Scattering of Radiation by Electrons in Relativistic Quantum Mechanics

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(Received July 30, 1951)

The theory of the scattering of radiation by Dirac electrons is revised and extended. Assuming negative energy states unoccupied, a formula for the cross section of coherent scattering of very hard quanta is derived. It is, furthermore, shown that the previously claimed and accepted one-to-one correspondence of the matrix elements for the cases of free or occupied negative energy states is generally untrue. It can be proved that for moderately small quanta the cross sections of coherent and incoherent scattering by bound electrons are approximately the same in the case of unoccupied negative energy states and in the pair theory proper. Characteristic differences are shown to exist for very hard radiation. The historical development of the problems here treated is also discussed.

I. INTRODUCTION

THE treatment of coherent x-ray scattering as presented in well-known textbooks[1] goes back to papers by Dirac[2] and Waller,[3] in which for the first time a relativistic theory of these phenomena was presented. Waller's paper[3] limits itself to the treatment of coherent scattering for incident frequencies whose $h\nu$ is large compared with the binding energy of the electron but small compared with mc^2.

The essential point in the relativistic theory is the treatment of the transitions to and from intermediate states of negative energy. In particular, the question arises as to whether the two assumptions: negative energy states free or occupied, lead to the same results for the scattering amplitude. Dirac,[2] in the paper quoted, gave a general proof, according to which there exists a one-to-one correspondence of the matrix elements for the two versions of the theory. The result, therefore, should be generally independent of any assumption as to whether the states of negative energy are empty or occupied. We shall, in future, refer to these two assumptions respectively as scheme I and scheme II.

In a brief communication[4] we presented a revision of these arguments customarily accepted. It was shown that no one-to-one correspondence of the various matrix elements exists in general if the exclusion principle is taken into account properly. We furthermore pointed out that the relation between schemes I and II becomes rather difficult to visualize if the interaction between the electrons is taken into account properly, and announced a more detailed treatment by us in a later publication.

The present paper contains a more complete elaboration of the ideas sketched in our first note. We here extend the treatment to the discussion of high frequency and inelastic scattering on the basis of scheme I as well as scheme II, and show how for certain cases agreement

between the two schemes can be analytically obtained. We also discuss deviations between the two schemes for special scattering problems.

Since we announced our views on this question, and our forthcoming detailed treatment, the problems raised by us have attracted the attention of two authors who have presented their versions already.[5] We shall here proceed with the exposition of our theory and reserve some comparative remarks for the closing section of this paper.

The present paper divides itself up as follows. In Sec. II, the coherent scattering of hydrogen for $h\nu \gg mc^2$ is presented as based on scheme I. Section III contains a detailed criticism of the present views as presented in the literature and text books. In Sec. IV, the approximate equivalence of schemes I and II is shown for those cases in which the interaction between the electrons is neglected. In Sec. V, we show that the one-electron treatment is insufficient for both schemes I and II, and present in Sec. VI a general method based on scheme II for coherent and incoherent scattering. Section VII contains a discussion of the scattering of very large quanta according to scheme II, while finally in Sec. VIII the differences are examined between earlier theories and the results obtained in this investigation.

II. THE SCATTERING OF LARGE QUANTA ACCORDING TO SCHEME I

The differential cross section for coherent scattering by a single atomic electron may be written in the form

$$d\sigma = (e^2/mc^2)^2 d\Omega |A_1{}^+ + A_1{}^-|^2. \qquad (2.1)$$

The symbols in Eq. (2.1) are self-explanatory apart from the partial amplitudes $A_1{}^+$ and $A_1{}^-$, which will be defined subsequently.

The quantity $A_1{}^+$ shall denote in scheme I as well as in scheme II the scattering amplitude due to transitions which involve positive energy states only. Defining the matrix elements M, M' through the Eqs. (2.3), we can

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write for $A_1{}^+$ the expression,

$$A_1{}^+ = \sum_{E>0} \left(\frac{M_{E_0E}(-k_0)M'_{EE_1}(k)}{E_0+k_0-E} \right.$$

$$\left. + \frac{M'_{E_0E}(k)M_{EE_1}(-k_0)}{E_0-k-E} \right). \quad (2.2)$$

In Eq. (2.2), E_0 represents the energy of the original bound state, E the energy in the intermediate state, while the vectors $\mathbf{k}_0$, $\mathbf{k}$ are the propagation vectors of the incident and scattered radiation; in the case of coherent scattering $k_0 = k$, $E_1 = E_0$.

In scheme I, the partial scattering amplitude $A_1{}^-$ is the same as $A_1{}^+$ except that the summation must be extended over negative values of E. We finally give the definition of the matrix elements,

$$M_{E_0E}(-k_0) = \int \psi_{E_0}{}^*(\boldsymbol{\alpha} \cdot \mathbf{e}_0)\psi_E e^{-i\mathbf{k}_0 \cdot \mathbf{r}} dV,$$

$$(2.3)$$

$$M'_{EE_1}(k) = \int \psi_E{}^*(\boldsymbol{\alpha} \cdot \mathbf{e})\psi_{E_1} e^{i\mathbf{k} \cdot \mathbf{r}} dV.$$

The matrix element M corresponds to the absorption of the incident quantum k_0 whose polarization vector is assumed to be parallel to the unit vector $\mathbf{e}_0$. The matrix element M' refers to the emission of the scattered quantum which is polarized parallel to $\mathbf{e}$. All quantities are expressed throughout this paper in relativistic units, i.e., mc^2 for energy, $\hbar/mc$ for length, and mc for momenta.

In the limiting case of large quanta, since $h\nu \gg mc^2$, terms of the order $1/k_0$ will always be negligible compared with unity. We, furthermore, assume that the generalized fine structure constant $\alpha = Z/137$ will be so small that terms of the order α^2 can be neglected.

An inspection of the matrix elements M and M' entering into $A_1{}^+$ and $A_1{}^-$ makes it obvious that transitions from the bound state will occur only to such intermediate states ψ_E which have a momentum p which equals the momentum of the light quantum plus a correction of the order of magnitude of the average momentum in the bound state. This means that

$$\mathbf{p} = \mathbf{k}_0 + \mathbf{p}_0 \quad (2.4)$$

with $p_0 \cong O(\alpha)$; and since $k_0 \gg p_0$ we have

$$p_0 \cong k_0 + (\mathbf{k}_0 \cdot \mathbf{p}_0)/k_0 \cong k_0 + O(\alpha). \quad (2.5)$$

The energy denominator $E_0 + k_0 - E$, therefore, takes on the approximate value

$$E_0 + k_0 - p, \quad \text{to} \quad O(1/k_0) \quad (2.6)$$

or,

$$E_0 - (\mathbf{k}_0 \cdot \mathbf{p}_0)/k_0, \quad (2.7)$$

where we replace $E_0 = (1-\alpha^2)^{\frac{1}{2}}$ by one, since α^2 is being neglected consistently. The term $(\mathbf{k}_0 \cdot \mathbf{p}_0)/k_0$ in the sum over intermediate states can also give rise to a correction

of $O(\alpha^2)$, which is also neglected. The energy denominator $E_0 + k_0 - E$ may vanish at certain points of the integration range over E. This does not cause any divergencies; in fact, a more detailed study shows that these points do not contribute appreciably to the values of the scattering amplitude. The reason for this can be found in a simple argument referring to the method of variation of constants which underlies the derivation of all our expressions for $d\sigma$. A more correct formulation would show that the population of the initial state actually decreases like $\exp(-\Gamma t)$, where the quantity Γ with which we are familiar from the theory of line breadth was neglected in the derivation of $d\sigma$. Otherwise, the energy denominator would have had the form

$$E_0 + k_0 - E + i\Gamma/2 \quad (2.8)$$

and would never have vanished. Integration over this region containing an apparent singularity shows that it contributes to the value of A only a term which is proportional to a higher power of α^2.

