

**Physics.** — *The use of charge-conjugated wave-functions in the hole-theory of the electron.* By H. A. KRAMERS.

(Communicated at the meeting of November 27, 1937.)

From the 4-component DIRAC wave-function  $\psi_k$  ( $k = 1, 2, 3, 4$ ) satisfying

$$\{\vec{\alpha}, \vec{p} - e\vec{\mathcal{A}}\} + e\Phi + \beta m \psi = i\hbar \frac{\partial \psi}{\partial t}, \dots \dots \dots (1)$$

another 4-component wave-function  $\psi^L$  can be derived, which satisfies the same equation, but with the sign of  $e$  reversed:

$$\{\vec{\alpha}, \vec{p} + e\vec{\mathcal{A}}\} - e\Phi + \beta m \psi^L = i\hbar \frac{\partial \psi^L}{\partial t}, \dots \dots \dots (2)$$

We call  $\psi^L$  the *charge-conjugated* function of  $\psi$ . The relation between  $\psi$  and  $\psi^L$  is a very simple one, when we choose for the matrices  $\vec{\alpha}, \beta$  that particular representation, which causes the two components  $\psi_1, \psi_2$  to transform like a relativistic spinor  $u, v$ , and  $\psi_3, \psi_4$  like a spin-conjugated spinor  $U^\dagger (= -V^*), V^\dagger (= U^*)$ , when a LORENTZ-transformation is applied<sup>1</sup>). In fact, writing

$$\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix} = \begin{pmatrix} u \\ v \\ -V^* \\ U^* \end{pmatrix} \dots \dots \dots (3)$$

and defining the charge-conjugated wave-function by

$$\psi^L = \begin{pmatrix} \psi_1^L \\ \psi_2^L \\ \psi_3^L \\ \psi_4^L \end{pmatrix} = \begin{pmatrix} U \\ V \\ -v^* \\ u^* \end{pmatrix} = \begin{pmatrix} \psi_4^* \\ -\psi_3^* \\ -\psi_2^* \\ \psi_1^* \end{pmatrix} \dots \dots \dots (4)$$

it is easily verified that  $\psi^L$  satisfies (2) when  $\psi$  satisfies (1).

In order to prove this, consider for a moment  $\psi_k$  as a function of two variables  $s, r$  which each take only the values  $+1/2$  and  $-1/2$ :

$$\psi = \psi_{s,r}, \quad \psi_1 = \psi_{1/2, 1/2}, \quad \psi_2 = \psi_{-1/2, 1/2}, \quad \psi_3 = \psi_{1/2, -1/2}, \quad \psi_4 = \psi_{-1/2, -1/2}.$$

<sup>1</sup>) Compare for instance H. A. KRAMERS, Hand u. Jahrb. d. Chem. Physik, I, § 63, 64.

If  $\vec{\sigma}(\sigma_x, \sigma_y, \sigma_z)$  and  $\varrho_x, \varrho_y, \varrho_z$  are the PAULI matrices operating on  $s$  and  $r$ , the representation of  $\vec{\alpha}, \beta$  under consideration takes the form:

$$\vec{\alpha} = \varrho_z \vec{\sigma}, \quad \beta = \varrho_x. \quad \dots \quad (5)$$

Now the following formulae are easily seen to hold for each of the three  $\sigma$ - and three  $\varrho$ -operators:

$$(\sigma \psi)^L = -\sigma \psi^L \quad (\varrho \psi)^L = -\varrho \psi^L.$$

From this follows:

$$(\vec{\alpha} \psi)^L = \vec{\alpha} \psi^L \quad (\beta \psi)^L = -\beta \psi^L.$$

Since we have furthermore:

$$\begin{aligned} (\vec{p} \psi)^L &= \hbar (-i \nabla \psi)^L = \hbar i \nabla \psi^L = -\vec{p} \psi^L, & \left( i \hbar \frac{\partial \psi}{\partial t} \right)^L &= -i \hbar \frac{\partial \psi^L}{\partial t} \\ (\mathfrak{A} \psi)^L &= \vec{\mathfrak{A}} \psi^L & (\Phi \psi)^L &= \Phi \psi^L \end{aligned}$$

we see that the charge-conjugated of the left and right side of (1) are equal to the left and right side of (2), both multiplied by  $-1$ .

