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predecessors, and hence that the degree of pre-existing ionization in the channel governs the velocity of the dart leader.

The downward-branching of lightning and its characteristic zig-zag form are shown to arise during the stepped-leader process before the first return stroke.

An account, based upon 24 cases examined, is given of the nature of the stepped leader. The velocity of the streamers making up the steps is of the order of $5 \times 10^9$ cm/sec. The range of variation of the time intervals between steps is small ($31-91$ $\mu$-sec) compared with that of the step-lengths themselves ($10-206$ metres).

A decrease in the intensity of the return portion of a stroke in passing branch-points is found to be general, and it is deduced that the leader process lowers into the air a very considerable fraction of the cloud charge tapped.

Discharges into the air exhibit no return stroke but sometimes show a slow recoil effect from their ends.

The Relativistic Self-Consistent Field

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(Communicated by D. R. Hartree, F.R.S.—Received June 12, 1935)

1—The method of the self-consistent field for determining the wave functions and energy levels of an atom with many electrons was developed by Hartree,† and later derived from a variation principle and modified to take account of exchange and of Pauli’s exclusion principle by Slater‡ and Fock.§ No attempt was made to consider relativity effects, and the use of “spin” wave functions was purely formal. Since, in the solution of Dirac’s equation for a hydrogen-like atom of nuclear charge $Z$, the difference of the radial wave functions from the solutions of Schrödinger’s equation depends on the ratio $Z/137$, it appears that for heavy atoms the relativity correction will be of importance; in fact, it may in some cases be of more importance as a modification of Hartree’s original self-

§ ‘Z. Physik,’ vol. 61, p. 126; vol. 62, p. 793 (1930); vol. 81, p. 195 (1933); V. Fock and M. Petrasch, ‘Phys. Z. Sowjet.,’ vol. 6, p. 368 (1934).

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consistent field equation than "exchange" effects. The relativistic self-consistent field equation neglecting "exchange" terms can be formed from Dirac's equation by a method completely analogous to Hartree's original derivation of the non-relativistic self-consistent field equation from Schrödinger's equation. Here we are concerned with including both relativity and "exchange" effects and we show how Slater's variational method may be extended for this purpose.

A difficulty arises in considering the relativistic theory of any problem concerning more than one electron since the correct wave equation for such a system is not known. Formulae have been given for the interaction energy of two electrons, taking account of magnetic interactions and retardation, by Gaunt,† Breit‡, and others. Since, however, none of these is to be regarded as exact, in the present paper the crude electrostatic expression for the potential energy will be used. The neglect of the magnetic interactions is not likely to lead to any great error for an atom consisting mainly of closed groups, since the magnetic field of a closed group vanishes. Also, since the self-consistent field type of approximation is concerned with the interaction of average distributions of electrons in one-electron wave functions, it seems probable that retardation does not play an important part. These effects are in any case likely to be of less importance than the improvement in the grouping of the wave functions which arises from using a wave equation which involves the spins implicitly.

It is first shown that Dirac's equations for a single electron can be derived from a variation principle and this is extended to the case of many electrons when the magnetic interactions and retardation are ignored. The wave functions for individual electrons are assumed to be quantities with four components of the types found for a single electron in a central field.§ and the anti-symmetrical wave function for the whole atom to be a "determinant" built up from these in the same way as the non-relativistic wave function for a whole atom is built up from one-electron wave functions. It is then possible to obtain an expression for the total energy of the atom in terms of radial functions only. This necessitates the construction of tables analogous to those given by Slater.|| Then by a variation method differential equations for these radial wave functions can be obtained. As an example, we derive the equations for the two different types of $2p$ wave function for copper.

† 'Phil. Trans.,' A, vol. 228, p. 151 (1929).
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2—Dirac's expression† in atomic units for the hamiltonian $H$ for a single electron moving in a field of force of scalar potential $V$ and zero vector potential is the matrix

$$H = -VU + c\alpha \cdot p + c^2\beta,$$

(1)

where $c$ is equal to 137 in atomic units, $p = -i\nabla$, $U$ is the unit matrix with four rows and columns, and the components of $\alpha$ ($\alpha_1$, $\alpha_2$, $\alpha_3$) and $\beta$ are given by

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

$$\alpha_3 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}.$$

(2)

We form the volume integral

$$E = \int \psi^* \psi \, d\tau$$

(3)

taken over all space. The suffixes $\rho, \sigma$ go from 1 to 4, and we use the summation convention throughout. We shall show that Dirac's equations can be obtained by requiring that this integral shall be stationary for arbitrary independent variations of the four components of $\psi$, subject only to a normalizing condition. We first show that the integral (3) is real for any $\psi$ obeying a given boundary condition, not only for solutions of Dirac's equations. For

$$E = \int \psi^* \left( -VU_{\rho\sigma} - ic\alpha_{\rho\sigma} \cdot \nabla + c^2\beta_{\rho\sigma} \right) \psi \, d\tau,$$

(4)

and since $U$ and $\beta$ are real, the conjugate complex quantity $E^*$ is

$$E^* = \int \psi^* \left( -VU_{\rho\sigma} + ic\alpha_{\rho\sigma}^* \cdot \nabla + c^2\beta_{\rho\sigma} \right) \psi \, d\tau.$$

(5)

Now,

$$U_{\rho\sigma} = U_{\sigma\rho}, \quad \beta_{\rho\sigma} = \beta_{\sigma\rho} \quad \text{and} \quad \alpha_{\rho\sigma}^* = \alpha_{\sigma\rho}.$$

† Pauli, 'Handb. der Physik,' vol. 24, p. 233.
Therefore\[ E^* = \int \psi_\alpha^* (\mathbf{VU}_{\alpha\beta} - i c \mathbf{\alpha}_{\alpha\beta} \cdot \nabla + \epsilon^{\alpha\beta\gamma}_{\nu \rho} \psi_{\nu} d\tau 
 + i c \int (\psi_\alpha \mathbf{\alpha}_{\alpha\beta}^* \psi_{\beta}^*) \cdot \mathbf{dS}, \quad (6) \]

where the surface integral is taken over the sphere at infinity and therefore vanishes if all the components $\psi_p$ are $O(1/r)$ for large $r$. The volume integral in (6) is the same as (4) with a change of the dummy suffixes. It follows that, subject to the condition for the behaviour at infinity, $E = E^*$, so that for any such $\psi$ $E$ defined by (3) is real.