The second term in Eq. (2.2) corresponds to an inverted order process, emission followed by absorption. The energy denominator, therefore, becomes of the order $E_0 - k_0 - E$, which allows us to neglect this term as compared to the first, since the matrix elements in the numerator are similar in both cases except that $-k_0$ and k are interchanged. We, therefore, arrive with these simplifications at the following expression for $A_1{}^+$, $A_1{}^-$:

$$A_1{}^+ \cong \sum_{E>0} M_{E_0E}(-k_0)M'_{EE_0}(k),$$

$$A_1{}^- \cong \sum_{E<0} M'_{E_0E}(k)M_{EE_0}(-k_0). \quad (2.9)$$

Using the completeness theorem and the well-known factor

$$\tfrac{1}{2}(1 + H/|E|), \quad (2.10)$$

we can extend our summation now over all values of E (negative as well as positive). The sharp dependence of the matrix elements in Eq. (2.9) on p allows us to write

$$1/|E| \cong 1/k_0, \quad (2.11)$$

so that the factor (2.10) can be written in the form

$$\tfrac{1}{2}(1 + H/k_0). \quad (2.12)$$

Here, H is the Hamiltonian operator defined by the Dirac equation $H\psi = E\psi$:

$$H = -[\boldsymbol{\alpha} \cdot (1/i) \,\mathrm{grad} + \beta - V]. \quad (2.13)$$

Now, the insertion of Eq. (2.12) into Eq. (2.9) leads to

$$A_1{}^+ \cong \sum_{E \gtrless 0} \int \psi_{E_0}{}^*(\boldsymbol{\alpha} \cdot \mathbf{e}_0)e^{-i\mathbf{k}_0 \cdot \mathbf{r}}\tfrac{1}{2}(1 + H/k_0)\psi_E dV$$

$$\times \int \psi_E{}^*(\boldsymbol{\alpha} \cdot \mathbf{e})e^{i\mathbf{k} \cdot \mathbf{r}}\psi_{E_0} dV \quad (2.14)$$

$$\cong \int_E \psi_0(\boldsymbol{\alpha} \cdot \mathbf{e}_0)e^{-i\mathbf{k}_0 \cdot \mathbf{r}}\tfrac{1}{2}(1 + H/k_0)(\boldsymbol{\alpha} \cdot \mathbf{e})$$

$$\times e^{i\mathbf{k} \cdot \mathbf{r}}\psi_{E_0} dV; \quad (2.15)$$

and since according to Eq. (2.13),

$$He^{i\mathbf{k}\cdot\mathbf{r}} = e^{i\mathbf{k}\cdot\mathbf{r}}(H - \boldsymbol{\alpha}\cdot\mathbf{k}), \qquad (2.16)$$

we have, with the abbreviation

$$\mathbf{q} = \mathbf{k}_0 - \mathbf{k} \qquad (2.17)$$

$$A_1{}^+ \cong \int \psi_{E_0}{}^*(\boldsymbol{\alpha}\cdot\mathbf{e}_0)e^{-i\mathbf{q}\cdot\mathbf{r}}$$

$$\times \tfrac{1}{2}(1 + (H - \boldsymbol{\alpha}\cdot\mathbf{k})/k_0)(\boldsymbol{\alpha}\cdot\mathbf{e})\psi_{E_0}dV. \qquad (2.18)$$

In the integrand of Eq. (2.18) we can neglect the whole term

$$(\boldsymbol{\alpha}\cdot\mathbf{e}_0)[(H - \boldsymbol{\alpha}\cdot\mathbf{k})/k_0](\boldsymbol{\alpha}\cdot\mathbf{e}). \qquad (2.19)$$

The part of the numerator containing H is independent of k_0; and this part is, therefore, small of the order $1/k_0$, while the other term

$$(\boldsymbol{\alpha}\cdot\mathbf{e}_0)(\boldsymbol{\alpha}\cdot\mathbf{k})(\boldsymbol{\alpha}\cdot\mathbf{e})/k_0 \qquad (2.20)$$

contains an odd number of α factors, and, therefore, vanishes for bound stationary states.

Our expression for $A_1{}^+$, therefore, takes on the form

$$A_1{}^+ \cong \frac{1}{2} \int \psi_{E_0}{}^*(\boldsymbol{\alpha}\cdot\mathbf{e}_0)(\boldsymbol{\alpha}\cdot\mathbf{e})e^{-i\mathbf{q}\cdot\mathbf{r}}\psi_{E_0}dV. \qquad (2.21)$$

The partial scattering amplitude $A_1{}^-$ can be treated in an entirely similar manner; it turns out only during the derivation that the processes of emission and absorption are interchanged, which means that in the final formula $\mathbf{e}_0$ must be replaced by $\mathbf{e}$ and vice versa. Now,

$$\tfrac{1}{2}[(\boldsymbol{\alpha}\cdot\mathbf{e}_0)(\boldsymbol{\alpha}\cdot\mathbf{e}) + (\boldsymbol{\alpha}\cdot\mathbf{e})(\boldsymbol{\alpha}\cdot\mathbf{e}_0)] = (\mathbf{e}_0\cdot\mathbf{e}), \qquad (2.22)$$

which, therefore, gives

$$A_1 = A_1{}^+ + A_1{}^-$$
$$\cong (\mathbf{e}_0\cdot\mathbf{e}) \int \psi_{E_0}{}^*\psi_{E_0}e^{-i\mathbf{q}\cdot\mathbf{r}}dV. \qquad (2.23)$$

The integral expression for the scattering amplitude exhibits the usual form factor as originally derived by Waller for the scattering of very small quanta. No further discussion of A_1 seems indicated in this connection, except that attention should be called here to a point which acquires even greater significance in scheme II. For sufficiently large values of q, that means for scattering angles larger than α/k_0, the form factor in Eq. (2.23) becomes quite small (of the order of a high power of α). Since all terms of the order α^2 have been consistently neglected in the derivation given, we cannot be sure that our final result is correct at large angles, where terms of the order α^2 become dominant.

It is easy to see how one can extend the treatment to the case of many electrons.

III. GENERAL REMARKS ON THE RELATION BETWEEN SCHEMES I AND II

It has first been argued by Dirac[2] and since accepted by Waller[3] and in various textbooks[1] that there exists a one-to-one correspondence between the matrix elements leading to intermediate states of the two schemes. The argument for this statement runs about as follows:

If the intermediate states are of positive energy, then the contributions are obviously the same for both schemes. If, on the other hand, the intermediate state is one of negative energy according to scheme I, then it gives rise to an expression of the type,

$$A_1{}^- = \sum_{\epsilon < 0} \frac{M_{E_0\epsilon}(-k_0)M'_{\epsilon E_1}(k)}{E_0 + k_0 - \epsilon} + \text{Em-Abs.} \qquad (3.1)$$

Here, the electron goes first from its state of positive energy E_0 to the intermediate state of negative energy ϵ, the matrix element being $M_{E_0\epsilon}$, and then it passes from the state of negative energy ϵ to the final state E_1. The energy denominator is obviously given by $E_0 + k_0 - \epsilon$.

If, on the other hand, the negative energy states are filled (scheme II), then Dirac[2] studies the following process.

He considers an electron passing first from the negative energy state ϵ to the final state E_1, and then another electron from its initial state E_0 to the vacated state of negative energy ϵ. The energy denominator in this case is the same as above. Obviously, these two expressions are equal; and if we sum over all intermediate states of negative energy, the total contribution to the scattering amplitude is the same in both cases, since all individual matrix elements are identical, even if changed in order. This argument of Dirac, was, for example, used for the calculation of the relativistic Compton effect and led to satisfactory agreement with experiment.

It was now pointed out by us[4] that as correct as this argument may be for the case of free electrons (Compton effect), it becomes inapplicable when we are dealing with coherent scattering or the incoherent scattering by bound electrons. It is very clear that in the case of coherent scattering the inverted order of transitions proposed by Dirac is just as forbidden by the exclusion principle as is the original arrangement of terms. The final state to which the electron of negative energy should pass is identical with the initial state, and therefore, occupied. All these matrix elements, therefore, do not exist in scheme II.