Any other representation of the  $\alpha, \beta$  matrices corresponds to a transformation of the wave-function

$$\psi' = S \psi, \quad \psi'^L = S \psi^L, \quad \dots \quad (6)$$

where  $S$  is an arbitrary non-singular matrix and we have

$$\vec{\alpha}' = S \vec{\alpha} S^{-1}, \quad \beta' = S \beta S^{-1}.$$

In the particular case

$$S = \frac{e^{\frac{\pi i}{4}}}{\sqrt{2}} (1 + i \varrho_y \sigma_y), \quad S^{-1} = \frac{e^{-\frac{\pi i}{4}}}{\sqrt{2}} (1 - i \varrho_y \sigma_y). \quad \dots \quad (7)$$

we find

$$\alpha'_x = \alpha_x = \varrho_z \sigma_x, \quad \alpha'_z = \alpha_z = \varrho_z \sigma_z, \quad \alpha'_y = -\beta = -\varrho_x, \quad \beta' = \alpha_y = \varrho_z \sigma_y.$$

The matrices  $\vec{\alpha}'$  are now purely real whereas  $\beta'$  is purely imaginary. From (6) we find:

$$\begin{pmatrix} \psi'_1 \\ \psi'_2 \\ \psi'_3 \\ \psi'_4 \end{pmatrix} = \frac{e^{\frac{\pi i}{4}}}{\sqrt{2}} \begin{pmatrix} \psi_1 - i \psi_4 \\ \psi_2 + i \psi_3 \\ \psi_3 + i \psi_2 \\ \psi_4 - i \psi_1 \end{pmatrix}, \quad \begin{pmatrix} \psi'^L_1 \\ \psi'^L_2 \\ \psi'^L_3 \\ \psi'^L_4 \end{pmatrix} = \frac{e^{-\frac{\pi i}{4}}}{\sqrt{2}} \begin{pmatrix} \psi_4^* - i \psi_1^* \\ -\psi_3^* - i \psi_2^* \\ -\psi_2^* - i \psi_3^* \\ \psi_1^* - i \psi_4^* \end{pmatrix} = \begin{pmatrix} \psi_1^* \\ \psi_2^* \\ \psi_3^* \\ \psi_4^* \end{pmatrix}.$$

Thus, for this particular representation, charge-conjugation and complex-conjugation are identical:

$$\psi'^L = \psi'^* \dots \dots \dots (8)$$

It is immediately seen that equation (2) in this case is the conjugate complex of eq. (1).

The property (8) must be invariant with respect to LORENTZ-transformations; this is directly verified, since — with the representation under consideration — the coefficients of the LORENTZ-transformation of  $\psi'_1, \psi'_2, \psi'_3, \psi'_4$  are real. In fact, an infinitesimal LORENTZ-transformation corresponds to the operator

$$I_{op.} = \frac{1}{2} S (i d_x \sigma_x + i d_y \sigma_y + i d_z \sigma_z + l_x \rho_x \sigma_x + l_y \rho_y \sigma_y + l_z \rho_z \sigma_z) S^{-1},$$

where  $d_x, d_y, d_z$  (infinitesimal rotation) and  $l_x, l_y, l_z$  (infinitesimal pure LORENTZ-transformation) are all real. Inserting the value (7) for  $S$ , we find for  $I_{op.}$  a purely real matrix.

A representation where  $\vec{\alpha}, i\beta$  are real has been used by MAJORANA <sup>1)</sup> in his recent work on the quantum theory of the negaton and the positon. The concept of charge conjugation is, however, independent of the particular choice of the representation. By its means we will in this article represent some results of the MAJORANA-calculus (and, thereby, also of the DIRAC-HEISENBERG formulation of the hole theory, with which it is practically equivalent) in a general form, which on account of its simplicity might be of some interest.

