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# The Theory of Collisions of Electrons with Atoms

G. F. DRUKAREV

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The collision between an electron and an arbitrary atom is considered. The wave function of the system "atom + electron" with given spin is described by the coordinate and spin functions of this system. The coordinate function of the system is constructed from the atomic and one-electron functions in such a way that it possesses in explicit form the correct symmetry properties relative to a transposition of the arguments. A system of integrodifferential equations, similar to the Fock self-consistent field equations have been obtained for the one-electron coordinate functions. These equations can be transformed into integral equations. The angular variables have been separated and integral equations have been obtained for the radial one-electron functions. The integral equations can be simplified if approximate atomic functions are used. The problem is reduced to a system of Volterra integral equations which are suitable both for general investigations and for computations. An analysis of the asymptotic expressions is carried out and formulas are derived for effective cross sections.

## INTRODUCTION

**R**ECENT investigations (see, for example, Ref. 1) have revealed the unsuitability of the Born approximation (and its modification which takes exchange into account --- the method of Born-Oppenheimer) for calculation of collisions of slow electrons with atoms. Especially poor results are obtained in the calculation of the effective cross section for excitation near the threshold in those cases in which exchange effects play a role.

In a number of cases the effective excitation cross section calculated according to the Born-Oppenheimer method exceeds the theoretical limit imposed by conservation of the number of particles. For example, the effective excitation cross section of the 2S level of the hydrogen atom in the antisymmetric case (parallel spins) for 13.5 ev is twice the theoretical limit. For the excitation of the  $2^{3}S$  level of helium at 22.5 ev the cross section computed according to Born-Oppenheimer is 1.1 times the theoretical limit and exceeds experimental values by a factor of 20.

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In the methods of Born and Born-Oppenheimer, the interaction of the electron with the atom is considered weak, and therefore the wave function of the electron is taken in the form of a plane wave. Refinement of the methods of calculation is obtained by consideration of the perturbation of the electronic wave function by the strong field of the atom and by exchange interaction.

Representing the wave function of the system "atom + electron" in the form of a properly symmetrized sum of products of atomic and oneelectron functions, and carrying out the computations based on the use of the Schrödinger equation, one can obtain a system of integro-differential equations for the one-electron functions. These equations, similar to the self-consistent field equations of V. A. Fock, describe the interaction of the electron with the atom. The simplest equations of such form for the elastic collisions of electrons with atoms of hydrogen and helium were first considered by Morse and Ellis<sup>2</sup> and were integrated numerically. For excitation of the 2S level of the hydrogen, and of the  $2^{1}S$  and  $2^{3}S$  levels of the helium atom, such equations were considered in the researches of Massey and Erskine<sup>3</sup> and Massey and Moiseiwitsch<sup>4</sup> which were devoted to the application of variational methods to collision problems.

In 1953 it was shown by the author<sup>5</sup> that the integro-differential equations of the type obtained in Refs. 2 and 3 could be transformed into a system of Volterra integral equations and a system of algebraic equations for certain constants. The integral equations to which the problem reduces are suitable both for general investigations and for computations.

In the present work we consider the general problem of the collision of an electron with an arbitrary atom or ion. An expression for the coordinate wave function of the system "electron + atom" is constructed from atomic functions and one-electron functions which possesses in explicit form the appropriate properties of symmetry relative to a transposition of arguments. In this case some results of Fock<sup>6</sup> are used that are concerned with the waye functions of manyelectron systems. Integro-differential equations are obtained for one-electron functions. The potential energy of interaction of the electron with the atom and the exchange operator are expressed by quantities which are constructed from atomic functions according to the type of the density matrix\*. Integro-differential equations are transformed into integral equations. Separation of angular quantities is carried out and integral equations for the radial functions are obtained.

In practice, the atomic wave functions are expressed approximately in the calculations in the

\* The general equations for the collision of electrons with an atom were also considered by Seaton<sup>7</sup>. However, Seaton began from a wave function system in which the spin and coordinate variables were not separated; therefore, his equations have a symbolic character. form of a combination of products of one-electron functions. If this approximation is used, then the equations for the radial functions reduce to a system of integral equations of the Volterra type and to a system of algebraic equations.