While in the case now discussed the difficulty arises primarily from the exclusion principle and only secondarily from the fact that scheme II always leads to a $Z+1$ electron problem, while scheme I is always a Z electron problem, the case is slightly different for the incoherent scattering by bound electrons. All the principal points can here, as well as in the case of coherent

scattering, be understood by an analysis of the one-electron problem (for example, H). Consider, for example, the incoherent scattering in which the electron is transferred from the ground state to the second excited state. Here, it would in principle be possible to invert the scheme I transitions as sketched by Dirac to lead to a scheme II transition. But the difficulty is now of the following nature. In scheme I, we are always dealing with a one-electron problem, while in scheme II the intermediate state would be formed in such a way that we have the hydrogen nucleus surrounded by two electrons, one in the ground state and one in the second excited state. This intermediate state exists only if, most unrealistically, the interaction between the electrons is neglected. Otherwise, essentially only intermediate states with one bound and one excited electron in the continuum can occur. There is, therefore, no identity of the individual matrix elements of scattering for the two schemes, not so much on account of the exclusion principle, but on account of the fact that certain matrix elements exist in the one- but not in the two-electron problem.

It is very clear that this difference in the number of electrons occurring in the intermediate states of positive energy constitutes a fundamental difference between the two schemes, also for all coherent scattering processes. The treatment, according to scheme II, will, therefore, have to take into account not only the exclusion principle, but also the change in the number of electrons; that is, the different effective fields and the eigenfunctions corresponding to them. The principal difficulty of the treatment which, therefore, requires various methods, lies in the fact that this effective field is not a constant; that means that it depends on the different intermediate states. It, therefore, becomes advisable to proceed in the treatment of scheme II in various steps of approximation, isolating the changes between the two schemes. We, therefore, treat first in Sec. IV the changes brought about by the Pauli principle alone, neglecting unrealistically the interaction between the electrons, while later on in the paper we include these interactions and their possible influence on the form factor. We have already pointed out in our first note[4] that any changes between the two schemes can be expected to show themselves, if at all, in the form factor of the scattering amplitude.

It is thus proved that the individual matrix elements of scheme I corresponding to electronic transitions from an occupied state of positive energy to a state of negative energy and back have no counterpart in scheme II, where all matrix elements refer to transitions from occupied states of negative energy to unoccupied states of positive energy and back. The remainder of this paper will now be devoted to an analysis of the question how far the *s u m* over the individual matrix elements, in the absence of their one-to-one correspondence, depends on the use of scheme I or scheme II.

IV. SCATTERING ACCORDING TO SCHEME II. NO ELECTRON INTERACTION

Proceeding by various steps of approximation, we treat in this paragraph the coherent scattering by a nuclear atom (for example, H) under the assumption that interaction between the electrons can be neglected. Furthermore, we drop all terms of the order α^2, k_0^2 or higher. For the electrons in the negative energy states or in the intermediate states of positive energy we now make two different assumptions.

A. The Use of Plane Waves

In this crudest approximation, we allow for interaction only between the nucleus and the bound electron, while treating the electrons in the negative energy states or in their transitions from negative energy states to intermediate states of positive energy, and back, as being perfectly free.

Following the procedure in II, we can again write the total scattering amplitude in the form

$$A_2 = A_2^+ + A_2^-. \tag{4.1}$$

Here, A_2^+ can be neglected for small frequencies ($\alpha^2 mc^2/2 \ll h\nu \ll mc^2$) and can be described by Eq. (2.21) for large frequencies, since the calculation of the positive positive transitions is not influenced, in our approximation, by the electrons in the negative energy states.

A_2^-, on the other hand is now given by the following expression:

$$A_2^- = \sum_A \sum_I \frac{\int \Psi_A^* O \Psi_I \int \Psi_I^* O' \Psi_A}{E_A + k_0 - E_I} + \text{Em-Abs.} \tag{4.2}$$

In the eigenfunctions appearing in Eq. (4.2), the exclusion principle must be taken into account. One is here, strictly, dealing with an infinite number of electrons in the negative energy states, plus one electron in the bound state. Since all electrons are equivalent, it is sufficient to calculate one term in the operator O, which more completely would have to be written as an infinite sum

$$\begin{aligned}
O &= O_1 + O_2 + \cdots \\
&= (\alpha_1 \cdot e_0) e^{-i k_0 \cdot r_1} + \cdots, \\
O' &= O_1' + O_2' + \cdots \\
&= (\alpha_1 \cdot e) e^{-i k \cdot r_1} + \cdots.
\end{aligned} \right\} \tag{4.3}$$

A similar simplification can be carried out for the eigenfunctions $\Psi_{A,I}$. Since Ψ is antisymmetrical in all the electron coordinates, one can limit the treatment in the present case to eigenfunctions referring to two electrons only. The initial eigenfunction will then read

$$\Psi_A = \tfrac{1}{2}\sqrt{2}[\psi_{E_0}(x_1) U_\epsilon(x_2) - \psi_{E_0}(x_2) U_\epsilon(x_1)], \tag{4.4}$$

where $\epsilon < 0$. The intermediate eigenfunction will be given

by

$$\Psi_I = \tfrac{1}{2}\sqrt{2}[\psi_{E_0}(x_1)U_E(x_2) - \psi_{E_0}(x_2)U_E(x_1)], \quad (4.5)$$

where $E > 0$, and the final eigenfunction will agree with the initial eigenfunction. ψ_{E_0} shall denote the eigenfunction of the bound state, while $U_{\epsilon, E}$ are plane wave eigenfunctions. A_2^- thus takes on the form

$$A_2^- = \sum_{\epsilon, E} \frac{\int \Psi_A{}^* O \Psi_I \int \Psi_I{}^* O' \Psi_A}{\epsilon + k_0 - E} + \text{Em-Abs.}, \quad (4.6)$$

where O, O' now contain only two terms.

It should be pointed out that all the eigenfunctions U_ϵ and U_E are mutually orthogonal, while ψ_{E_0} is not strictly orthogonal to any of them; but, according to well-known properties of the Dirac equation,

$$\int \Psi_A{}^* \Psi_I dV_1 dV_2 = -(E_0/\epsilon)(E/E_0) \quad (4.7)$$

is always sufficiently small in relation to

$$\int \Psi_{A,\,I}{}^* \Psi_{A,\,I} dV_1 dV_2. \quad (4.8)$$

Evaluating now exactly the expression corresponding to Eq. (4.6), we find

$$\left. \begin{aligned} M &= \int \Psi_A{}^* O \Psi_I dV_1 dV_2 \\[4pt] &= (E_0|O|E_0)(\epsilon/E) + (\epsilon|O|E) \\[4pt] &\quad - (E_0|O|E)(\epsilon/E_0) - (\epsilon|O|E_0)(E_0/E). \end{aligned} \right\} \quad (4.9)$$

According to the orthogonality mentioned, the term containing (ϵ/E) vanishes and the term $(E_0|O|E)(\epsilon/E_0)$ is small. So we find

$$M \cong (\epsilon|O|E) - (\epsilon|O|E_0)(E_0/E) \quad (4.10)$$

and by analogous procedure a similar expression for the second matrix element

$$M' \cong (E|O'|\epsilon) - (E/E_0)(E_0|O'|\epsilon). \quad (4.11)$$

In the product

$$\left. \begin{aligned} MM' &\cong (\epsilon|O|E)(E|O'|\epsilon) \\[4pt] &\quad + (E_0/E)(E/E_0)(E_0|O|\epsilon)(\epsilon|O|E_0) \\[4pt] &\quad - (E_0|O'|\epsilon)(\epsilon|O|E)(E/E_0) \\[4pt] &\quad - (E_0/E)(E|O'|\epsilon)(\epsilon|O|E_0) \end{aligned} \right\} \quad (4.12)$$

the first term vanishes for all angles of scattering except $\vartheta = 0$. This δ-function has obviously no physical meaning; its contribution is reabsorbed in the incident beam, and it can be put equal to zero.

