetrical form by putting

$$\alpha_1 = -\gamma(\ \ )\alpha\ , \quad \alpha_2 = -\gamma(\ \ )\beta\ , \quad \alpha_3 = -\gamma(\ \ )\gamma\ , \quad \alpha_4 = i\alpha(\ \ )$$

and we thus get the quaternion form of the equation

[1] $$\frac{\partial\psi}{\partial t} = -\gamma\psi\nabla - k_0\alpha\psi$$

and its conjugate

[2] $$\frac{\partial\psi^*}{\partial t} = -\nabla\psi^*\gamma + k_0\psi^*\alpha$$

of these [2] is the easier form to work with.

Multiplying [1] by ψ^* from the left and [2] by ψ from the right and taking the scalar product we get

$$\frac{\partial}{\partial t} S\psi^*\psi = -S\nabla\psi^*\gamma\psi = -S\nabla\overline{V}\psi^*\gamma\psi\ .$$

Which shows $-e\overline{V}\psi^*\gamma\psi$ is the vector flux.

Other mean densities connected with the equation are in quaternion form

the magnetic moment

[i] $$\frac{e\hbar V\psi^*\alpha\psi}{2m}$$

the electric moment

[ii] $$-\frac{e\hbar V \psi^* \beta \psi}{2m}$$

the spin

[iii] $$-\frac{1}{2} i \hbar V \psi^* \psi$$

two scalars

[iv] $$I_1 = -iS\psi^* \alpha \psi \; ; \qquad I_4 = -iS\psi^* \beta \psi$$

We proceed to consider these.

IV. — TRANSFORMATION OF THE WAVE FUNCTIONS

Consider the function $f(\;) = l(\;) + m\gamma(\;)\varepsilon$ we see at once that

$$f^{-1}(\;) = l(\;) - m\gamma(\;)\varepsilon$$

and if $\psi = f\psi'$ we hawe

$$\gamma\psi = \gamma f \psi' = f \gamma \psi'$$
$$\alpha \psi = \alpha f \psi' = f^{-1} \alpha \psi' \; .$$

We consider the function

$$H = \frac{\partial \psi}{\partial t} + \gamma \psi \nabla + k_0 \alpha \psi$$

and we calculate

$$f(H) = f \left\{ \frac{\partial}{\partial t} f(\psi') + \gamma f(\psi') \nabla + k_0 \alpha f(\psi') \right\} .$$

For the last term

$$k_0 f \alpha f \psi' = k_0 \alpha f^{-1} f \psi'$$
$$= k_0 \alpha \psi' \; .$$

The first term gives

$$\frac{\partial}{\partial t} f^2 \psi' = (l^2 + m^2) \frac{\partial \psi'}{\partial t} + 2\, lm\, \gamma \frac{\partial \psi'}{\partial t} \varepsilon$$

The first and second terms give

$$(l^2+m^2)\frac{\partial\psi'}{\partial t} - lm\,\psi'(\varepsilon\nabla+\nabla\varepsilon) + \gamma\left\{\psi'(l^2\nabla - m^2\varepsilon\nabla\varepsilon) + 2lm\frac{\partial\psi'}{\partial t}\varepsilon\right\}.$$

Collecting terms we have by

$$f(\mathrm{H}) = \frac{\partial\psi'}{\partial t} + \gamma\psi'\nabla' + k_0\alpha\psi' .$$

Hence if

$$\nabla' + i\frac{\partial}{\partial t'} = (l+mi\varepsilon)\left(\nabla + i\frac{\partial}{\partial t}\right)(l+mi\varepsilon)$$

$$\psi' = l\psi - m\gamma\psi\varepsilon$$

the Dirac equation remains unchanged in form.