The PAULI-principle is introduced in the usual way by promoting the wave-function  $\psi$  to a "matrix-operator"  $\psi$  satisfying

$$\psi^*(q) \psi(q') + \psi(q') \psi^*(q) = \delta(q, q') \dots \dots \dots (9)$$

where  $q$  stands for the complete set of positional and spin-coordinates. The same relation will hold for the charge-conjugated function:

$$\psi^{L*}(q) \psi^L(q') + \psi^L(q') \psi^{L*}(q) = \delta(q, q') \dots \dots \dots (10)$$

In these expressions, the asteric means hermitic conjugation.

In ordinary, non-relativistic, quantummechanics an operator  $F^{total}$ , which is symmetrical with respect to the electrons and which consists simply of a sum of identical hermitic operators  $F(i)$

$$F^{total} = \sum_i F(i)$$

( $F(i)$  operates on the coordinates of the  $i^{th}$  electron), is promoted to a matrix operator  $F$  by the well known formula:

$$F = \int \psi^* F \psi,$$

where  $\int$  means integration over the three space coordinates and summa-

<sup>1)</sup> Nuovo Cimento, April, p. 171 (1937).

tion over the spin coordinates. With DIRAC's equation (1) and its charge-conjugated equation (2), we would have the choice between the two completely analogous hermitic expressions

$$\int \psi^* F \psi \quad \text{and} \quad \int \psi^{L*} F^L \psi^L, \dots \dots \dots (11)$$

where  $F$  is obtained from  $F$  by changing the quantity  $e$  representing the electric charge (and which in general may occur in  $F$ ) into  $-e$ :

$$F^L(e) = F(-e) \dots \dots \dots (12)$$

MAJORANA's calculus can now be simply expressed by stating that the arithmetic mean of the two expressions (11) has to be taken:

$$F = \frac{1}{2} \int (\psi^* F \psi + \psi^{L*} F^L \psi^L) \dots \dots \dots (13)$$

A particular representation of  $\psi$  is obtained by developing  $\psi$  in terms of the eigenfunctions of the free electron. Those corresponding to "positive" energies will be denoted by  $\varphi_\lambda$ ; those corresponding to "negative" energies by  $\varphi_\lambda^L$ . For the latter we may indeed take the charge-conjugated of the former. The  $\varphi_\lambda$  may be taken to correspond to definite values of the impuls-vector  $\vec{p}$ ; for each  $\vec{p}$  there will still be two  $\varphi_\lambda$ 's, which may be taken to correspond to spin parallel ( $\varphi_\lambda^p$ ) and antiparallel ( $\varphi_\lambda^a$ ) to  $\vec{p}$ . Taking for simplicity the eigenfunctions to be normalized eigenfunctions in a big cubical space (volume  $\Omega$ ) with periodic boundary conditions, and using the representation (5), we may write for every possible impuls-vector  $\vec{p}_\lambda$  with components  $h \Omega^{-1/3} k_x, h \Omega^{-1/3} k_y, h \Omega^{-1/3} k_z$  ( $k_x, k_y, k_z$  integers)<sup>1)</sup>

$$\left. \begin{aligned} \varphi_\lambda^p &= \frac{1}{\sqrt{\Omega}} \begin{pmatrix} C \alpha \\ C \beta \\ S \alpha \\ S \beta \end{pmatrix} e^{\frac{i(\vec{p} \vec{r})}{\hbar}}, & \varphi_\lambda^a &= \frac{1}{\sqrt{\Omega}} \begin{pmatrix} -S \beta^* \\ S \alpha^* \\ -C \beta^* \\ C \alpha^* \end{pmatrix} e^{\frac{i(\vec{p} \vec{r})}{\hbar}} \\ \varphi_\lambda^{pL} &= \frac{1}{\sqrt{\Omega}} \begin{pmatrix} S \beta^* \\ -S \alpha^* \\ -C \beta^* \\ C \alpha^* \end{pmatrix} e^{-\frac{i(\vec{p} \vec{r})}{\hbar}}, & \varphi_\lambda^{aL} &= \frac{1}{\sqrt{\Omega}} \begin{pmatrix} C \alpha \\ C \beta \\ -S \alpha \\ -S \beta \end{pmatrix} e^{-\frac{i(\vec{p} \vec{r})}{\hbar}} \end{aligned} \right\} (14)$$