Summing now over the expression

$$MM'/(\epsilon + k_0 - E), \quad (4.13)$$

we put the denominator $\epsilon + k_0 - E \cong -2$, an approximation valid for $h\nu \ll mc^2$. The problem thus reduces to the summation of the remaining three terms of MM' over E_1, ϵ. Each of these two summations extends within the approximation used over a complete set of wave functions, so that we have

$$\sum_{E > 0} (E_0/E)(E/E_0) \cong 1, \quad (4.14)$$

$$\sum_{\epsilon < 0} (E_0|O'|\epsilon)(\epsilon|O|E_0) \cong (E_0|O'O|E_0). \quad (4.15)$$

In the sum of MM' over ϵ, E each of the three terms in question thus has the same value apart from the sign, so that we finally obtain

$$\sum_{\epsilon,\,E} MM'/(\epsilon + k_0 - E) \cong \tfrac{1}{2}(E_0|O'O|E_0). \quad (4.16)$$

Interchanging the order of the emission and absorption process and adding the result to Eq. (4.16) gives us again, as in Eq. (2.23)

$$A_2 \cong (e_0 \cdot e) \int \psi_{E_0}{}^* \psi_{E_0} e^{-i\mathbf{q}\cdot\mathbf{r}} dV. \quad (4.17)$$

The agreement obtained in Eq. (4.17) with Waller's result is exclusively due to the antisymmetrization of the complete wave function. It cannot be called very surprising, since we have deliberately, for the purpose of analysis, neglected electron interaction.

B. Use of Coulomb Eigenfunction

While still neglecting interaction between the electrons, we describe the state of all electrons by coulombian eigenfunctions under the influence of the nuclear charge. We can again obtain expressions in analogy to Eqs. (4.4), (4.5) and proceed with the evaluation as before, leading up to the expression (4.12) for MM', except that now all wave functions in the matrix elements pertain to coulomb states and are, therefore, strictly orthogonal. A_2^- can now be evaluated with some slight difference only as compared with Eq. (4.16). We thus obtain

$$\left. \begin{aligned} A_2^- = &\sum_{\epsilon,\,E} [(\epsilon|O|E)(E|O'|\epsilon)/(\epsilon + k_0 - E)] \\[4pt] &+ \sum_{\epsilon,\,E} \{ (E_0/E)(E/E^4)(E_0|O'|\epsilon)(\epsilon|O|E_0) \\[4pt] &\quad - (E_0|O'|\epsilon)(\epsilon|O|E)(E/E_0) \\[4pt] &\quad - (E_0/E)(E|O'|\epsilon)(\epsilon|O|E_0)\}/\epsilon + k_0 - E \\[4pt] &\qquad\qquad\qquad\qquad\qquad + \text{Em-Abs.} \end{aligned} \right\} \quad (4.18)$$

In Eq. (4.18), terms of the structure

$$\sum_{\epsilon,\,E} (\epsilon|O|E)(E|O'|\epsilon)/(\epsilon + k_0 - E) \quad (4.19)$$

appear for the first time. They would be present also if we were dealing with a bare nucleus; one could even generalize them by assuming any potential field in the absence of electrons and using the eigenfunctions corresponding to that potential. For the case of a bare nucleus they represent a scattering phenomenon to which attention was first called shortly after the dis-

covery of the pair theory and which has received an approximate treatment by various authors.[6] For small quanta, the value of Eq. (4.19) has been found to be negligibly small indeed, while it must assume very large values for $h\nu \gg mc^2$ and sufficiently small angles of scattering. Estimates in the literature justify our assumption that for moderate values of $h\nu$, Eq. (4.19) can be totally neglected.

We shall, in the future, refer to terms of the structure (4.19) as nuclear terms, without distinguishing the cases of a bare nucleus with a coulomb field or any other constant potential.

The remaining terms in the sum over E in (4.18) now vanish exactly on account of the orthogonality conditions unless $E=E_0$, so one finds Eq. (4.17) for A_2^-. Apart from the nuclear terms which are vanishingly small for $h\nu \ll mc^2$, we have, therefore, again established equivalence between scheme I and scheme II. It has, on the other hand, already become clear that a strict separation in the scattering amplitude of electronic and nuclear terms will, in general, not be feasible if terms of higher order in α^2, k_0^2 are included.

V. DIFFICULTIES OF THE ONE-ELECTRON MODEL TREATMENT

The procedure followed by Waller[3] and also adopted so far in the present paper will now be shown to be not satisfactory if we consider systems with more than one electron. The difficulties appear already in calculations done according to scheme I, although in this case it is sometimes not difficult to justify the approximation used. Analogous calculations according to scheme II, on the other hand, can in general not be carried out on account of mathematical difficulties; this will require the introduction of some new method like that presented in VI.

Turning first to a two-electron problem in scheme I, we want to discuss the scattering of small quanta by, for example, the neutral helium atom; this sufficiently illustrates the essential points. If we write again, as before,

$$A_1 = A_1^+ + A_1^-, \qquad (5.1)$$

one can readily verify that for the present case A_1^+ is again negligible compared with A_1^-.

The formal expression for A_1^- is again given by

$$A_1^- = \sum_I \frac{M_{AI}(-k_0)M_{IA}'(k)}{E_A + k_0 - E_I} + \text{Em-Abs.} \qquad (5.2)$$

The point of importance is now the exact expression for the eigenfunctions in the intermediate state.

Since we are dealing with a two-electron problem, we have to antisymmetrize the eigenfunctions, and we can

[6] M. Delbrueck, Z. Physik **84**, 144 (1933); N. Kemmer, Helv. Phys. beta **10**, 112 (1937); A. Achieser and T. Pomerantschuk, Physik Z. Sowjetunion **11**, 478 (1937); R. Gluckstern and F. Rohrlich, Phys. Rev. **83**, 218 (1951).

in a suitable approximation again assume that the eigenfunctions for the two-electron system are separable into products of eigenfunctions referring to one electron alone. We thus obtain for the eigenfunction of the ground state the expression

$$\Psi_A = \tfrac{1}{2}\sqrt{2}[\psi_{E_1}(x_1)\psi_{E_2}(x_2) - \psi_{E_1}(x_2)\psi_{E_2}(x_1)]. \qquad (5.3)$$

Here, ψ_{E_1, E_2} stands for the coulombian eigenfunctions of opposite spin for the ground state corresponding to an effective nuclear charge $Z-s$. It is well known from the study of light elements that such an eigenfunction is a good approximation of the actual conditions if $s \cong 0.3$.

Similarly, we write for a representative eigenfunction of an intermediate state

$$\Psi_I = \tfrac{1}{2}\sqrt{2}[\psi_{E_0}(x_1)\psi_\epsilon(x_2) - \psi_{E_0}(x_2)\psi_\epsilon(x_1)]. \qquad (5.4)$$