### 1. THE WAVE FUNCTION OF THE SYSTEM "ATOM + ELECTRON"

Let us consider the wave function of the N-electron system  $\Phi(\mathbf{r}_1 \sigma_1, \ldots, \mathbf{r}_N \sigma_N)$ . It must be antisymmetric relative to a permutation of any pair  $(\mathbf{r}_i, \sigma_i)$  and  $(\mathbf{r}_j, \sigma_j)$ . Neglecting spin-orbit interaction, we can subject  $\Phi$  to the condition that it be an eigenfunction of the square of the spin

$$S^2 \Phi = s \left( s + 1 \right) \Phi \tag{1.1}$$

 $(\pi = 1)$ . As Fock<sup>6</sup> has pointed out, the wave function  $\Phi$  satisfying (1.1) can be chosen from the coordinate function  $\Psi(\mathbf{r}_1 \dots \mathbf{r}_k | \mathbf{r}_{K+1} \dots \mathbf{r}_N)$ , where

$$k = \frac{1}{2}N - s, \qquad (1.2)$$

and the spin function  $\chi(\sigma_1 \dots \sigma_k | \sigma_{k+1} \dots \sigma_N)$ which possess definite properties of symmetry relative to permutation of the arguments. (In what follows, we shall write

$$\begin{split} & \Psi(1 \dots k | k + 1 \dots N) \text{and} \chi(1 \dots k | k + 1 \dots N) \\ & \text{in place of } \Psi(\mathbf{r}_1 \dots \mathbf{r}_k | \mathbf{r}_{k+1} \dots \mathbf{r}_N) \text{ and} \\ & \chi(\sigma_1 \dots \sigma_k | \sigma_{k+1} \dots \sigma_N), \text{ or even } \Psi, \chi \text{ where} \\ & \text{these would not lead to misunderstanding.}) \end{split}$$

The function  $\Psi$  is antisymmetric relative to a permutation of arguments up to or after the vertical bar; this can be described with the help of the permutation operator  $P_{ii}$  in the form

$$(1 + P_{ij})\Psi = 0; i, j < k \text{ or } i, j > k.$$
 (1.3)

Moreover,  $\Psi(1 \dots k | k + 1 \dots N)$  possesses the property of cyclic symmetry

$$\left(1-\sum_{j=k+1}^{N}P_{kj}\right)\Psi=0.$$
 (1.4)

The function  $\chi$  is symmetric relative to a permutation of arguments up to or after the vertical bar:

$$(1 - P_{ij})\chi = 0$$
, *i*, *j* < *k* or *i*, *j* > *k*. (1.5)

Following Fock<sup>6</sup>, we construct the expression

$$\Phi = \left[\frac{(N-k)!k!}{N!}\right]^{1/2}$$

$$\times \sum_{\lambda_1 \dots \lambda_k} (-1)^p \Psi'(\lambda_1 \dots \lambda_k \mid \lambda_{k+1} \dots \lambda_N)$$
(1.6)

 $\times \chi (\lambda_1 \ldots \lambda_k | \lambda_{k+1} \ldots \lambda_N),$ 

where  $\lambda_1 \ldots \lambda_N$  is a set of N different numbers from the series  $1 \ldots N$  and P is the parity of the permutation  $\begin{pmatrix} 1 & 2 & \ldots & N \\ \lambda_1 \lambda_2 & \ldots & \lambda_N \end{pmatrix}$ .

By virtue of the properties (1.3)-(1.5) and the relations (1.2), the function (1.6) satisfies the relation (1.1) and possesses the necessary asymmetry property relative to the permutation of  $(\mathbf{r}_i, \sigma_i)$  and  $(\mathbf{r}_j, \sigma_j)$ . The coefficient of the sum in Eq. (1.6) is introduced so that, in the normalization of  $\Psi$  and  $\chi$  to unity,  $\Phi$  will also be normalized to unity.

If we choose  $\chi$  in the form

$$\chi = \beta_1 \dots \beta_k \alpha_{k+1} \dots \alpha_N, \qquad (1.7)$$



where  $\alpha = \delta_{\sigma,1}$ ,  $\beta = \delta_{\sigma,-1}$ then  $\Phi$  will be the eigenfunctions of the operator  $S_z$  which correspond to the eigenvalue s (i.e., the spin of the system is directed along the z axis). The function  $\Psi$  which possesses the properties (1.3) and (1.4) can be obtained by subjecting an arbitrary function of N arguments to symmetrization according to the scheme of

Young pictured in the Figure(Landau and Lifshitz<sup>8</sup>), i.e., we first carry out symmetrization over the variables entering into a row and then alternation over the variables entering into the columns\*. We shall denote such a scheme by the symbol (k; N - K).