where  $C, S, \alpha, \beta$  are defined by

$$\left. \begin{aligned} C &= \cos \frac{1}{2} \chi, & S &= \sin \frac{1}{2} \chi, & \text{ctg } \chi &= \frac{p}{m}, \\ p_z &= p \cos \vartheta, & p_x + i p_y &= p \sin \vartheta e^{i\psi}, \\ \alpha &= \cos \frac{\vartheta}{2} e^{-i\psi/2}, & \beta &= \sin \frac{\vartheta}{2} e^{i\psi/2} \end{aligned} \right\} \dots \dots \dots (15)$$

<sup>1)</sup> Compare H. A. KRAMERS, loc. cit. p. 292.

The representation in question can now be defined as

$$\psi = \sum_{\lambda} a_{\lambda} \varphi_{\lambda} + \sum_{\lambda} b_{\lambda}^* \varphi_{\lambda}^L \dots \dots \dots (16)$$

To it corresponds the following representation for  $\psi^L$

$$\psi^L = \sum_{\lambda} b_{\lambda} \varphi_{\lambda} + \sum_{\lambda} a_{\lambda}^* \varphi_{\lambda}^L \dots \dots \dots (17)$$

In these formulae the summation over  $\lambda$  includes summation over the two opposite spin-directions. The  $a_{\lambda}$ ,  $b_{\lambda}$  and their hermitic conjugates  $a_{\lambda}^*$ ,  $b_{\lambda}^*$  are WIGNER-JORDAN matrices satisfying

$$a_{\lambda}^* a_{\lambda} + a_{\lambda} a_{\lambda}^* = 1, \quad b_{\lambda}^* b_{\lambda} + b_{\lambda} b_{\lambda}^* = 1. \\ \text{(all other pairs anticommute).}$$

In a continuous description (16) and (17) have to be replaced by integrals. Such a description is particularly appropriate to the discussion of the LORENTZ-invariance of the calculus, but we will not enter upon it here.

We will now discuss some particular examples of the application of (13). Consider first the case of free electrons, i. e. electrons in the absence of external fields and without interaction. We compute *the energy operator*  $H^0$

$$H^0 = \frac{1}{2} \int (\psi^* H^0 \psi + \psi^{L*} H^0 \psi^L)$$

where

$$H^0 = H^{0L} = \vec{(\alpha p)} + \beta m.$$

Now, since

$$H^0 \varphi_{\lambda} = E_{\lambda} \varphi_{\lambda}, \quad E_{\lambda} = +\sqrt{p_{\lambda}^2 + m^2}, \\ H^0 \varphi_{\lambda}^L = -E_{\lambda} \varphi_{\lambda}^L,$$

we find

$$\left. \begin{aligned} H^0 &= \frac{1}{2} \sum_{\lambda} E_{\lambda} (a_{\lambda}^* a_{\lambda} - b_{\lambda} b_{\lambda}^*) + \frac{1}{2} \sum_{\lambda} E_{\lambda} (b_{\lambda}^* b_{\lambda} - a_{\lambda} a_{\lambda}^*) \\ &= \frac{1}{2} \sum_{\lambda} E_{\lambda} \{ (a_{\lambda}^* a_{\lambda} - a_{\lambda} a_{\lambda}^*) + (b_{\lambda}^* b_{\lambda} - b_{\lambda} b_{\lambda}^*) \} \\ &= \sum_{\lambda} E_{\lambda} \{ a_{\lambda}^* a_{\lambda} + b_{\lambda}^* b_{\lambda} - 1 \}, \end{aligned} \right\} \dots (18)$$