Here, ψ_ϵ stands for the coulombian eigenfunction of a free electron of negative energy ϵ under the influence of a nuclear charge $Z-1$, while ψ_{E_0} represents the coulombian eigenfunction of a bound electron with a nuclear charge Z. Attention is now called to the fact that the integral

$$(E_{1,2}/E_0) = \int \psi^*_{E_{1,2}}\psi_{E_0}dV, \qquad (5.5)$$

though close to one, is no longer equal to one. If this difference between $\psi_{E_{1,2}}$ and ψ_0 is kept in mind, then a direct transfer of the previously used methods to the two-electron problem would lead to a change in the scattering cross section by the factor $(E_1/E_0)^4$. This can immediately be verified by following through the previous calculations leading to A_1^- if we sum over all intermediate states of negative energy but let—erroneously—the second electron always occupy the ground state of the He+ ion. Correctly, what should be done is a summation over all possible intermediate states, which include excited states of positive energy of the second electron. Written in detail, M_{AI} takes on the form

$$M_{AI} = (E_2|O|\epsilon)(E_1/E_0) - (E_1|O|\epsilon)(E_2/E_c) \\ + (E_1|O|E_0)(E_2/\epsilon) - (E_2|O|E_0)(E_1/\epsilon) \qquad (5.6)$$

with a similar expression for M'. Dropping now small terms of the form $(E_1|O|E_0)(E_2/\epsilon)$ and summing first over ϵ, we find

$$\sum_\epsilon MM'/D \\ \cong \sum_\epsilon \{(E_0/E_1)(E_1/E_0)(E_2|O|\epsilon)(\epsilon|O'|E_2) \\ + (E_0/E_2)(E_2/E_0)(E_1|O|\epsilon)(\epsilon|O'|E_1)\}/ \\ [E_1 + E_2 + k_0 - (E_0 + \epsilon)] \qquad (5.7)$$

or

$$\sum MM'/D \cong \{(E_0/E_2)(E_2/E_0)(E_1|OO'|E_1) \\ + (E_0/E_1)(E_1/E_0)(E_2|OO'|E_2)\}/ \\ (E_1 + E_2 + k_0) \qquad (5.8)$$

where, in the sum over ϵ we have set $E_0 + \epsilon \cong 0$. Now, the

sum over the matrix elements

$$\sum_{E_1>0} (E_0/E_1)(E_1/E_0)$$
$$=\sum_{E_2>0} (E_0/E_2)(E_2/E_0)\cong 1 \quad (5.9)$$

up to terms of the order α^2, as we have already utilized before in IV. The calculation from here on follows exactly the scheme indicated by Waller and will lead again, after putting the energy denominator $E_1+E_2+k_0\cong 2$ and adding the emission-absorption terms, to

$$A_1=(\mathbf{e_0}\cdot\mathbf{e})\left[\int \psi_{E_1}{}^*\psi_{E_1}e^{-i\mathbf{q}\cdot\mathbf{r}}dV \right.$$

$$\left. +\int \psi_{E_2}{}^*\psi_{E_2}e^{-i\mathbf{q}\cdot\mathbf{r}}dV\right]. \quad (5.10)$$

This expression (5.10) constitutes a generalization of the Waller formula for the two-electron case.

It is obvious that in the case of scheme II the various excited states of positive energy have similarly to be taken into account. But a straightforward procedure on this basis does not seem to be practical. Consider, for example, the case of the Li$^+$ ion, where all intermediate states contain three electrons of positive energy. The various excited states do not permit any longer a description utilizing one and the same potential energy; one has to take into explicit account the interaction energy between the electrons and is, therefore, unable to give simple, complete expressions for the matrix elements which describe the transitions to the intermediate states. We have, for example, carried out calculations with an approximate potential constructed in analogy with the Heisenberg potential used in the calculation of excited He terms. We refrain from reproducing these calculations here in any detail, since they clearly show that residual differential effects depending upon the form of the potential for the excited states will be obtained. Since the method developed in VI shows that these differential effects between scheme I and scheme II are, for small values of $h\nu$, not existant, we refrain from a reproduction of these approximate calculations. The whole discussion is here only presented to illustrate the incompleteness of a method which is based on the use of a one-electron model in a constant average potential field.

The difficulties become even more obvious, and in our opinion insoluble, for the simple model-theory if one attempts to study inelastic scattering processes, e.g., the scattering accompanying the transition of a hydrogenic electron from the ground state to some excited state. There does not exist any intermediate state in which the hydrogen nucleus would be capable of binding two electrons, one of them excited, and therefore, no one-electron model procedure is feasible in scheme II. Cases of this type, which require the consideration of all possible states of a two-electron system, can only be calculated with the use of a general method of the kind presented in the following paragraph.

VI. A GENERAL METHOD FOR THE TREATMENT OF THE SCATTERING OF MODERATELY LARGE QUANTA

The case of coherent or incoherent scattering of quanta with $h\nu\ll mc^2$ will now be treated for both schemes with a general method that makes it possible to overcome the various difficulties discussed in the preceding paragraphs. We shall primarily limit the explicit discussion to the scattering by hydrogen; the method permits extension to many-electron problems, but no explicit presentation is given in this paper for reasons of economy of space and also because the generalization, carried out by us, follows well-marked lines.

Obviously, we have again

$$A_1{}^+=A_2{}^+ \quad (6.1)$$

and so want to study first the expression for $A_1{}^-$ which takes on the form

$$A_1{}^-=\sum_{\epsilon<0} \frac{MM'}{E_0+k_0-\epsilon}+\text{Em-Abs.} \quad (6.2)$$

Since we include inelastic scattering, the final state may now in general differ from the initial state. We expand the energy denominator

$$\frac{1}{D}=\frac{1}{E_0+k_0-\epsilon}\cong\frac{1}{2+k_0}\left(1+\frac{\epsilon+2-E_0}{2+k_0}+\cdots\right) \quad (6.3)$$

under the assumption that $|\epsilon+2-E_0|\ll 1$. The summation over $\epsilon<0$ can now be extended over a complete set of hydrogenic states by adding and subtracting the summation over $\epsilon>0$. In this way, the absorption-emission part of $A_1{}^-$ takes on the form

$$\sum_{\epsilon<0} \frac{MM'}{D}\cong\sum_{\epsilon<0} \frac{MM'}{2+k_0}\left(1+\frac{\epsilon+2-E_0}{2}\right) \quad (6.4)$$

$$\left.\begin{aligned}&\cong\frac{1}{2+k_0}\int \psi_0{}^*O\\ &\qquad\times\left(1+\frac{H+2-E_0}{2}\right)O'\psi_1 dV\\ &-\sum_{E>0} \frac{MM'}{2+k_0}\left(1+\frac{E+2-E_0}{2}\right)\end{aligned}\right\}. \quad (6.5)$$

We have here replaced ϵ by the Hamiltonian in the second part of (6.3). It is, furthermore, clear that we had to place the operator H after the first operator O, making it act on ψ_ϵ so as to obtain the proper factor in (6.4). In (6.5) the terms which have to be summed over $E>0$ are, as shown before, small of second order due to the properties of the Dirac matrices contained in them; it is, therefore, only consistent to neglect k_0 in the denominator, and, equally, to put $E+2-E_0$ equal to 2. We now add the emission-absorption terms which

are to be treated similarly, remembering that $E_0 + k_0 = E_1 + k$, and thus finally obtain

$$
\left.
\begin{aligned}
A_1{}^- \cong & \frac{1}{2+k_0} \int \psi_0{}^* O\left(1 + \frac{H+2-E_0}{2}\right) O'\psi_1 dV \\
& + \frac{1}{2-k_0} \int \psi_0{}^* O'\left(1 + \frac{H+2-E_1}{2}\right) O\psi_1 dV \\
& - \sum_{E>0} \left\{ \int \psi_0{}^* O\psi_E dV \int \psi_E{}^* O'\psi_1 dV \right. \\
& \left. + \int \psi_0{}^* O'\psi_E dV \int \psi_E{}^* O\psi_1 dV \right\}
\end{aligned}
\right\}
\quad (6.6)
$$

The later comparison with $A_2{}^-$ makes it advisable to rewrite the first two terms in (6.6). Introducing a commutator

$$C' = HO' - O'H, \quad (6.7)$$

we obtain by elementary matrix algebra

$$O[1 + \tfrac{1}{2}(H+2-E_0)]O' = 2OO' - \tfrac{1}{2}CO' \quad (6.8)$$

and, similarly

$$O'[1 + \tfrac{1}{2}(H+2-E_1)]O = 2O'O + \tfrac{1}{2}O'C \quad (6.9)$$

so that the expression for $A_1{}^-$ may now be put into the form

$$
\left.
\begin{aligned}
A_1{}^- \cong & (2+k_0)^{-1} \int \psi_0{}^*(2OO' - \tfrac{1}{2}CO')\psi_1 dV \\
& + (2-k_0)^{-1} \int \psi_0{}^*(2O'O + \tfrac{1}{2}O'C)\psi_1 dV \\
& - \sum_{E>0} \{M_{E_0E}M'_{EE_1} + M'_{E_0E}M_{EE_1}\}
\end{aligned}
\right\}
\quad (6.10)
$$