As an illustration, we consider the example of a

function of three variables, symmetrized according to the scheme (1; 2). The scheme (1; 2) corresponds to the action of the operator  $(1 - P_{23})$  $(1 + P_{12})$ . It is evident that by using such an operator, we obtain a function which is antisymmetric relative to the permutation of the indices 2 and 3. It is not difficult to prove further that, using the operator  $(1 - P_{12} - P_{13})(1 - P_{23})(1 + P_{12})$  on an arbitrary function of three variables we obtain zero. Thus the function obtained as a result of symmetrization according to the scheme (1; 2) actually possesses the properties of symmetry which ought to be had by  $\Psi(1 | 23)$ .

We return to the problem of interest to us, namely, the construction of a coordinate function system "atom + electron" from atomic and one-electron coordinate functions. For this purpose we consider the particular case  $\Psi(1 \dots k | k + 1 \dots n + 1)$ which is formed from the product of the functions  $\psi(1 \dots j | j + 1 \dots n)$  and F(n + 1).

We note that in the expression for  $\Psi$  there can enter only two types of function  $\psi$ :

$$\psi_1 = \psi(1...k | k + 1...n),$$
 (1.8)

$$\psi_2 = \psi (1 \dots k - 1 \mid k \dots n).$$

This follows from consideration of the Young scheme. Actually, one can obtain the scheme (k; n - k + 1) by adding one cell either in the second column of the scheme (k; n - k) or in the first column of the scheme (k - 1; n - k + 1).

The same result follows from the rule for the addition of momenta. Actually, for a given square of the spin moment of the (n + 1)-electron system. s(s+1), there are two possible states of the *n*electron system:  $s_1 = s - \frac{1}{2}$  and  $s_2 = s + \frac{1}{2}$ . In the first case, in accord with (1.2),  $j_1 = \frac{1}{2}n - (s - \frac{1}{2})$ , in the second,  $j_2 = \frac{1}{2}n - (s + \frac{1}{2})$ . In asmuch as  $k = \frac{1}{2}(n+1) - s$ , then  $j_i = k$ ,  $j_2 = k - 1$ . The expression for  $\Psi$ , which consists of the products  $\psi_1 F$  and  $\psi_2 F$ , which satisfy the conditions (1.3) and (1.4) (for N = n + 1), can be got by carrying out symmetrization of these products according to the Young scheme (k; n - k + 1) and making use of the fact that  ${\boldsymbol \psi}_1$  and  ${\boldsymbol \psi}_2$  were already symmetrized according to the schemes (k; n - k) and (k - 1;n - k + 1).

However, this leads to cumbersome calculations; therefore, we proceed otherwise: we set up the

<sup>\*</sup> This circumstance was brought out as a result of discussions with Iu. N. Demkov.

expressions\*

$$\Psi_{1} = \sum_{j=k+1}^{n+1} a_{i} P_{i,n+1} \psi_{1} (1...k | k+1...n) \quad (1.9)$$

$$\times F(n+1);$$

$$\Psi_{2} = \sum_{t=1}^{k} \sum_{i=k}^{n+1} b_{t, i} P_{t, k} P_{i, n+1}$$

$$\times^{\psi_{2}} (1 \dots k - 1 | k \dots n) F (n+1)$$

$$(1.10)$$

and we determine the coefficients  $a_i$  and  $b_{t,i}$  so that  $\Psi_1$  and  $\Psi_2$  satisfy Eqs. (1.3) and (1.4).