where the  $-1$  corresponds to the well known infinite negative zero point energy of the hole-theory. Generalising the  $a$  and  $b$  to time-dependent matrices  $a(t)$ ,  $b(t)$ , which for  $t=0$  become equal to  $a$  and  $b$ , we find immediately from

$$\dot{a}_{\lambda} = \frac{i}{\hbar} (H^0 a_{\lambda} - a_{\lambda} H^0), \quad \dot{b}_{\lambda} = \frac{i}{\hbar} (H^0 b_{\lambda} - b_{\lambda} H^0).$$

the well known time-dependence

$$a_\lambda(t) = a_\lambda e^{-\frac{iE_\lambda t}{\hbar}}, \quad b_\lambda(t) = b_\lambda e^{-\frac{iE_\lambda t}{\hbar}}.$$

Promoting also  $\psi$  to a time-dependent operator  $\psi(t)$ , the formula (16) takes the form:

$$\psi_k(x, y, z, t) = \sum_\lambda a_\lambda \varphi_\lambda^0 e^{-\frac{i}{\hbar}(\vec{p}_\lambda \cdot \vec{r} - E_\lambda t)} + \sum_\lambda b_\lambda^* \varphi_\lambda^{0L} e^{-\frac{i}{\hbar}(\vec{p}_\lambda \cdot \vec{r} - E_\lambda t)},$$

where  $\varphi_\lambda^0$  and  $\varphi_\lambda^{0L}$  are the values of  $\varphi_\lambda$  and  $\varphi_\lambda^L$  at the origin. It is of interest to compare this formula with the analogous formula for the quantized radiation field of vacuum-electrodynamics<sup>1)</sup>, where a similar formalism imposes itself automatically and ensures positive energy-values for the light-quanta.

The operator  $e$  of the total charge of the electrons will be given by choosing in (13):

$$F = -F^L = e,$$

and we find:

$$e = \frac{e}{2} \int (\psi^* \psi - \psi^{L*} \psi^L) = \frac{e}{2} \sum_\lambda (a_\lambda^* a_\lambda + b_\lambda b_\lambda^*) - \frac{e}{2} \sum_\lambda (b_\lambda^* b_\lambda + a_\lambda a_\lambda^*) \left. \vphantom{\int} \right\} (19)$$

$$= e \sum_\lambda (a_\lambda^* a_\lambda - b_\lambda^* b_\lambda) = -e \sum_\lambda (b_\lambda^* b_\lambda - a_\lambda^* a_\lambda)$$

This leads us to consider  $a_\lambda^* a_\lambda$  as the operator of the number of electrons with charge  $e$  in the state  $\lambda$  (we will call them *negatons*) and  $b_\lambda^* b_\lambda$  as that of the electrons with charge  $-e$  in this state (*positons*). This interpretation is in accordance with the usual interpretation of the formulae to which one is led when external fields are taken into consideration and when the non relativistic limiting case is discussed. It must, however, be remarked that the total number of electrons

$$N = \sum_\lambda (a_\lambda^* a_\lambda + b_\lambda^* b_\lambda) \dots \dots \dots (20)$$

is not given by (13) when we put  $F = F^L = 1$ ; we find indeed for  $F = 1$  formally a constant:

$$1 = \sum_\lambda 1.$$

On the other hand, the simple but non-analytical operator

$$F = F^L = \frac{H^0}{|H_0|}$$

<sup>1)</sup> H. A. KRAMERS, loc. cit. p. 434. Eq. (103).

would give

$$\left( \frac{\mathbf{H}^0}{|\mathbf{H}^0|} \right) = \sum_{\lambda} (\mathbf{a}_{\lambda}^* \mathbf{a}_{\lambda} + \mathbf{b}_{\lambda}^* \mathbf{b}_{\lambda} - 1) = \mathbf{N}_{\lambda} - \sum_{\lambda} 1.$$

The last sum might be called the negative zero-point number of electrons; it corresponds to the negative zero-point energy in (18).