In calculating

$$A_2{}^- = \sum_{A,I} \frac{M_{AI}M_{IF}'}{E_A+k_0-E_I} + \text{Em-Abs.} \quad (6.11)$$

with an analogous method, we have to observe several differences from scheme I which have their origin in the fact that we now deal with a two-electron problem. The essential advantage of the method consists, of course, as will be seen, in the fact that we do not require an explicit knowledge of Ψ_I. We can again limit ourselves as far as antisymmetrization is concerned to the consideration of two electrons. We shall assume that the initial energy E_A as well as the expression $E_I - 2$ shall both be small of the second order. This assumption is not quite as obvious as an analogous assumption made in scheme I and will be discussed below. We can then expand the

energy denominator as follows

$$\frac{1}{D} = \frac{1}{E_A + k_0 - E_I}$$

$$\cong \frac{1}{-2+k_0}\left(1 + \frac{2+E_A-E_I}{2} + \cdots\right). \quad (6.12)$$

The summation over intermediate states in (6.11) is meant to extend over all states in which two electrons occupy states of positive energy, while all other electrons occupy states of negative energy. If we now extend the summation over a complete set of Ψ_I, we have added to the allowed intermediate states those in which one electron has a positive energy and all others a negative energy, as well as all those states in which more than two electrons have positive energy. The second addition is insignificant because the matrix elements are all of smaller order of magnitude. The first addition, on the other hand, must be corrected for, because it refers apart from the energy denominator, to intermediate states which are already taken into account in $A^+_{1,2}$. We can, therefore, write the absorption-emission part of $A_2{}^-$ in the following form:

$$
\left.
\begin{aligned}
\sum_{A,I} \frac{MM'}{D} \cong & \frac{1}{-2+k_0} \sum_A \int \Psi_A{}^* O \\
& \times \left(1 + \frac{2+E_A-H}{2}\right) O'\Psi_F dV_1 dV_2 \\
& - \sum' \frac{1}{-2+k_0} M_{AI}M'_{IF} \\
& \times \left(1 + \frac{2+E_A-E_I}{2}\right)
\end{aligned}
\right\}
\quad (6.13)
$$

In $\sum'$ the prime indicates that the summation is to be extended over all excited states of positive energy, leaving all states of negative energy fully occupied.

In the last sum, $E_I = \epsilon + E$, so that we have $E_A - E_I = E_0 - E$. This is small and may, therefore, be neglected, since, as before, the expressions for M and M' are small. We thus arrive at the following expression for

$$
\left.
\begin{aligned}
\sum \frac{MM'}{D} \cong & \frac{1}{-2+k_0} \sum_A \int \Psi_A{}^* O \\
& \times \left(1 + \frac{2+E_A-H}{2}\right) O'\Psi_F dV_1 dV_2 \\
& + \sum_{E>0} MM'
\end{aligned}
\right\}
\quad (6.14)
$$

Apart from the difference in sign, we observe that the sum over $E>0$ is the same as in (6.5) of scheme I.

The assumption leading to (6.12) will now be dis-

cussed more closely. It is, strictly speaking, not justified to assume that E_A and $E_I - 2$ are both small of second order in the transitions considered. So, for example, the assumption turns out to be wrong if the electron in the negative energy states has originally an energy the absolute value of which is very large compared to mc^2. Since we have to sum over all negative energy states, we will encounter an infinity of such electrons. A similar remark could be made with respect to $E_I - 2$.

Nevertheless, for small quanta the assumption still seems to be quite justified. Transitions in which such electrons with exceptionally large energies are involved contribute only to the modified nuclear terms which are assumed to be very small. We can, therefore, be sure that the error introduced is of no significance.

We obtain the complete expression for A_2^- by adding, as before, the similarly treated emission-absorption terms. Before doing this, however, we proceed as follows:

To compare A_1^- and A_2^-, we must evaluate the spur in (6.14). We can write

$$(E_F - H)O' = O'H - HO'. \qquad (6.15)$$

Now the Hamiltonian H can be written in the form

$$H = H_1 + H_2 + V_{12}. \qquad (6.16)$$

Here the interaction with the nuclear field is contained in H_1 and H_2, while V_{12} refers to the electronic interaction. The symmetrical part played by all the electrons clearly shows that

$$\begin{aligned} O'H - HO' &= 2(O_1'H_1 - H_1O_1') \\ &= -2C_1', \end{aligned} \qquad (6.17)$$

where C_1' is defined similarly as in (6.7) by the relation

$$C_1' = H_1O_1' - O_1'H_1. \qquad (6.18)$$

We can thus write for

$$\sum \frac{MM'}{D} \cong \frac{1}{-2+k_0} \sum_A \int \Psi_A{}^* O \\ \cdot 2\left[O_1' + \frac{(2+E_0-E_1)O_1' - C_1'}{2} \right] \Psi_F \\ + \sum_{E>0} MM' \qquad (6.19)$$

and introduce the abbreviation

$$P_1' = O_1' + \tfrac{1}{2}[(2+E_0-E_1)O_1' - C_1']. \qquad (6.20)$$

Recalling that

$$O_1' = (\alpha_1 \cdot \mathbf{e})e^{i\mathbf{k}\cdot\mathbf{r}_1} \qquad (6.21)$$

we note that P_1' contains O', i.e., one Dirac matrix in each term.

We now introduce explicit expressions for Ψ_A and Ψ_F. It is assumed that the wave function is separable in the coordinates of the atomic electron and of the electron

in the negative energy state

$$\Psi_A = \tfrac{1}{2}\sqrt{2}[\psi_0(x_1)U_\epsilon(x_2) - \psi_0(x_2)U_\epsilon(x_1)], \qquad (6.22)$$

$$\Psi_F = \tfrac{1}{2}\sqrt{2}[\psi_1(x_1)U_\epsilon(x_2) - \psi_1(x_2)U_\epsilon(x_1)]. \qquad (6.23)$$

Here ψ_0 and ψ_1 are hydrogenic functions for the initial and final states, respectively, while U_ϵ is an appropriately screened eigenfunction of negative energy. One then obtains

$$\left.\begin{aligned} &\int \Psi_A{}^* O 2P_1' \Psi_F dV_1 dV_2 \\ &= (E_0|OP'|E_1) + (E_0/E_1)(\epsilon|OP'|\epsilon) \\ &\quad + (E_0|P'|E_1)(\epsilon|O|\epsilon) + (E_0|O|E_1)(\epsilon|P'|\epsilon) \\ &\quad - (E_0|OP'|\epsilon)(\epsilon/E_1) - (E_0/\epsilon)(\epsilon|OP'|E_1) \\ &\quad - (E_0|P'|\epsilon)(\epsilon|O|E_1) - (E_0|O|\epsilon)(\epsilon|P'|E_1) \end{aligned}\right\} . \qquad (6.24)$$

Of the eight terms appearing on the right side of (6.24), only three are found to be significant for the coherent case $E_1 = E_0$. The second term here corresponds to the nuclear terms discussed in IV and is again neglected for moderate $h\nu$. In the incoherent case, this term vanishes on account of the orthogonality $(E_0/E_1) = 0$. The third and fourth terms are exchange terms which vanish in the coherent case on account of the property of the Dirac matrices in stationary states, while in the inelastic case, one term vanishes and the other becomes small of the fourth order. The fifth and sixth terms are also small of at least fourth order due to the approximate orthogonality of U_ϵ and $\psi_{0,1}$, combined with the properties of the Dirac matrix elements connecting states of opposite sign of energy. This can perhaps be illustrated by looking at the largest term in OP' for parallel polarization, which will be of the order one. Thus the fifth term becomes of the order

$$(E_0/\epsilon)(\epsilon/E_{0,1}) \lesssim 4\text{th order.} \qquad (6.25)$$

In this way, one eventually finds

$$\int \Psi_A{}^* O 2P_1' \Psi_F dV_1 dV_2 \cong (E_0|OP'|E_1) \\ - (E_0|P'|\epsilon)(\epsilon|O|E_1) - (E_0|O|\epsilon)(\epsilon|P'|E_1). \qquad (6.26)$$

To sum (6.26) over all screened states U_ϵ, $\epsilon < 0$, we extend the sum over a complete set including all $\epsilon > 0$ and subtract the (small) part for $\epsilon > 0$.

$$\sum_A \int \Psi_A{}^* O 2P_1' \Psi_F dV_1 dV_2 \cong - (E_0|P'O|E_1) \\ + \sum_{E>0}\{(E_0|P'|E)(E|O|E_1) \\ + (E_0|O|E)(E|P'|E_1)\}_S. \qquad (6.27)$$

In (6.27), the subscript S indicates that the wave functions U_E differ from those of energy E in (6.6) by virtue of the screening.