We normalize the $\psi$'s to unity, thus

\[ \int \psi_p^* \psi_p d\tau = 1, \quad (7) \]

and consider the result of putting

\[ \delta E = 0 \quad (8) \]

subject to

\[ \delta \int \psi_p^* \psi_p d\tau = 0. \]

This is in complete analogy to the procedure in the non-relativistic case, since, if the $\psi_p$ are wave functions, (3) is the expression for the total energy of the system while $\psi_p^* \psi_p$ is the charge density. We have then

\[ \int (\delta \psi_p^* \mathbf{H}_{\alpha\beta} \psi_\alpha + \psi_\alpha^* \mathbf{H}_{\alpha\beta} \delta \psi_p) d\tau = \varepsilon \int (\delta \psi_p^* \psi_p + \psi_p^* \delta \psi_p) d\tau = 0, \quad (9) \]

where $\varepsilon$ is real since it is equal to a stationary value of

\[ \frac{\int \psi_p^* \mathbf{H}_{\alpha\beta} \psi_\alpha d\tau}{\int \psi_p^* \psi_p d\tau}, \]

which is real as proved above.

Now,

\[ \int \psi_\alpha^* \mathbf{H}_{\alpha\beta} \delta \psi_p d\tau = \int \delta \psi_p \mathbf{H}_{\alpha\beta}^* \psi_\alpha^* d\tau - i \int (\psi_\alpha^* \mathbf{\alpha}_{\alpha\beta} \delta \psi_p) \cdot \mathbf{dS}, \quad (10) \]

\[ \dagger \] Here and in equation (10) we apply the divergence theorem to $\int \nabla \cdot (\psi_p \mathbf{\alpha}_{\alpha\beta}^* \psi_\alpha) d\tau$

instead of to $\int \nabla \cdot (\psi \nabla \psi) d\tau$ as in the non-relativistic case.
and the surface integral over the sphere at infinity vanishes under the given conditions. (9) may therefore be written in the form

\[ \int \left[ R(\delta \psi_{\rho}) (H_{\rho\sigma} \psi_{\sigma} + H_{\rho\sigma}^* \psi_{\sigma}^* - \varepsilon \psi_{\rho} - \varepsilon \psi_{\rho}^*) + I(\delta \psi_{\rho}^*) (H_{\rho\sigma} \psi_{\sigma}^* - H_{\rho\sigma} \psi_{\sigma} + \varepsilon \psi_{\rho} - \varepsilon \psi_{\rho}^*) \right] \, d\tau = 0. \]  

(11)

If we are considering a general variation of \( \psi \) we must regard each of its components as capable of variation independently of the others and also must contemplate independent variations of \( R(\delta \psi_{\rho}) \) and \( I(\delta \psi_{\rho}^*) \), the real and imaginary parts of \( \delta \psi_{\rho} \). The coefficient of \( R(\delta \psi_{\rho}) \) is purely real and that of \( I(\delta \psi_{\rho}^*) \) purely imaginary. We have therefore

\[ H_{\rho\sigma} \psi_{\sigma} + H_{\rho\sigma}^* \psi_{\sigma}^* - \varepsilon \psi_{\rho} - \varepsilon \psi_{\rho}^* = 0 \]  

(12)

and

\[ H_{\rho\sigma}^* \psi_{\sigma}^* - H_{\rho\sigma} \psi_{\sigma} + \varepsilon \psi_{\rho} - \varepsilon \psi_{\rho}^* = 0. \]  

(13)

By adding and subtracting these equations we have

\[ H_{\rho\sigma} \psi_{\sigma} - \varepsilon \psi_{\rho} = 0 \]  

(14)

\[ H_{\rho\sigma}^* \psi_{\sigma}^* - \varepsilon \psi_{\rho}^* = 0, \]  

(15)

which are Dirac's equations for \( \psi \) and \( \psi^* \) and are written more fully as

\[ (-VU_{\rho\sigma} - ic \alpha_{\rho\sigma} \cdot \nabla + c^2 \beta_{\rho\sigma} - \varepsilon U_{\rho\sigma}) \psi_{\sigma} = 0 \]  

(16)

and

\[ -V \psi_{\sigma}^* U_{\sigma\rho} + ic \nabla \psi_{\sigma}^* \cdot \alpha_{\rho\sigma} + c^2 \psi_{\sigma}^* \beta_{\sigma\rho} - \varepsilon \psi_{\rho} U_{\sigma\rho} = 0. \]  

(17)

For an electron in a field of potential \( V \), a function of \( r \) only, equations (16), written out in full, become

\[
\begin{align*}
  i\left(-\frac{\varepsilon + V}{c} + c\right)\psi_1 + \left(\frac{\partial}{\partial x} - i \frac{\partial}{\partial y}\right)\psi_2 + \frac{\partial}{\partial z} \psi_3 &= 0 \\
  i\left(-\frac{\varepsilon + V}{c} + c\right)\psi_2 + \left(\frac{\partial}{\partial x} + i \frac{\partial}{\partial y}\right)\psi_3 - \frac{\partial}{\partial z} \psi_4 &= 0 \\
  -i\left(\frac{\varepsilon + V}{c} + c\right)\psi_3 + \left(\frac{\partial}{\partial x} - i \frac{\partial}{\partial y}\right)\psi_2 + \frac{\partial}{\partial z} \psi_1 &= 0 \\
  -i\left(\frac{\varepsilon + V}{c} + c\right)\psi_4 + \left(\frac{\partial}{\partial x} + i \frac{\partial}{\partial y}\right)\psi_1 - \frac{\partial}{\partial z} \psi_2 &= 0
\end{align*}
\]

(18)