The operator of the charge-density in space is given by

$$\rho(x, y, z) = \sum_k \frac{e}{2} (\psi_k^* \psi_k - \psi_k^{*L} \psi_k^L). \quad \dots \quad (21)$$

If necessary it can be expressed explicitly in terms of the  $\mathbf{a}$ ,  $\mathbf{b}$ ,  $\mathbf{a}^*$ ,  $\mathbf{b}^*$ . It is a particular case of the more general operator:

$$\mathbf{P}(q', t'; q, t) = \frac{e}{2} (\psi^*(q, t) \psi(q', t') - \psi^{*L}(q, t) \psi^L(q', t')) \quad \dots \quad (22)$$

where  $q$  and  $q'$  stand for two arbitrary, different choices of the space coordinates  $x, y, z$  and the spin coordinate  $k$ . The meaning of  $\mathbf{P}$  is of course only well defined when the HAMILTONIAN  $\mathbf{H}$  of the system is known, which governs the time dependence of all operators. In the particular case where the electrons are free, we have  $\mathbf{H} = \mathbf{H}^0$ . The corresponding  $\mathbf{P}$ -operator will be denoted by  $\mathbf{P}^0$ . It is closely related to

$$R^0(q', t'; q, t) = e \sum_{\lambda} \left( \varphi_{\lambda}^* \varphi_{\lambda} e^{\frac{i E_{\lambda}(t-t')}{\hbar}} - \varphi_{\lambda}^{*L} \varphi_{\lambda}^L e^{-\frac{i E_{\lambda}(t-t')}{\hbar}} \right) \dots \quad (23)$$

This function is identical with the density matrix, which has been computed in DIRAC's paper on the hole-theory of 1934<sup>1)</sup>.  $\mathbf{P}$  in (22) may be called the general operator of the matrix density of the electric charge.

If the electrons are subject to an external field with potentials  $\vec{\mathcal{A}}, \Phi$ , we introduce in (13) for  $F, F^L$  the operators:

$$H = H^0 + e (\Phi - (\vec{\alpha} \vec{\mathcal{A}}))$$

$$H^L = H^0 - e (\Phi - (\vec{\alpha} \vec{\mathcal{A}}))$$

and we find for the energy-operator of the system:

$$\mathbf{H} = \mathbf{H}^0 + \mathbf{H}^1$$

$$\mathbf{H}^1 = \frac{e}{2} \int \{ \psi^* (\Phi - (\vec{\alpha} \vec{\mathcal{A}})) \psi - \psi^{*L} (\Phi - (\vec{\alpha} \vec{\mathcal{A}})) \psi^L \}. \quad \dots \quad (24)$$

<sup>1)</sup> Proc. Cambr. Philos. Soc., 30, 150 (1934).

If the action of the operator  $\Phi - (\vec{\alpha} \vec{\mathfrak{U}})$  is described by means of the two-point operator-function  $\Omega(q, q')$ :

$$(\Phi - (\vec{\alpha} \vec{\mathfrak{U}})) f(q) = \int_{q'} \Omega(q, q') f(q'),$$