For the general LORENTZ transformation for which

$$\nabla' + i\frac{\partial}{\partial t'} = \bar{b}\left(\nabla + i\frac{\partial}{\partial t}\right)\bar{a} ,$$

where

$$a = (l - mi\varepsilon)r, \quad b = r^{-1}(l - mi\varepsilon)$$

we easily obtain

$$\psi + i\gamma\psi = (\psi' + i\gamma\psi')b$$

$$\psi - i\gamma\psi = (\psi' - i\gamma\psi')a^{-1}$$

$$\psi = l\psi' r^{-1} + m\gamma\psi' r^{-1}\varepsilon .$$

As an example let us consider the functions

$$\mathrm{V}\,\psi^*\beta\psi \qquad \text{and} \qquad \mathrm{V}\,\psi^*\alpha\psi$$

we have

$$\psi' = l\psi - m\gamma\psi\varepsilon$$

$$\psi^{*\prime} = l\psi^* - m\varepsilon\psi^*\gamma$$

$$\beta\psi' = l\beta\psi - m\alpha\psi\varepsilon .$$

From which

$$\mathrm{V}\,\psi^{*\prime}\beta\psi' = l^2\,\mathrm{V}\,\psi^*\beta\psi + m^2\varepsilon(\mathrm{V}\,\psi^*\beta\psi)\varepsilon - lm\}\overline{\mathrm{V}}\,\psi^*\alpha\psi\varepsilon - \overline{\mathrm{V}}\varepsilon\psi^*\alpha\psi\{$$

Or putting

$$\bar{\pi} = -\frac{e\hbar}{2m} \mathrm{V}\, \psi^* \beta \psi \;, \quad \bar{\mu} = \frac{e\hbar}{2m} \mathrm{V}\, \psi^* \alpha \psi$$

$$\bar{\pi}' = l^2 \bar{\pi} + m^2 \varepsilon \bar{\pi} \varepsilon + lm(\bar{\mu} \varepsilon - \varepsilon \bar{\mu})$$

and in the same manner

$$\bar{\mu}^1 = l^2 \bar{\mu} + m^2 \varepsilon \mu \varepsilon - lm(\bar{\pi} \varepsilon - \varepsilon \bar{\pi})$$

V. — WAVE FUNCTION AS SPINORS

Any wave-function can be expressed in terms of the units

$$\gamma,\ \varepsilon,\ \varepsilon\gamma,\ 1\ .$$

Putting

$$\psi = \psi_1 \gamma + \psi_2 \varepsilon + \psi_3 \varepsilon\gamma + \psi_4$$

$$\psi' = \psi'_1 \gamma + \psi'_2 \varepsilon + \psi'_3 \varepsilon\gamma + \psi'_4$$

We have

$$\psi' = l\psi - m\gamma\psi\varepsilon$$

and finally

$$\psi'_1 = l\psi_1 + m\psi_2 \;; \qquad \psi'_3 = l\psi_3 - m\psi_4$$

$$\psi'_2 = m\psi_1 + l\psi_2 \;; \qquad \psi'_4 = l\psi_4 - m\psi_3$$

The transformations $(\psi_1, \psi_2) \rightarrow (\psi'_1, \psi'_2)$ and $(\psi_3, \psi_4) \rightarrow (\psi'_3, \psi'_4)$ have the appearance of equal and opposite hyperbolic transformations but geometrically they are not except in the very special case $S\varepsilon\gamma = 0$.

VI. — THE FREE ELECTRON

The equation of the free electron is

$$\frac{\partial \psi}{\partial t} = -\gamma \psi \nabla - k_0 \alpha \psi$$

or

$$\frac{\partial \psi^*}{\partial t} = -\psi^* \gamma + k_0 \psi^* \alpha\ .$$

Putting

$$\psi = \psi_0 \, e^{-i(kt - xp_x - yp_y - zp_z)}$$

where ψ_0 is a constant quaternion we get, on putting

$$\omega = \alpha p_x + \beta p_y + \gamma p_z \,, \quad p^2 = |\omega|^2 \ ,$$

and

$$p\,\omega_1 = \omega \ ,$$

$$k\psi_0 = p\gamma\,\psi_0\,\omega_1 - k_0\,i\,\alpha\,\psi_0$$

There are various methods for finding ψ_0. The following is lengthy but it introduces a rather general treatment.