Darwin\(^\dagger\) has shown that two types of solution in polar co-ordinates

\(^\dagger\) ' Proc. Roy. Soc.,' A, vol. 118, p. 654 (1928). The spherical harmonics used here are the conventional ones, not the modified ones used by Darwin. Differences in sign between equations (19) and Darwin's (7.1) are due to a different formulation of Dirac's hamiltonian. The notation used here is that used by Pauli ('Handbuch der Physik,' vol. 24).
may be obtained for these equations, the one corresponding in the usual notation to \((l, j = l + \frac{1}{2}, m = u + \frac{1}{2})\) and given by†

\[
\begin{align*}
\psi_1 &= -iF_l (l - u + 1) P_{l+1}^u (\mu) e^{i u \phi} \\
\psi_2 &= -iF_l P_{l+1}^{u+1} (\mu) e^{i(u+1)\phi} \\
\psi_3 &= G_l (l + u + 1) P_l^u (\mu) e^{i(u+1)\phi} \\
\psi_4 &= -G_l P_l^{u+1} (\mu) e^{i(u+1)\phi} \\
\end{align*}
\]

\[
\begin{align*}
\psi_1 &= -iF_l P_{l+1}^{-u} (\mu) e^{i u \phi} \\
\psi_2 &= iF_l (l + u + 2) P_{l+1}^{-(u+1)} (\mu) e^{i(u+1)\phi} \\
\psi_3 &= G_l P_{l+1}^{-u} (\mu) e^{i u \phi} \\
\psi_4 &= G_l (l - u) P_{l+1}^{-(u+1)} (\mu) e^{i(u+1)\phi} \\
\end{align*}
\]

\[0 \leqslant u \leqslant l \tag{19A}\]

\[-(l + 1) \leqslant u \leqslant -1 \tag{19B} \]

where \(F_l, G_l\) are functions of \(r\) only and \(\mu = \cos \theta\); the other, corresponding to \((l, j = l - \frac{1}{2}, m = u + \frac{1}{2})\) given by

\[
\begin{align*}
\psi_1 &= -iF_{l-1} (l + u) P_{l-1}^u (\mu) e^{i u \phi} \\
\psi_2 &= iF_{l-1} P_{l-1}^{u+1} (\mu) e^{i(u+1)\phi} \\
\psi_3 &= G_{l-1} (l - u) P_l^u (\mu) e^{i u \phi} \\
\psi_4 &= G_{l-1} P_l^{u+1} (\mu) e^{i(u+1)\phi} \\
\end{align*}
\]

\[
\begin{align*}
\psi_1 &= iF_{l-1} P_{l-1}^{-u} (\mu) e^{i u \phi} \\
\psi_2 &= iF_{l-1} (l - u - 1) P_{l-1}^{-(u+1)} (\mu) e^{i(u+1)\phi} \\
\psi_3 &= -G_{l-1} P_{l}^{-u} (\mu) e^{i u \phi} \\
\psi_4 &= G_{l-1} (l + u + 1) P_{l}^{-(u+1)} (\mu) e^{i(u+1)\phi} \\
\end{align*}
\]

\[0 \leqslant u \leqslant l - 1 \tag{20A}\]

\[-l \leqslant u \leqslant -1 \tag{20B}\]

The functions \(F_l, G_l\) are solutions of the differential equations

\[
\begin{align*}
\left(-\frac{\varepsilon + V}{c} + c\right) F_l + \frac{dG_l}{dr} - \frac{l}{r} G_l &= 0 \\
\left(\varepsilon + V + c\right) G_l + \frac{dF_l}{dr} + \frac{l + 2}{r} F_l &= 0 \\
\end{align*}
\]

Putting

\[
\begin{align*}
P_l &= rG_l \\
Q_l &= rF_l \\
\end{align*}
\]

\[\tag{21}\]

\[\tag{22}\]


‡ See footnote †, p. 629.
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Equations (21) become

\[
\begin{align*}
\left(-\frac{\varepsilon + V}{c} + c\right)Q_i + \frac{dP_i}{dr} - \frac{l + 1}{r} P_i &= 0 \\
\left(-\frac{\varepsilon + V}{c} + c\right)P_i + \frac{dQ_i}{dr} + \frac{l + 1}{r} Q_i &= 0
\end{align*}
\]

(23)

The second-order equation derived for \( P_i \) from these equations is, when the relativistic terms are neglected, the same as the non-relativistic equation for the function \( P_i \) defined as \( r \) times the radial wave function, i.e., \( P_i \) corresponds to the non-relativistic \( P_i \) used by Hartree.† We could at once build up the relativistic self-consistent field equation without "exchange" terms by taking for \( V \) the sum of the potential due to a nucleus of charge \( Z \) and that of the charge distribution \( \Sigma \psi_p^* \psi_p \) where the summation is taken over the electrons in other wave functions than the particular one considered. In what follows we show how to derive the relativistic self-consistent field equations including "exchange" terms.

3—We follow the line suggested by Slater for the non-relativistic case for an atom with \( N \) electrons.

We first construct an expression for the total energy of the system in terms of one-electron wave functions. Let the expression

\[
\psi_{\rho s}(\alpha_p | s), \quad (\rho_s = 1 \ldots 4)
\]
denote the wave function for the state \( \alpha_p \), specified by the four quantum numbers \((n, l, j, m)\), expressed as a function of the co-ordinates of the \( s \)th electron. That is, the \( s \)th electron is in the state \( \alpha_p \). We consider the integral

\[
\int \sum_{\rho_1, \ldots, \rho_N = 1}^{4} \sum_{\sigma_1, \ldots, \sigma_N = 1}^{1} (-1)^P \psi_{\rho_1}^* (\alpha_1 | 1) \ldots \psi_{\rho_N}^* (\alpha_N | N) H_{\rho_1, \ldots, \rho_N, \sigma_1, \ldots, \sigma_N} \psi_{\sigma_1} (\beta_1 | 1) \ldots \psi_{\sigma_N} (\beta_N | N) d\tau_1 \ldots d\tau_N,
\]