Now $\sum_{E>0}$ in (6.27) can be simplified. Since all terms in this sum are already small of second order on account of the properties of the Dirac matrices, we may neglect in the expression P' appearing in them the term E_0-E_1 and simply put

$$P' = 2O' - C'/2 \qquad (6.28)$$

instead of (6.20). Now, since

$$(E_0|C'|E_1) = (1/i)(E_0|\dot{O}'|E_1) \qquad (6.29)$$

$$= (E_0 - E_1)(E_0|O'|E_1), \qquad (6.30)$$

it is clear that all these terms will be not larger than of fourth order and may be dropped. Furthermore, we have

$$\left.\begin{array}{c}(E_0|P'|E)(E|O|E_1)\cong 2(E_0|O'|E)(E|O|E_1)\\ \cong 2M'_{E_0E}M_{EE_1}\end{array}\right\}, \qquad (6.31)$$

and so obtain

$$\left.\begin{array}{c}\sum_A\int \Psi_A{}^*O2P_1'\Psi_FdV_1dV_2\cong -(E_0|P'O|E_1)\\ +2\sum_{E>0}(M_{E_0E}M'_{EE_1}+M'_{E_0E}M_{EE_1})_S\end{array}\right\}. \qquad (6.32)$$

To complete the comparison of A_1^- and A_2^-, we now have to examine the term

$$(E_0|P'O|E_1) \qquad (6.33)$$

Here, the second-order terms in P' must be retained. It is now possible to write out the complete expression for A_2^- combining (6.11), (6.19) and (6.32) and including both sequences of emission and absorption processes

$$\left.\begin{array}{c}A_2^-\cong(2+k_0)^{-1}\int \psi_0{}^*(2OO'-\tfrac{1}{2}CO')\psi_1dV\\ \\ +(2-k_0)^{-1}\int \psi_0{}^*(2O'O+\tfrac{1}{2}O'C)\psi_1dV\\ \\ +\sum_{E>0}(M_{E_0E}M'_{EE_1}+M'_{E_0E}M_{EE_1})\\ \\ -2\sum_{E>0}(M_{E_0E}M'_{EE_1}+M'_{E_0E}M_{EE_1})_S\end{array}\right\}. \qquad (6.34)$$

The results (6.6) and (6.34) for A_1^- and A_2^- appear to differ in the terms $\sum_{E>0}$, but these terms are already small of the second order and their difference is only due to differences in the screening of the wave functions which makes it appear that A_1^- and A_2^- will differ only by terms that are smaller than α^2 or k_0^2 from each other.

VII. THE SCATTERING OF HARD QUANTA ACCORDING TO SCHEME II

The theoretical treatment according to scheme II of the scattering of quanta $h\nu\gg mc^2$ encounters various difficulties by which we were forced to limit ourselves in this paper to the discussion of some important special cases and of some qualitative differences between schemes I and II.

No scheme analogous to the procedure in VI could be

devised for the scattering of very hard quanta; this is due to the fact that simplified expressions for the energy denominator like those used in (6.12) are no longer valid in the case of large quanta. One cannot, therefore, use the general methods of summing over complete sets which form the basis of the procedure in VI.

We proceed, therefore, with the treatment on the basis of a model, keeping well in mind the unsatisfactory features of such an attempt which have been discussed before. We treat here, for purposes of illustration, the scattering by a hydrogen atom. The antisymmetrization, as discussed in IV, has then again to be extended to two electrons only; there is, furthermore, no difference in the calculation of A_1^+ and A_2^+ as given in II.

The eigenfunctions for the initial and intermediate states which have to be used for the purpose of calculating A_2^- can then be written

$$\Psi_A\cong\tfrac{1}{2}\sqrt{2}[\psi_{E_0}(x_1)U_\epsilon(x_2)-\psi_{E_0}(x_2)U_\epsilon(x_1)], \qquad (7.1)$$

$$\Psi_I\cong\tfrac{1}{2}\sqrt{2}[\psi_{E_0}(x_1)U_E(x_2)-\psi_{E_0}(x_2)U_E(x_1)]. \qquad (7.2)$$

In (7.1, 2), the symbol ψ_{E_0} denotes the coulombian eigenfunction of the electron in its ground state. U_ϵ and U_E form together a complete orthogonal system of eigenfunctions of negative and positive energy, respectively, originating from some suitable potential which takes into account the effect of the nucleus as well as that of the electron in the ground state.

For A_2^- we then write in complete analogy to earlier discussions in II and IV.

$$A_2^-\cong\sum_A\sum_I\frac{M_{AI}M_{IA}'}{E_A+k_0-E_I}+\text{Em-Abs}, \qquad (7.3)$$

where

$$E_A=E_0+\epsilon, \quad E_I=E_0+E.$$

Introducing the explicit expressions M, M' for the operators (4.3), we now find for M_{AI} the following expression

$$M_{AI}=(E_0|O|E_0)(\epsilon/E)+(\epsilon|O|E)$$
$$-(E_0|O|E)(\epsilon/E_0)-(\epsilon|O|E_0)(E_0/E), \qquad (7.4)$$

which consists of four terms. The first of these terms is obviously zero.

Constructing a similar expression for M_{IA}' and carrying out the multiplication, we arrive at the following expression for MM'

$$\left.\begin{array}{c}MM'\cong(\epsilon|O|E)(E|O'|\epsilon)\\ +(E_0/E)^2(E_0|O'|\epsilon)(\epsilon|O|E_0)\\ -(E_0|O'|\epsilon)(\epsilon|O|E)(E/E_0)\\ -(E_0/E)(E|O'|\epsilon)(\epsilon|O|E_0)\\ +(E_0|O|E)[(E|O'|\epsilon)\\ -(E/E_0)(E_0|O'|\epsilon)](\epsilon/E_0)\\ +(E_0/\epsilon)[(\epsilon|O|E)\\ -(\epsilon|O|E_0)(E_0/E)](E|O'|E_0)\\ +(E_0/\epsilon)(\epsilon/E_0)(E_0|O|E)(E|O'|E_0)\end{array}\right\}. \qquad (7.5)$$

MM' consists of nine terms, which will now be discussed for two special cases.

a. Scattering into Sufficiently Small Angles

The first term in (7.5) represents the well-known modified nuclear scattering. In the case of very large quanta, the differential scattering cross section due to it alone becomes rather large in the forward direction and can no longer be neglected compared with the ordinary electron scattering.

The following three terms all carry factors of the form (E_0/E). These Fourier coefficients of the eigenfunction describing the ground state, expanded into eigenfunctions which are very similar to plane waves have a sizeable value only for values of E with a momentum which is comparable to αmc. One can now show easily that for sufficiently small angles which will soon be defined more quantitatively these three terms are of the same order of magnitude and are all complete analogs of the generalized Waller terms discussed in II. We illustrate this statement by a simple discussion of the second of these three terms. The same discussion can be almost literally transposed to the other two terms mentioned.