Let τ be a solution of

[1] $$i\alpha\tau = \tau$$

and let

[2] $$\gamma\,\tau\,\omega_1 = \tau'$$

then

[3] $$\gamma\,\tau'\,\omega_1 = \tau$$

and

$$i\alpha\gamma\,\tau\,\omega_1 = -\gamma(i\alpha\tau)\,\omega_1$$

or

[4] $$i\alpha\tau' = -\tau'$$

Substitute $\psi_0 = u\tau + u'\tau'$ where u, u' are scalars and making use of [1], [2], [3], [4]

$$\}(k + k_0)\,u - p\,u'\{\,\tau + \}(k - k_0)\,u' - p\,u\{\,\tau' = 0$$

From which since

$$i\alpha\tau - \tau = 0 \qquad \text{and} \qquad i\alpha\tau' + \tau' = 0$$

we get

$$(k + k_0)\,u = p\,u' \ ; \quad (k - k_0)\,u' = p\,u$$

and

$$k^2 - k_0{}^2 = p^2 \ .$$

As an example, one value of τ is

$$\beta + i\gamma \qquad \text{so that} \qquad \tau' = \gamma(\beta + i\gamma)\,\omega_1 = -(\alpha + i)\,\omega_1$$

and we have

$$\begin{aligned} \psi_0 &= u\,\tau + \alpha'\,\tau' \\ &= u(\beta + i\gamma) - u'(\alpha + i)\,\omega_1 \end{aligned}$$

and

$$\psi_0{}^* = u(-\beta + i\gamma) - u'\,\omega_1(\alpha + i)$$

Normalising to unit volume we get

$$1 = \mathrm{S}\,\psi_0{}^*\,\psi_0 = 2(u^2 + u'^2)$$

From which

$$u = \frac{p}{2\sqrt{\{k(k+k_0)\}}} \ , \quad u' = \frac{k + k_0}{2\sqrt{\{k(k+k_0)\}}}$$

The vector

$$\mathrm{V}\,\psi_0{}^*\,\gamma\,\psi_0$$

$$= \mathrm{V}\}u(-\beta + i\gamma) - u'\,\omega_1(\alpha + i)\{\ \} - u(\alpha + i) - u'(\beta + i\gamma)\,\omega_1\{$$

$$= -4\,u\,u'\,\omega_1 = -\frac{p}{k}\,\omega_1 \qquad \left(\frac{k}{p} \text{ is the wave velocity}\right)$$

Further examples are

$$\bar{\mu} = \frac{e\hbar}{2m}\,\mathrm{V}\,\psi^*\alpha\,\psi = -\frac{e\hbar}{m}\,\omega_1\,\mathrm{V}\,\alpha\,\omega_1$$

$$\bar{\pi} = -\frac{ek}{2m}\,\overline{\mathrm{V}}\,\psi^*\beta\,\psi = \frac{e\hbar}{m}\,\frac{p}{k}\,\mathrm{V}\,\alpha\,\omega_1$$

VII. — ELECTRON IN A FIELD OF FORCE.

If A_0, $\mathbf{A}$ denote the 4-potential of a field then in the equation

$$\frac{\partial\psi}{\partial t} = -\gamma\psi\nabla - k_0\alpha\psi \qquad \left(k_0 = \frac{m}{\hbar},\ c = 1\right)$$

$$\frac{\partial}{\partial t} \to \frac{\partial}{\partial t} - \frac{iA_0 e}{\hbar}\,, \qquad \nabla \to \nabla + \frac{i\mathbf{A}e}{\hbar}$$

and the conjugate equation can be written

$$\left(\frac{\partial}{\partial t} + \frac{iA_0 e}{\hbar}\right)\psi^* + \left(\nabla - \frac{i}{\hbar}\mathbf{A}e\right)\psi^*\gamma - k_0\psi^*\alpha = 0$$