(24)

where \( H_{\rho_1, \ldots, \rho_N, \sigma_1, \ldots, \sigma_N} \), the hamiltonian for the whole atom is the sum of several terms; firstly, the hamiltonians of the separate electrons in the field of the nucleus, for example, that of electron 1, namely,

\[
\left(-\frac{Z}{r_1} U_{\rho_1 \sigma_1} + c\alpha_{p_1 \sigma_1} \cdot p_1 + c^2 \beta_{p_1 \sigma_1} \right) U_{\rho_1 \sigma_1} \ldots U_{\rho_N \sigma_N},
\]

(25)

and secondly, terms due to the interaction between pairs of electrons, which, as we have pointed out, we take to be the crude electrostatic interaction, so that these terms are of the type

\[
\frac{1}{r_{12}} U_{\rho_1 \sigma_1} \ldots U_{\rho_N \sigma_N},
\]

(26)

† No confusion should arise between \( P_i \) and the Legendre functions.
where $r_{12}$ is the distance between electrons 1 and 2. The summation \( \Sigma (-1)^{\nu} \) means that the summation is to be taken over all permutations of the electrons among the different wave functions, the positive or negative sign to be taken according as the permutation is even or odd.

We contemplate only wave functions constructed of \( \psi \)'s of the forms (19) and (20) as regards their dependence on \( \theta \) and \( \phi \). As in the non-relativistic case, we work with orthogonal one-electron wave functions. We determine the differential equations for the radial wave functions \( P, Q \), by making (24) take a stationary value for variations of \( P \) and \( Q \) subject to the normalizing and orthogonalizing conditions for the one-electron wave functions. The normalizing factors for the solutions (19a), (19b), (20a), (20b) are respectively

\[
\left[ \frac{1}{4\pi} \frac{(l - u)!}{(l + u + 1)!} \right]^\frac{1}{2} \left[ \frac{1}{4\pi} \frac{(l + u + 1)!}{(l - u)!} \right]^\frac{1}{2} \left[ \frac{1}{4\pi} \frac{(l - u - 1)!}{(l + u)!} \right]^\frac{1}{2} \left[ \frac{1}{4\pi} \frac{(l + u)!}{(l - u - 1)!} \right]^\frac{1}{2},
\]

with

\[
\int_0^\infty (P_1^2 + G_1^2) r^2 dr = \int_0^\infty (P_1^2 + Q_1^2) dr
\]
\[
= \int_0^\infty (F_{\alpha l_{-1}} + G_{\alpha l_{-1}}) r^2 dr = \int_0^\infty (P_{\alpha l_{-1}} + Q_{\alpha l_{-1}}) dr = 1.
\]

(27)

We therefore multiply the solutions (19) and (20) by the appropriate factors (27) and the normalizing condition for the radial wave functions \( P_{n, l}, Q_{n, l} \) for a state \( (n, l, j = l + \frac{1}{2}, m) \) is

\[
\int_0^\infty (P_{n, l}^2 + Q_{n, l}^2) dr = 1,
\]

(29)

while that for \( P_{n, -l-1}, Q_{n, -l-1} \), corresponding to a state \( (n, l, j = l - \frac{1}{2}, m) \), is

\[
\int_0^\infty (P_{n, -l-1}^2 + Q_{n, -l-1}^2) dr = 1.
\]

(30)

Two wave functions of the types (19) and (20) are orthogonal (that is to say, \( \int \psi_{\alpha p} (\alpha_p | s) \psi_{\alpha q} (\alpha_q | s) d\tau = 0 \)), unless the triad of quantum numbers \( (l, j, m) \) is the same for both; for two functions corresponding to states \( (n, l, j, m), (n', l, j, m) \) the orthogonalizing condition is

\[
(P_{n, l - l - 1} + Q_{n, l - l - 1}) (P_{n', l - l - 1} + Q_{n', l - l - 1}) dr = 0.
\]

(31)

We proceed to the evaluation of (24) in terms of integrals involving these radial wave functions only. The terms of the type (25) involv-
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ing the co-ordinates of a single electron only give, for completed subgroups,

\[ N! \sum_{n, l \geq 0, j = l + \frac{1}{2}} (2j + 1) \int_{0}^{\infty} \left[ -\left( \frac{Z}{cr} + c \right) Q_{n,l}^{a} + Q_{n,l} \left( \frac{dP_{n,1}}{dr} - \frac{l + 1}{r} P_{n,1} \right) \right. \]

\[ \left. -\left( \frac{Z}{cr} + c \right) P_{n,l}^{a} - P_{n,l} \left( \frac{dQ_{n,1}}{dr} + \frac{l + 1}{r} Q_{n,1} \right) \right] dr \]

\[ + N! \sum_{n, l \geq 1, j = l - \frac{1}{2}} (2j + 1) \times \]

\[ \int_{0}^{\infty} \left[ -\left( \frac{Z}{cr} + c \right) Q_{n,l-1}^{a} + Q_{n, l-1} \left( \frac{dP_{n,l-1}}{dr} + \frac{l}{r} P_{n,l-1} \right) \right. \]

\[ \left. -\left( \frac{Z}{cr} + c \right) P_{n,l-1}^{a} - P_{n,l-1} \left( \frac{dQ_{n,l-1}}{dr} - \frac{l}{r} Q_{n,l-1} \right) \right] dr. \] \( \text{(32)} \)