We note that all the calculations necessary for the determination of  $a_i$  and  $b_{t,i}$  can be put in compact form if we make use of the "permutation relations"

$$P_{ab}P_{bc} = P_{ac}P_{ab} = P_{bc}P_{ac}.$$
 (1.11)

We shall not carry out the calculations here, but shall at once write the result:

$$\Psi_{1} = \left(1 - \sum_{i=k+1}^{n} P_{i, n+1}\right) \psi_{1} F, \qquad (1.12)$$

$$\Psi_{2} = \left(1 - \sum_{t=1}^{k-1} P_{t, k}\right) \left(1 - \sum_{i=k+1}^{n} P_{i, n+1} + (n - 2k + 2) P_{k, n+1}\right) \psi_{2} F.$$

It is shown in Appendix I that (1.12) satisfy the conditions (1.3)- (1.4). From (1.12), in particular for n = 1, we get

$$\Psi(|12) = \psi(1) F(2) - \psi(2) F(1), \qquad (1.12a)$$

$$\Psi(1 \mid 2) = \psi(1) F(2) + \psi(2) F(1), \quad (1.12b)$$

for n = 2

$$\begin{split} \Psi_{1} (1 | 23) &= \psi (1 | 2) F (3) - \psi (1 | 3) F (2), \\ \Psi_{2} (1 | 23) &= \psi (| 12) F (3) \\ &- \psi (| 13) F (2) + 2\psi (| 32) F (1). \end{split}$$

On the basis of the result (1.12) we now construct the coordinate function of the system "atom + electron." Let  $\psi_{A1}$  and  $\psi_{A2}$  be atomic coordinate functions; the indices A show the value of the energy, the orbital momentum and its projection on the z axis. (1) and (2) have the same meaning as above. We can then write

$$\Psi = \sum_{A} \left( 1 - \sum_{i=k+1}^{n} P_{i,n+1} \right) \psi_{A1} F_{A1}$$

$$+ \sum_{A} \left( 1 - \sum_{t=1}^{k-1} P_{t,k} \right) \left( 1 - \sum_{i=k+1}^{n} P_{i,n+1} + (n - 2k + 2) P_{k,n+1} \right) \psi_{A2} F_{A2}.$$
(1.13)

We note that in this case, if  $\psi_{A-1,2}$  are expressed approximately by the product of one-electron functions (or are themselves one-electron functions) we can carry out the transformation

$$F_{Aa} \to F'_{Aa} + \xi_{Aa} \quad (a = 1, 2)$$
 (1.14)

in (1.13), which does not change  $\Psi$  essentially. Thus, for  $\Psi(|12)$ ,

$$\xi_A = \sum_{A'} B_{AA'} \psi_{A'}, \qquad (1.15)$$

where  $B_{AA}$ , are constants which satisfy the condition  $B_{AA}$ ,  $= B_{A'A}$  but are otherwise arbitrary. For  $\Psi(1|2)\xi_A$  also has the form (1.15), but the constants  $B_{AA}$ , will satisfy the condition  $B_{AA}$ ,  $= -B_{A'A}$ .

If, in the expression for  $\Psi(1|23)$  we take  $\psi_{A|1}$ and  $\psi_{A|2}$  in the form

$$\psi_{A_{1,2}} = [V_A(1) W_A(2) \pm V_A(2) W_A(1)], (1.16)$$

then

$$\xi_{A_1} = \sum_{A'} (C_{AA'} V_{A'} + D_{AA'} W_{A'}), \quad (1.17)$$
  
$$\xi_{A_2} = \frac{1}{3} \sum_{A'} (D_{A'A} W_{A'} - C_{AA'} V_{A'}), \quad (1.17)$$

where  $C_{AA}$ , and  $D_{AA}$ , are arbitrary constants.

## 2. EQUATIONS FOR THE FUNCTIONS $F_{Aa}$

To derive the equations determining the functions

<sup>\*</sup> It is understood that application of the permutation operator to the product of two functions obeys the rule  $P_{ab}(fg) = (P_{ab}f)(P_{ab}g)$ .

 $F_{Aa}$ , we shall start out with the equation

$$(H - E) \Psi = 0. \tag{2.1}$$

Multiplying (2.1) by  $\psi_{Aa}^* d\tau$ , where  $a = 1, 2; d\tau = d\mathbf{r}_1, \ldots d\mathbf{r}_n$ , and integrating, we get

$$\int \psi_{Aa}^* \left( H - E \right) \Psi \, d\tau = 0. \tag{2.2}$$

If  $\Psi$  is expressed approximately by a finite number of atomic functions, so that the number totaled in the sum (1.13) is finite, then (2.1) is not satisfied. In this case we shall consider that  $\Psi$  no longer satisfies (2.1), but satisfies Eq. (2.2) as before.