(24) can also be written in the form

$$H^1 = \int \int_q \mathbf{P}(q', q) \Omega(q, q') \dots \dots \dots (25)$$

where  $\mathbf{P}(q', q)$  is obtained from (22) by putting  $t$  and  $t'$  equal to zero. The  $H^1$  in (24) or (25) corresponds to the prescription of the DIRAC-HEISENBERG hole-theory; expressed in the  $\mathbf{a}_\lambda$  and  $\mathbf{b}_\lambda$  it contains on one hand the terms

$$\left. \begin{aligned} \frac{e}{2} \sum_{\lambda \lambda'} (\Omega_{\lambda \lambda'} + \Omega_{\lambda \lambda'}^*) (\mathbf{a}_\lambda^* \mathbf{a}_{\lambda'} - \mathbf{b}_\lambda^* \mathbf{b}_{\lambda'}) \\ \Omega_{\lambda \lambda'} = \int \varphi_\lambda^* (\Phi - (\vec{\alpha} \vec{\mathfrak{U}})) \varphi_{\lambda'} \end{aligned} \right\} \dots \dots \dots (26)$$

which commute with  $\mathbf{N}$ , and on the other hand the terms

$$\left. \begin{aligned} \frac{e}{2} \sum_{\lambda \lambda'} (\Omega_{\lambda \bar{\lambda}'} + \Omega_{\lambda \bar{\lambda}'}^*) (\mathbf{a}_\lambda^* \mathbf{b}_{\lambda'}^* + \mathbf{b}_{\lambda'} \mathbf{a}_\lambda) \\ \Omega_{\lambda \bar{\lambda}'} = \int \varphi_\lambda^* (\Phi - (\vec{\alpha} \vec{\mathfrak{U}})) \varphi_{\lambda'}^L \end{aligned} \right\} \dots \dots \dots (27)$$

The terms (27) do not commute with  $\mathbf{N}$ ; they correspond to pair-formation ( $\mathbf{a}^* \mathbf{b}^*$ ) and to pair-annihilation ( $\mathbf{b} \mathbf{a}$ ).

If the potentials of the external field are time-independent, the operator  $H = H^0 + e(\Phi - (\vec{\alpha} \vec{\mathfrak{U}}))$  will have eigenfunctions  $\chi_e$  and corresponding eigenvalues  $E_e$ . The question arises if, and in what way, they correspond to stationary states of the one-electron problem in the field in question. It seems very difficult to give any definite answer at all to this question if no specification of the  $\vec{\mathfrak{U}}, \Phi$  field is given. This difficulty is related to the unsatisfactory and preliminary character of the hole-theory in its present condition.

In the particular case, where the external field is due to a positive electric charge, smaller than  $137|e|$ , fixed at some point in space (hydrogen-like atom), the  $\chi_e$  and  $E_e$  can be naturally divided into two groups. The first of these corresponds to positive values of  $E_e$ , which we will denote by  $E_n$  (eigenfunctions  $\chi_n$ ). For the second group the  $E_e$ 's are negative; we denote them by  $-\bar{E}_n$  (eigenfunctions  $\bar{\chi}_n^L$ ). From comparison with the non-relativistic treatment, we expect that if  $e$  is taken to be negative, the first group corresponds to one negative electron



in the field of the nucleus (ordinary hydrogen atom), whereas the second group corresponds to one positive electron in this field. When the nuclear charge continuously decreases to zero, the set of  $\chi_m$ -functions merges continuously into the set of  $\varphi_\lambda$ -functions defined by (14), whereas the set of  $\bar{\chi}_m^L$ -functions merges into the  $\varphi_\lambda^L$ -functions. In this case we are therefore led to introduce the following representation of  $\psi$  and  $\psi^L$ :

$$\left. \begin{aligned} \psi &= \sum_m \mathbf{c}_m \chi_m + \sum_n \mathbf{d}_n^* \bar{\chi}_n^L \\ \psi^L &= \sum_n \mathbf{d}_n \bar{\chi}_n + \sum_m \mathbf{c}_m^* \chi_m^L \\ \mathbf{c}_m^* \mathbf{c}_m + \mathbf{c}_m \mathbf{c}_m^* &= 1, \quad \mathbf{d}_n^* \mathbf{d}_n + \mathbf{d}_n \mathbf{d}_n^* = 1 \end{aligned} \right\} \dots (28)$$

(all other pairs anticommute).