The contributions from terms of the type (26) will be of two kinds, the direct interaction integrals for which the permutation among the \( \psi^* \)'s is the same as that among the \( \psi \)'s and the "exchange" integrals for which the permutation of the electrons among the \( \psi^* \)'s differs from that among the \( \psi \)'s by the interchange of two electrons. As in the non-relativistic case, all other permutations give zero contributions when the orthogonality relations are satisfied. These terms therefore give altogether

\[ \frac{N!}{c} \sum_{n, l, j, \bar{u}} \left[ J(n, l, j, u; n', l', j', u') - K(n, l, j, u; n', l', j', u') \right], \] \( \text{(33)} \)

where \( J \) is the direct integral, \( K \) the exchange integral. Now,

\[ \frac{1}{r_{12}} = \sum_{k} \left( \frac{k - m}{k + m} \right)! \frac{r(a)^{k}}{r(b)^{k+1}} P_{k}^{(1)}(\mu_{1}) P_{k}^{(2)}(\mu_{2}) e^{im(\psi_{1} - \psi_{2})}, \] \( \text{(34)} \)

where \( r(a) \) is the smaller and \( r(b) \) the greater of \( r_{1} \) and \( r_{2} \) and \( \mu_{1} = \cos \theta_{1}, \mu_{2} = \cos \theta_{2}. \) We have, therefore, for \( u, u' \geq 0 \)

\[ J(n, l, l + \frac{1}{2}, u; n', l', l' + \frac{1}{2}, u') = \frac{1}{4\pi^{2}} \frac{(l-u)!}{(l+u+1)!} \frac{(l'-u')!}{(l'+u'+1)!} \]

\[ \times \sum_{k} \int \left\{ Q_{n,l}^{a} \left( r_{1} \right) \left[ (l-u+1)^{a} (P_{l+1}^{u} (\mu_{1}))^{2} + (P_{l+1}^{u+1} (\mu_{1}))^{2} \right] \right. \]

\[ + P_{n,l}^{a} \left( r_{1} \right) \left[ (l+u+1)^{a} (P_{l}^{u} (\mu_{1}))^{2} + (P_{l}^{u+1} (\mu_{1}))^{2} \right] \}

\[ \times \left\{ Q_{n',l'}^{a} \left( r_{2} \right) \left[ (l'-u'+1)^{a} (P_{l'+1}^{u'} (\mu_{2}))^{2} + (P_{l'+1}^{u'+1} (\mu_{2}))^{2} \right] \right. \]

\[ + P_{n',l'}^{a} \left( r_{2} \right) \left[ (l'+u'+1)^{a} (P_{l'}^{u'} (\mu_{2}))^{2} + (P_{l'}^{u'+1} (\mu_{2}))^{2} \right] \}

\[ \times \left. P_{k}^{(1)}(\mu_{1}) P_{k}^{(2)}(\mu_{2}) \frac{r(a)^{k}}{r(b)^{k+1}} d\tau_{1} d\tau_{2} \right] \]

\[ = \sum_{k} a_{k} \left( l, l + \frac{1}{2}, u; l', l' + \frac{1}{2}, (u'+1) \right) F_{k}(n, l; n', l'), \] \( \text{(35)} \)

\[ \text{where } \left\{ \begin{array}{l}
\end{array} \right. \]
where

$$a_k(l, l - \frac{1}{2}, -(u + 1); l', l' - \frac{1}{2}, -(u' + 1))$$

$$= \frac{(l - u)! (l' - u')!}{(l + u + 1)! (l' + u' + 1)!} \left[ \int_0^1 [(l + u + 1)^2 (P_l^u(\mu_1))^2 + (P_{l+1}^{u+1}(\mu_1))^2] P_l^u(\mu_1) \frac{d\mu_1}{2} \right.$$  

$$\times \left\{ \int_0^1 [(l' + u' + 1)^2 (P_{l'}^{u'}(\mu_2))^2 + (P_{l'+1}^{u'+1}(\mu_2))^2] P_{l'}^{u'}(\mu_2) \frac{d\mu_2}{2} \right\}$$

$$= \int_0^1 \left[ P_{n_1}^{l_1}(r_1) P_{n_1'}^{l_1'}(r_2) + Q_{n_1}^{l_1}(r_1) Q_{n_1'}^{l_1'}(r_2) \right]$$

$$\times \frac{r(a)^{n_1} b^{l_1+1}}{r(b)^{n_1'+1}} dr_1 dr_2.$$  

The proof that in (35) the coefficients of all the different products of $P_{n_1}^{l_1}, Q_{n_1}^{l_1}, P_{n_1'}^{l_1'}, Q_{n_1'}^{l_1'}$ are equal is given in Hartree's paper A. The notation is analogous to that used by Slater.

We find similarly that

$$J(n, l, l - \frac{1}{2}, -(u + 1); n', l', l' - \frac{1}{2}, -(u' + 1))$$

$$= \sum a_k(l, l - \frac{1}{2}, -(u + 1); l', l' - \frac{1}{2}, -(u' + 1))$$

$$= \sum a_k(l - 1, l - \frac{1}{2}, -(u + 1); l' - 1, l' - \frac{1}{2}, -(u' + 1))$$

$$= a_k(l - 1, l - \frac{1}{2}, -(u + 1); l' - 1, l' - \frac{1}{2}, -(u' + 1))$$

and

$$J(n, l, l + \frac{1}{2}, -(u + 1); n', l', l' - \frac{1}{2}, -(u' + 1))$$

$$= \sum a_k(l, l + \frac{1}{2}, -(u + 1); l', l' - \frac{1}{2}, -(u' + 1))$$

$$= \sum a_k(l, l + \frac{1}{2}, -(u + 1); l', l' - \frac{1}{2}, -(u' + 1))$$

$$= a_k(l, l + \frac{1}{2}, -(u + 1); l', l' - \frac{1}{2}, -(u' + 1))$$

$$F_k(n, l; n', -(l' + 1)), \quad (39)$$

$$F_k(n, l; n', -(l' + 1)), \quad (40)$$
The Relativistic Self-Consistent Field

where

\[ a_k \left( l, l + \frac{1}{2}, -\frac{u}{u + 1}; l', l' - \frac{1}{2}, -\frac{u'}{(u' + 1)} \right) \]

\[ = a_k \left( l, l + \frac{1}{2}, -\frac{u}{u + 1}; l' - 1, l' - \frac{1}{2}, -\frac{u'}{(u' + 1)} \right). \tag{41} \]

In all these formulae the four values, \( u, -\frac{u}{u + 1}; u', -\frac{u'}{(u' + 1)} \) can be taken together in any of the four possible ways. The table of \( a' \)'s can be very simply constructed from the set given by (37). Table I gives the values of the \( a' \)'s for all pairs of \( s, p, \) and \( d \) wave functions.