Operating on this expression with

$$\left(\frac{\partial}{\partial t} + \frac{iA_0 e}{\hbar}\right)(\quad) - \left(\nabla - \frac{i\mathbf{A}e}{\hbar}\right)(\quad)\gamma + k_0(\quad)\alpha$$

we get

$$\left\{\left(\frac{\partial}{\partial t} + \frac{iA_0 e}{\hbar}\right)^2 + \left(\nabla - \frac{i\mathbf{A}e}{\hbar}\right)^2 + k_0^2\right\}\psi^* - \frac{ie}{\hbar}\mathbf{H}\psi^* + \frac{ie}{\hbar}\mathbf{E}\,\psi^*\gamma$$

The last two terms are more usually written in the conjugate form and multiplied by $-\hbar^2$ and become

$$ie\hbar(\psi\mathbf{H} + \gamma\psi\mathbf{E})$$

VIII. — THE HYDROGEN LINE SPECTRUM AND ITS FINE STRUCTURE.

In ordinary units putting $A_0 = \frac{e}{r}$ we have

$$[1] \qquad \frac{i}{c\hbar}\left(E + \frac{e^2}{r}\right)\psi^* = -\nabla\psi^*\gamma + \frac{mc}{\hbar}\psi^*\alpha$$

From II[1] and

$$\gamma\alpha = -\alpha\gamma$$

we see that

$$(\overline{V}\rho\nabla + 1)(\quad)\alpha$$

commutes with every term of [1]. Hence we have an integral

[2] $$(V\rho\nabla + 1)\psi^*\alpha = -ni\psi^*$$

or

[3] $$V\rho\nabla\psi^* = -\psi^* + ni\psi^*\alpha$$

using II [3], [1] becomes

[4] $$\frac{i}{c\hbar}\left(E + \frac{e^2}{r}\right)\psi^* = -\rho_1\left(\frac{\partial\psi^*}{\partial r} + \frac{\psi^*}{r}\right)\gamma + \frac{n}{r}\rho_1 i\psi^*\alpha\gamma + \frac{mc}{\hbar}\psi^*\alpha$$

Introducing the quaternions τ, τ' defined by

[5] $$\left\{\begin{array}{l} i\tau\alpha = \tau\ ; \qquad \rho_1\tau\gamma = \tau' \\ \text{and therefore} \\ i\tau'\alpha = -\tau'\ ; \qquad \rho_1\tau'\gamma = \tau \end{array}\right.$$

Assume $\psi^* = u\tau - iv\tau'$ where u and v are functions of τ and we get from [4]

$$i\tau\left\{\left(E + \frac{e^2}{r} + mc\right)u - \frac{\partial v}{\partial r} - \frac{n+1}{r}v\right\} + \tau'\left\{\left(E + \frac{e^2}{r} - mc\right)v + \frac{\partial u}{\partial r} + \frac{n-1}{r}u\right\} = 0$$

and since $i\tau\alpha - \tau = 0$ and $i\tau'\alpha + \tau' = 0$ we get the differential equation for u, and v

[6] $$\left\{\begin{array}{l} \dfrac{\partial v}{\partial r} + \dfrac{n+1}{r}v = \left(E + \dfrac{e^2}{r} + mc\right)u \\ \dfrac{\partial u}{\partial r} - \dfrac{n-1}{r}u = -\left(E + \dfrac{e^2}{r} - mc\right)v \end{array}\right.$$