Since (E/E_0) is of the order one only if p_E is of the order α, we have thereby a defined range for E; the same argument, therefore, leads to a range for ϵ which lies in momentum space in the range of $-\mathbf{k}+O(\alpha)$. But the remaining factor in this term, $(\epsilon|O|E)$, will be of order one also only if the range of $\mathbf{p}_E$ overlaps through action of the operator O with the range of $O(\mathbf{k}_0+\mathbf{p}_E)$. This requires, therefore, that

$$\mathbf{p}_E \sim \mathbf{k}_0 + \mathbf{p}_\epsilon \sim \mathbf{k}_0 - \mathbf{k} \sim O(\alpha). \qquad (7.6)$$

If we study the scattering into angles satisfying the condition $|\mathbf{k}_0-\mathbf{k}| \simeq k_0\theta \lesssim \alpha$, the matrix element here discussed will have its maximum value and take on the form of the generalized Waller matrix element given in II; summation over all values of ϵ, E makes this term equal to

$$\left.
\begin{array}{l}
\displaystyle\sum_{\epsilon,E} \frac{-(E_0|O'|\epsilon)(\epsilon|O|E)(E/E_0)}{\epsilon+k_0-E} \\[3mm]
\displaystyle\simeq\sum_{\epsilon<0} \frac{-(E_0|O'|\epsilon)(\epsilon|O|E_0)}{\epsilon+k_0-1} \\[3mm]
\cong(E_0|O'O|E_0)
\end{array}
\right\}. \qquad (7.7)$$

As mentioned before, the same argument holds true for the other terms containing the factor (E/E_0). We have thus rederived the scattering formula presented in II.

Obviously, for this small angle scattering, the remaining five terms in (7.5) are small, since all of them carry a very small factor (E_0/ϵ). One can, therefore, summarize that for sufficiently small angles the scattering amplitude A_2^- of hard quanta is composed by a super-

position of the amplitudes arising from the modified nuclear term and that given in II.

b. Scattering into Large Angles

In this second case, no quantitative discussion is attempted. We know from II that for large angles the form factor of the scattering according to scheme I becomes proportional to a high power of α/k_0. It, therefore, is no longer permissible to neglect terms which are perhaps of the order α^2 in the general formula, since the end result is obtained only by a large size cancellation of the various contributions. One can similarly see quite easily that the three terms carrying factors (E_0/E) which were the leading terms in the case of small angle scattering are no longer equal to each other. The remaining five terms in the expression (7.5) can be calculated only with difficulty, and cannot a priori be considered to be small compared to those terms retained in the case of small angle scattering. One must, therefore, be prepared to find as a result of a calculation left to later endeavors that the wide angle scattering of hard radiation differs considerably from the result suggested by II and may not in general be representable as a simple superposition of generalized Waller terms and modified nuclear terms.

VIII. GENERAL DISCUSSION

We may now perhaps summarize the main results of this investigation. It was proved that up to orders of α^2, k_0^2 the cross section for elastic and inelastic scattering of small quanta is the same in both schemes. The problem of the scattering of hard quanta is in a much less satisfactory state. While it was comparatively easy to extend the treatment for the case of scheme I, we had to limit ourselves to the not quite satisfactory method of a model for scheme II and were unable to transpose the general method used for small quanta. Furthermore, the appearance of modified nuclear terms affects the results appreciably and does not allow us to make, in the present state of the theory, a reliable prediction of the scattering under sufficiently large angles.

There are several points of contact between the paper[5] of Furry's and the present analysis. As to the formalism applied, Furry used recently-developed methods which guarantee the avoidance of divergence difficulties. We did not find it necessary to do so, since in the approximation used we encountered only one divergence, namely the δ function in IV, which obviously has to be put equal to zero.

In contrast to the present paper Furry has treated the transitions of the electron from the negative to the positive intermediate state and back as a one-electron problem under the influence of a constant potential somewhat analogous to the procedure in IVb. We believe to have proved that such a treatment is not satisfactory and is incomplete. The example of inelastic scattering by the H atom shows without calculation how necessary

it is to abandon the simplified concepts and use a general method as introduced by us in VI. We are not certain if Furry wants his results to apply to the scattering of very hard quanta; if this is the case then there exist basic differences with the content of VII.

We want to express the hope that later investigations of a deeper-reaching mathematical nature will lead not only to a formulation as given here, but also to a computation of the differences in the two schemes and thereby present opportunities for an experimental decision between the two forms of the theory, which in our opinion will doubtless show the validity of scheme II.

Reversibility of Quantum Electrodynamics

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(Received May 23, 1951)

The aim of this paper is to re-establish the reversibility of classical electrodynamics in terms of the "expectation values" given by quantum electrodynamics. The reversibility requirement combined with the charge conjugation necessitates that charged fields should obey certain types of statistics. However, the reversibility requirement as such does not determine the statistics, showing that it is the requirement of charge-invariance that has the power to determine the statistics of charged fields. A new interpretation will be given to the old problem concerning the conflict of electromagnetic reversibility *versus* "retarded" potential. Four different kinds of tensors, four different kinds of spinors (pseudospinors), bi-spinors (eight-component spinors) and bi-tensors are introduced as useful representation vectors of the entire congruent group including spatial and temporal inversions.

I. INTRODUCTION

IN connection with the proof that phenomenological irreversibility originates essentially from the process of observation, it seemed to the present author to be of importance to ascertain the complete time-reversibility of quantum mechanics. In an earlier paper,[1] reversibility of the Dirac equation was demonstrated in its one-particle interpretation, and the behavior of the spin, electric moment and magnetic moment of the electron in the "reversed" motion was examined in detail. Then, the reversibility of quantum electrodynamics was proved in the frame-work of Dirac's many-time theory.[2] It was thereafter noticed that the same method can be applied to the theory in which the electron field also is quantized if a correct treatment of charge conjugation is introduced.[3] In all these considerations, it was observed that commutation relations of the field quantities, under certain assumptions, played important roles in the proof of reversibility.

Now that many authors are interested in the problem of necessary general forms of commutation relations, it may be of some interest to publish a summary of the results hitherto obtained by the author, clarifying the relationship between reversibility and commutation relations. In the meantime, Schwinger is reported to have used in his lectures a similar consideration to deduce the commutation relations from the requirement of reversibility.[4] However, since his method as well as his conclusion seems to be at variance with those of the present author, perhaps they may justifiably be presented here.

Against a formal requirement of reversibility objections are often raised to the effect that we can never reverse the direction of time in our actual experience. However, we can formulate the "reversibility" in such a manner that it does not involve any hypothetical inversion of time.

The reversibility of classical point mechanics can be expressed in the following way. Let us call two states of a mechanical system mutually reversed states if particles have the same positions and the opposite velocities. Then the reversibility of mechanics means that, if a mechanical system, which was in the state S_1 at the initial instant ($t=0$), finds itself in the state S_2 at the final instant ($t=t_1$), then the fundamental laws allow for another solution representing the similar system which was in the reversed state of S_2 at the initial instant ($t=0$) and which finds itself in the reversed state of S_1 at the final instant ($t=t_1$).

To extend this notion of reversibility to electrodynamics, we need only to add to the definition of reversed states the condition that the electric field has the same value and the magnetic field has the same absolute value but opposite sign. Then the above statement of reversibility holds again in the Maxwellian theory.

It is to be noted that this concept of reversibility does not invoke any fictional time-reversal. Also, as far as

[1] S. Watanabe, *Le Deuxième Théorème de la Thermodynamique et la Mécanique Ondulatoire* (Hermann et Cie, Paris, 1935).
[2] S. Watanabe, Sci. Pap. Inst. Phys. Chem. Research (Tokyo) 31, 109 (1937).
[3] Unpublished.
[4] Lectures by J. Schwinger, notes taken by M. L. Goldberger.