We now proceed to the evaluation of the “exchange” integrals \( K \).

If \( u, u' > 0 \)

\[ K \left( n, l, l + \frac{1}{2}, -\frac{u}{u + 1}; n', l', l' + \frac{1}{2}, -\frac{u'}{(u' + 1)} \right) \]

\[ = \sum b_k \left( l, l + \frac{1}{2}, -\frac{u}{u + 1}; l', l' + \frac{1}{2}, -\frac{u'}{(u' + 1)} \right) G_k(n, l; n', l'), \tag{42} \]

where

\[ b_k \left( l, l + \frac{1}{2}, -\frac{u}{u + 1}; l', l' + \frac{1}{2}, -\frac{u'}{(u' + 1)} \right) \]

\[ = \frac{(l - u)!}{(l + u + 1) (l' + u' + 1)} \frac{(l' - u')!}{(k - |u' - u|)!} \frac{(k + |u' - u|)!}{(k - |u' - u|)!} \]

\[ \times \left[ \int_{-1}^{1} \left[ (l + u + 1) (l' + u' + 1) P_{l}^u(\mu) P_{l'}^{u'}(\mu) \right. \right. \]

\[ + P_{l+1}^{u+1}(\mu) P_{l'+1}^{u'+1}(\mu) \left. \right] \left. \frac{d\mu}{2} \right]^2 \]

\[ \tag{43} \]

and

\[ G_k(n, l; n', l') \]

\[ = \int \left[ P_{n, l}(r_1) P_{n', l}(r_2) P_{n, l'}(r_1) P_{n', l'}(r_2) + P_{n, l}(r_1) P_{n', l}(r_2) Q_{n, l}(r_1) Q_{n', l}(r_2) \right. \]

\[ + Q_{n, l}(r_1) Q_{n', l}(r_2) P_{n, l'}(r_1) P_{n', l'}(r_2) + Q_{n, l}(r_1) Q_{n', l}(r_2) Q_{n, l'}(r_1) Q_{n', l'}(r_2) \]

\[ \times \frac{r (a)^k}{r (b)^{k+1}} \frac{d\mu}{2} \frac{d\nu}{2} \right]^2 \]

\[ \tag{44} \]

Here \( u \) is to be taken with \( u' \) and \( -\frac{u}{u + 1} \) with \( -\frac{u'}{(u' + 1)} \).

The proof that the coefficients of all the different products of a given set of \( P_{n, l}, P_{n', l}, Q_{n, l}, Q_{n', l} \) are the same follows very simply from the properties of spherical harmonics.†

† See Hartree, A, p. 228 (7) and (8).
Further
\[ K\left(n, l, l + \frac{1}{2}, -\left(\frac{u}{u' + 1}\right); n', l', l' + \frac{1}{2}, -\left(\frac{u'}{u'} + 1\right)\right) \]
\[ = \sum_k b_k \left(l, l + \frac{1}{2}, -\left(\frac{u}{u' + 1}\right); l', l' + \frac{1}{2}, -\left(\frac{u'}{u'} + 1\right)\right) G_k(n, l; n', l'), \tag{45} \]
where
\[ b_k \left(l, l + \frac{1}{2}, -\left(\frac{u}{u' + 1}\right); l', l' + \frac{1}{2}, -\left(\frac{u'}{u'} + 1\right)\right) \]
\[ = \frac{(l - u)!}{(l + u + 1)!} \frac{(l' - u')!}{(l' + u' + 1)!} \frac{(k - |u' + u + 1|)!}{(k + |u' + u + 1|)!} \]
\[ \times \left[ \frac{1}{\Gamma(u + 1)} \frac{1}{\Gamma(u' + 1)} \right] \frac{1}{\Gamma(l + u + 1)} \frac{1}{\Gamma(l' + u' + 1)} \]
\[ \times P_{l'}^{u+1} \left(\mu\right) P_{l'}^{u'} \left(\mu\right) - (l + u + 1) P_{l'}^{u} \left(\mu\right) P_{l'}^{u'+1} \left(\mu\right) \]
\[ \times P_{l'}^{u+u+1} \left(\mu\right) \frac{d\mu}{2}. \tag{46} \]

Again the two upper and two lower signs are to be taken together.

We find also that
\[ K\left(n, l, l - \frac{1}{2}, -\left(\frac{u}{u' + 1}\right); n', l', l' - \frac{1}{2}, -\left(\frac{u'}{u'} + 1\right)\right) \]
\[ = \sum b_k \left(l, l - \frac{1}{2}, -\left(\frac{u}{u' + 1}\right); l', l' - \frac{1}{2}, -\left(\frac{u'}{u'} + 1\right)\right) \]
\[ G_k(n, -(l + 1); n', -(l' + 1)), \tag{47} \]
where
\[ b_k \left(l, l - \frac{1}{2}, -\left(\frac{u}{u' + 1}\right); l', l' - \frac{1}{2}, -\left(\frac{u'}{u'} + 1\right)\right) \]
\[ = b_k \left(l - 1, l - \frac{1}{2}, -\left(\frac{u}{u' + 1}\right); l' - 1, l' - \frac{1}{2}, -\left(\frac{u'}{u'} + 1\right)\right) \tag{48} \]
for all four possible combinations of \( u, -(u + 1); u', \) and \(-(u' + 1)\).