Comparing (28) with (16), we see that the  $\mathbf{c}_m$  and  $\mathbf{d}_n^*$  can be expressed in terms of the  $\mathbf{a}_\lambda$  and  $\mathbf{b}_\lambda^*$ , and reversely.

The energy operator will now be given by

$$\mathbf{H} = \frac{1}{2} \int (\psi^* H \psi + \psi^L H^L \psi^L) = \sum_m E_m \mathbf{c}_m^* \mathbf{c}_m + \sum_n \bar{E}_n \mathbf{d}_n^* \mathbf{d}_n - \frac{1}{2} \left( \sum_m E_m + \sum_n \bar{E}_n \right) \dots (29)$$

The total charge is given by

$$e = e \left( \sum_m \mathbf{c}_m^* \mathbf{c}_m - \sum_n \mathbf{d}_n^* \mathbf{d}_n \right).$$

Looking apart from the zero-point energy in (29), all stationary states have positive energy. Their SCHRÖDINGER-functions, in the  $m, n$  representation, are given by functions

$$A (\dots N_m \dots; \dots \bar{N}_n \dots), \quad (N_m, \bar{N}_n = 1 \text{ or } 0) \dots (30)$$

which are zero for all  $N_m, \bar{N}_n$  combinations with the exception of one particular combination  $N_m^0, \bar{N}_n^0$ , for which  $A$  equals 1. Every one of these states can also be interpreted in terms of "free electrons", but it appears not to be quite easy to determine how the  $A (\dots N_m \dots; \dots \bar{N}_n \dots)$ -description is transformed into the  $A (\dots N_\lambda \dots; \dots \bar{N}_\lambda \dots)$ -description, which would refer to free electrons.

One of the ordinary discrete states, say state  $m_0$ , of the hydrogen-like atom with one electron would correspond to  $A (\dots N_m \dots; \dots \bar{N}_n \dots)$  being different from zero only for that particular  $N_m^0, \bar{N}_n^0$  combination for which all the  $\bar{N}_n^0$  are zero, and for which also all  $N_m^0$  are zero with the exception of  $N_{m_0}^0$ . In the description in terms of free electrons, the

number of electrons in this state is of course not well-defined, there being a probability of finding only one (negative) electron, a probability of finding three electrons (two negative, one positive), and so on.

Now, the electrons have up to this point been considered as independent, whereas in reality they act on each other through the medium of the electromagnetic field. It is of course possible to describe this interaction in a formal way, by introducing a quantized  $E, H$ -field by the methods of quantum-electrodynamics. In view of the unsatisfactory nature of these methods we might, as an approximation, try to introduce directly the COULOMB interaction between the electrons, in order to improve our scheme of calculating stationary states.

Now, in non-relativistic quantum mechanics, this COULOMB interaction would be represented by a matrix-operator:

$$H_2 = \frac{e^2}{2} \int \int_q \psi^*(q) \psi^*(q') \frac{1}{r} \psi(q') \psi(q) \quad r = |\vec{r}(q) - \vec{r}(q')| \quad . \quad (31)$$

The simplest but perhaps not correct way of generalizing this formalism in the hole theory would be:

$$H_2 = \frac{e^2}{4} \int \int \left\{ \psi^*(q) \psi^*(q') \frac{1}{r} \psi(q') \psi(q) + \psi^{L*}(q) \psi^{L*}(q') \frac{1}{r} \psi^L(q') \psi^L(q) \right\} \quad (32)$$

For large atomic number this energy might be considered as a perturbation. Its influence on the energy of the stationary states would be given by its expectancy value; this value does not vanish automatically in the case of the hydrogen-like atom (with one electron), in contrast to the result of applying (31) to such a state in non-relativistic quantum-mechanics. One might say this is due to the fact that, in the hole theory, it can no longer be said that precisely one electron is present in the stationary states in question. As a result we expect that *a correction must be applied to the energy values of the stationary states of the hydrogen atom, as given by the DIRAC theory of 1928.*

In a later paper we will discuss more closely the possibility of actually computing this correction.