In order to solve [3], $(V\rho\nabla + 1)\psi^* = -ni\psi^*\alpha$ we get

$$u(V\rho\nabla + 1 + n)\tau - iv(V\rho\nabla + 1 - n)\tau' = 0$$

which becomes, since

$$(V\rho\nabla+1)\tau'=(V\rho\nabla+1)\rho_1\tau\gamma=-\rho_1(V\rho\nabla+1)\tau\gamma$$

by II [4]

$$u(V\rho\nabla+1+n)\tau+iv\rho_1(V\rho\nabla+1+n)\tau=0\ ,$$

so that

$$(V\rho\nabla+1+n)\tau=0$$

Let τ_0 be any constant solution of $i\tau_0\alpha=\tau_0$ and $\tau'_0=\rho_1\tau_0\gamma$ and let $\tau=\sum_n\tau_0$, $\tau'=\sum_n\tau'_0$ where $\sum_n$ is a function of the angles θ, φ, we have then

$$(V\rho\nabla+1+n)\textstyle\sum_n=0$$

It is obvious that we have a solution by putting

$$\textstyle\sum_n=(V\rho\nabla-n)\,S_n$$

where S_n is a surface harmonic (see II [3]) and thus

$$\tau=(V\rho\nabla-n)S_n\tau_0\ ,$$

and

$$\tau'=\rho_1(V\rho\nabla-n)S_n\tau_0\gamma$$

We easily see that

$$\}V\rho\nabla-(n-1)\{\tau'=0$$

So that τ' is a spherical harmonic of degree $(n-1)$. We get finally

$$\psi^*\tau=(u\textstyle\sum_n\tau_0-iv\rho_1\sum_n\tau_0\gamma)e^{\frac{iEt}{k}}$$

$$\psi=(u\tau_0^*\textstyle\sum_n^*+iv\gamma\tau_0\sum_n^*\rho_1)e^{-\frac{iEt}{k}}$$

In order to normalise ψ we must have

$$\int S\,\psi^*\psi\,dx\,dy\,dz=1$$

Where the integral is taken over all space.

We have

$$S\psi^*\psi = u^2 \sum \sum_n^* \tau_0 \tau_0^* - v^2 S \rho_1 \sum_n \tau_0 \tau_0^* \sum_n^* \rho_1$$
$$= (u^2 + v^2) \sum \sum_n^* S \tau_0 \tau_0^*$$

and we can normalise by making

$$\int (u^2 + v^2) r^2 \, dr = 1$$

$$\int \sum_n \sum_n^* \sin\theta \, d\theta \, d\varphi = 1.$$

$$S \tau_0 \tau_0^* = 1$$

From

$$\sum_n = (V\rho \nabla - n) S_n \quad , \qquad \sum_n^* = -(V\rho \nabla + n) S_n$$

we get

$$\sum_n \sum_n^* = -(V\rho \nabla S_n)^2 + n^2$$

$$-\int (V\rho \nabla S_n)^2 \sin\theta \, d\theta \, d\varphi = \int \left\{ (1-\mu^2) \left(\frac{\partial S_n}{\partial \mu} \right)^2 + \frac{1}{1-\mu^2} \left(\frac{\partial S_n}{\partial \varphi} \right)^2 \right\} d\mu \, d\varphi$$
$$(\mu = \cos\theta)$$

$$= n(n+1) \int S^2_n \, d\mu \, d\varphi$$

Hence

$$\int \sum_n \sum_n^* \sin\theta \, d\theta \, d\varphi = n(2n+1) \int S_n^2 \, d\mu \, d\varphi$$

If we take

$$\tau_0 = A(\gamma + i\beta) + B(i - \alpha)$$

then

$$\tau^*_0 = A^*(-\gamma + i\beta) - B(i + \alpha)$$

and

$$\tau_0 \tau_0^* = 2(AA^* + BB^*)(1 - i\alpha)$$

Hence

$$S \tau_0 \tau_0^* = 1 \; , \quad \text{if} \quad 2(AA^* + BB^*) = 2|A|^2 + 2|B|^2 = 1$$

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