There are two remaining different types of integral,
\[ K\left(n, l, l + \frac{1}{2}, -\left(\frac{u}{u' + 1}\right); n', l', l' - \frac{1}{2}, -\left(\frac{u'}{u'} + 1\right)\right) \]
and
\[ K\left(n, l, l + \frac{1}{2}, -\left(\frac{u}{u' + 1}\right); n', l', l' - \frac{1}{2}, -\left(\frac{u'}{u'} + 1\right)\right) \]
where, in each case, the two upper and two lower signs are to be taken together. For the first,
\[ K\left(n, l, l + \frac{1}{2}, -\left(\frac{u}{u' + 1}\right); n', l', l' - \frac{1}{2}, -\left(\frac{u'}{u'} + 1\right)\right) \]
\[ = \sum b_k \left(l, l + \frac{1}{2}, -\left(\frac{u}{u' + 1}\right); l', l' - \frac{1}{2}, -\left(\frac{u'}{u'} + 1\right)\right) \]
\[ G_k(n, l; n', -(l' + 1)), \tag{49} \]
where
\[
b_k \left( l, l + \frac{1}{2}, -\frac{u}{u+1}; l', l' - \frac{1}{2}, -(u'+1) \right)
= \frac{(l-u)!}{(l+u+1)!} \frac{(l'-u'-1)!}{(l'+u')!} \frac{(k+|u'-u|)!}{(k+|u' - u|)!}
\times \int_{-1}^{1} \{l+u+1\} \{l'-u\} P_{l}^{u} (\mu) P_{l'}^{u'} (\mu)
- P_{l+1}^{u+1} (\mu) P_{l'+1}^{u'+1} (\mu) \} P_{k}^{u'+u+1} (\mu) \frac{d\mu}{2} \] .
\quad (50)

For the second
\[
K \left( n, l, l + \frac{1}{2}, -\frac{u}{u+1}; n', l', l' - \frac{1}{2}, -(u'+1) \right)
= \Sigma b_k \left( l, l + \frac{1}{2}, -\frac{u}{u+1}; l', l' - \frac{1}{2}, -(u'+1) \right) G \left( n, l; n', l' \right),
\quad (51)

where
\[
b_k \left( l, l + \frac{1}{2}, -\frac{u}{u+1}; l', l' - \frac{1}{2}, -(u'+1) \right)
= \frac{(l-u)!}{(l+u+1)!} \frac{(l'-u'-1)!}{(l'+u')!} \frac{(k+|u'+u+1|)!}{(k+|u' + u+1|)!}
\times \int_{-1}^{1} \{l'-u\} P_{l+1}^{u+1} (\mu) P_{l'}^{u'} (\mu)
+ (l+u+1) P_{l}^{u} (\mu) P_{l'}^{u'} (\mu) \} P_{k}^{u'+u+1} (\mu) \frac{d\mu}{2} \] .
\quad (52)

The four different types of \( b \) given by (43), (46), (50), and (52) have been evaluated for all pairs of \( s, p, d \) wave functions and the values of all the \( b \)'s derivable from them are given in Table II.

To show the relation of our results to the corresponding results of the non-relativistic treatment, it is desirable to adapt the conventional notation which uses the letters \( s, p, d, \ldots \) for wave functions with \( l = 0, 1, 2, \ldots \); we shall distinguish those for which \( j = l - \frac{1}{2} \) by a bar, thus:

\[
\begin{array}{cccccc}
\text{l} & s & p & \bar{p} & d & \bar{d} \\
\bar{l} & 0 & 1 & 1 & 2 & 2 \\
\end{array}
\]

In Table I the groups of values for \( u, u' \) may be taken together in any of the possible combinations. In Table II only the values on the same level are to be taken together.

4—We now construct a table of the total coefficients of the \( F_k (n, l; n', l') \) and \( G_k (n, l; n', l') \) in the expression (33) for the interaction energy, for
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<th>$l'$</th>
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an atom built up of completed sub-groups, up to and including \(d\) and \(\bar{d}\) electrons. With the aid of this it is possible to construct very simply the expression for the total energy of any atom not containing \(f\) or higher electrons. We denote a sub-group by \((ns)\), \((np)\) \((n\bar{p})\), etc. The numbers opposite \((ns)\), for example, denote the coefficients of the \(F_k(n, 0; n, 0)\) or \(G_k(n, 0; n, 0)\) due to interactions within the \((ns)\) shell. The numbers opposite \((ns)\) \((n'p)\) denote the coefficients of the \(F_k(n, 0; n', 1)\) or \(G_k(n, 0; n', 1)\) due to interactions between the \((ns)\) and \((n'p)\) shells. In such expressions as \((np)\) \((n'p)\), \(n \neq n'\), but in those like \((ns)\) \((n'p)\), \(n\) and \(n'\) can take all values.

In the non-relativistic case there is no distinction between the four quantities

\[
F_k(n, -(l + 1); n', -(l' + 1)) \quad \text{or} \quad G_k(n, -(l + 1); n', -(l' + 1))
\]
The Relativistic Self-Consistent Field

If we put these four $F$’s equal to each other, and similarly the four $G$’s equal, the sums of the coefficients for the interaction of two completed whole groups are the same as the corresponding sums taken from Slater’s tables. This provides a useful check on the calculations. The coefficients for interactions within a group are quite different from the non-relativistic ones, as we should expect, since the classification of wave functions within a group is quite different.

5—We now give an example of the derivation of the wave equations. The complete expression for the energy is the sum of terms of the types in (32) and (34). We obtain the equations for the radial wave functions for the $2p$ and $2\bar{p}$ states of neutral Cu (29). This is sufficient to bring out all the important features of the method.

In the expression for the total energy we vary $P_{2,1}$, $P_{2,-2}$, $Q_{2,1}$, $Q_{2,-2}$ separately, subject to the normalizing conditions (29) and (30) for $n = 2$, $l = 1$, and the orthogonal conditions (31) for $n = 2$, $l = 1$, $n = 3$, $l = 1$. Before performing the variation all integrals must be written in a form symmetrical in the two variables $r_1$ and $r_2$. The $G$’s are already in such a form, but, when $(n, l)$ $(n', l')$ are different, $F_k(n, l; n', l')$ must be written as half the sum of (38) and (38) with $r_1, r_2$ interchanged. Similarly (32) must be re-written in a form symmetrical in $r_1, r_2$.

When $Q_{n,l}(r_1)$ only is varied,

$$
\delta F_k(n, l; n', l') = 2 \int \int Q_{n,l}(r_1) \delta Q_{n,l}(r_1) \left[ P_{n,l}^2(r_2) + Q_{n,l}^2(r_2) \right] \frac{r(a)^k}{r(b)^{k+1}} dr_1 dr_2.
$$

We write

$$
\int \left[ P_{n,l}^2(r_2) + Q_{n,l}^2(r_2) \right] \frac{r(a)^k}{r(b)^{k+1}} dr_2 \text{ as } V_k(n', l' | r_1).
$$

Similarly

$$
\delta G_k(n,l; n', l', s) = \int \int Q_{n,l}(r_1) \delta Q_{n,l}(r_1) \left[ P_{n,l}^2(r_2) P_{n,l}(r_2) + Q_{n,l}(r_2) Q_{n,l}(r_2) \right] \frac{r(a)^k}{r(b)^{k+1}} dr_1 dr_2,
$$

and we write

$$
\int \left[ P_{n,l}(r_2) P_{n,l}(r_2) + Q_{n,l}(r_2) + Q_{n,l}(r_2) \right] \frac{r(a)^k}{r(b)^{k+1}} \text{ as } V_h(n, l; n' l' | r_1).
$$

We obtain similar expressions when $P_{n,l}(r_1)$ only is varied. The equations
for the 2p wave-functions obtained by varying \(Q_{2.1}(r_1)\) and \(Q_{2.2}(r_1)\) independently become

\[
\frac{dP_{2.1}}{dr} = \frac{2}{r} P_{2.1} + \left( c - \frac{\varepsilon_{(2.1)}}{c} - \frac{Z}{cr} \right) Q_{2.1} - \frac{\varepsilon_{(2.1; 3.1)}}{c} Q_{3.1} \\
+ \frac{1}{c} \left[ 2 \sum_{n=1}^{3} V_n(n, 0, 1; r) + V_0(4, 0, 1; r) + 3V_0(2, 1; 1; r) + 2V_0(2, 1; -2; 1; r) \right. \\
- \frac{1}{25} V_2(2, 1; 1; r) + 4V_0(3, 1; 1; r) + 2V_0(3, -2; 1; r) \\
\left. + 6V_0(3, 2; 1; r) + 4V_0(3, -3; 1; r) \right] Q_{2.1} \\
- \frac{1}{c} \left[ 1/3 \sum_{n=1}^{3} V_1(n, 0, 2, 1; 1; r) Q(n, 0) + 1/6 V_1(4, 0, 2, 1; 1; r) Q_{4.0} \\
+ 2/25 V_2(2, 1; 2, 1; 1; r) Q_{2.1} + 1/5 V_2(2, 1; 2, -2; 1; r) Q_{2.2} \\
+ \{V_0(3, 1; 2, 1; 1; r) + 1/5 V_2(3, 1; 2, 1; 1; r)\} Q_{3.1} \\
+ 1/5 V_2(3, -2; 2, 1; 1; r) Q_{3.2} \\
+ \{3/5 V_1(3, 2; 2, 1; 1; r) + 6/35 V_3(3, 2; 2, 1; 1; r)\} Q_{3.2} \\
+ \{1/15 V_1(3, -3; 2, 1; 1; r) + 9/35 V_3(3, -3; 2, 1; 1; r)\} Q_{3.3} \right] = 0 \text{ (57)}
\]

\[
\frac{dP_{2.2}}{dr} = \frac{1}{r} P_{2.2} + \left( c - \frac{\varepsilon_{(2.2)}}{c} - \frac{Z}{cr} \right) Q_{2.2} - \frac{\varepsilon_{(2.2; 3.2)}}{c} Q_{3.2} \\
+ \frac{1}{c} \left[ 2 \sum_{n=1}^{3} V_n(n, 0, 1; r) + V_0(4, 0, 1; r) + 4V_0(2, 1; 1; r) + V_0(2, -2; 1; r) \right. \\
+ 4V_0(3, 1; r) + 2V_0(3, -2; 1; r) + 6V_0(3, 2; 1; r) + 4V_0(3, -3; 1; r) \right] Q_{2.2} \\
- \frac{1}{c} \left[ 1/3 \sum_{n=1}^{3} V_1(n, 0, 2, 1; 1; r) Q_{n.0} + 1/6 V_1(4, 0, 2, 1; 1; r) Q_{4.0} \\
+ 2/5 V_2(2, 1; 2, -2; 1; r) Q_{2.1} + V_0(3, -2; 2, -2; 1; r) Q_{3.2} \\
+ 2/5 V_2(3, 1; 2, -2; 1; r) Q_{3.1} + 2/3 V_1(3, -3; 2, -2; 1; r) Q_{3.2} \\
+ 3/7 V_3(3, 2; 2, -2; 1; r) Q_{3.2} \right] = 0 \text{ (58)}
\]

\(\varepsilon_{(2.1)}, \varepsilon_{(2.2)}, \varepsilon_{(3.1)}, \varepsilon_{(3.2)}\) and \(\varepsilon_{(2.2; 3.2)}\) are different undetermined parameters. The two corresponding equations for \(Q_{2.1}\) and \(Q_{2.2}\) are obtained by varying \(P_{2.1}\) and \(P_{2.2}\) independently.
The Relativistic Self-Consistent Field

If we put $P_{n, i} = P_{n, i-1}$, $Q_{n, i} = Q_{n, i-1}$ as in the non-relativistic treatment, equations (57) and (58) become the same except for the second term and the terms arising from interactions within the $(2p)$ group. These terms are outlined in the equations. The relativistic self-consistent field equations without exchange are derived from (57) and (58) by omitting terms in $Q$'s other than $Q_{2, 1}$ and $Q_{2, -2}$.

In conclusion, it is a pleasure to record my thanks to Professor D. R. Hartree, F.R.S., for suggesting the possibility of this extension of the self-consistent field method, and for his interest and criticism during the progress of the work.

Summary

A relativistic treatment of a many-electron atom on the lines of the self-consistent field method with "exchange," is developed. Magnetic interactions and retardation effects are, for the present, neglected. Tables are given from which the expression for the total energy of an atom containing $s$, $p$, $d$ electrons may be constructed. An example is given of the derivation of the relativistic self-consistent field equations, including "exchange" terms, by means of a variation principle.