The energy operator H has the form (in atomic units)

$$H = H_0(\mathbf{r}_1...\mathbf{r}_n) - \frac{1}{2}\Delta_{n+1} + U(\mathbf{r}_1...\mathbf{r}_{n+1}).$$
(2.3)

Here  $H_0$  is the energy operator of the *n*-electron system; U is the interaction operator of the (n+1)electron with the *n*-electron system and with the nucleus, and is defined by the expression

$$U = -\frac{z}{\mathbf{r}_{n+1}} + \sum_{i=1}^{n} \frac{1}{|\mathbf{r}_{n+1} - \mathbf{r}_i|} .$$
 (2.4)

We substitute (1.13), (2.3) and (2.4) in (2.2). We note that the functions  $\psi_{Aa}$  satisfy the equation

$$H_0 \psi_{Aa} = E_{Aa} \psi_{Aa} \tag{2.5}$$

and the normalization condition

$$\int \psi^*_{Aa} \psi_{A'a'} d\tau = \delta_{AA'} \delta_{aa'}. \qquad (2.6)$$

Carrying out a transformation based on the use of the symmetry properties of  $\psi_{Aa}$ , we obtain the following system of equations:

$$(\Delta + k_{Aa}^2) F_{Aa} (\mathbf{r}) = 2 \sum_{A'} U_{AA'a} F_{A'a}$$
(2.7)

$$+\sum_{A'a}\mathcal{A}_{AA'aa'}[F_{A'a'}(\mathbf{r}')]$$

Here  $U_{AA'a} = \int \psi_{Aa}^* U \psi_{A'a} d\tau$  is the matrix of the potential energy of interaction:  $k_{Aa}^2 = 2(E - E_{Aa})$ ; *A* is the exchange operator:

$$\mathcal{A}_{AA'aa'}[F_{A'a'}(r_{n+1})] \tag{2.8}$$

$$= \int \psi_{Aa}^{*} \left[ \rho_{aa'} P_{1, n+1} + q_{aa'} P_{n, n+1} \right] \left[ \Delta + k_{A'a'}^{2} - 2U \right] \psi_{A'a'} F_{A'a'} \, d\tau,$$

where  $p_{aa}$ , and  $q_{aa}$ , are equal to

$$p_{11} = p_{12} = p_{21} = 0; (2.9)$$

$$p_{22} = (k-1) (n-2k+3) / (n-2k+2);$$

$$q_{11} = (n-k); \ q_{12} = k (n-k) (n-2k+3);$$

$$q_{21} = (n-k) (n-k+1) / (n-2k+2);$$

$$q_{22} = -(n-k+1) / (n-2k+2).$$

Taking into account the explicit expression (2.4) for U, making use of the symmetry properties of  $\psi_{Aa}$  and the self-conjugate property of the operator  $\Delta$ , we can put the potential energy matrix and the exchange operator in the form

$$U_{AA'a} = \left[ -\frac{z}{r} \delta_{AA'} + \int \frac{\rho_{AA'a} \left(\mathbf{r}'\right)}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}' \right]; \qquad (2.10)$$

$$\mathcal{A}_{AA'aa'}\left[F_{A'a'}\left(\mathbf{r}'\right)\right] \tag{2.11}$$

$$= \int W_{AA'aa'}(\mathbf{r}', \mathbf{r}) F_{A'a'}(\mathbf{r}') d\mathbf{r}',$$
(2.12)

$$W_{AA'aa'}(\mathbf{r}', \mathbf{r})$$
 (2.12)

$$= \left(\Delta' + k_{A'a'}^2 + \frac{2z}{r'} - \frac{2}{|\mathbf{r} - \mathbf{r}'|}\right) \rho_{AA'aa'}(\mathbf{r}', \mathbf{r})$$
$$- 2 \int \rho_{AA'aa'}(\mathbf{r}'', \mathbf{r}', \mathbf{r}) / |\mathbf{r}' - \mathbf{r}''| d\mathbf{r}''.$$
$$AA'a(\mathbf{r}'), \rho_{AA'aa'}(\mathbf{r}, \mathbf{r}), \rho_{AA'aa'}(\mathbf{r}, \mathbf{r}', \mathbf{r}), \rho_{AA'aa'}(\mathbf{r}, \mathbf{r}', \mathbf{r}', \mathbf{r}') \text{ are}$$

 $\rho_{AA'a}(\mathbf{r}'), \rho_{AA'aa'}(\mathbf{r}', \mathbf{r}), \rho_{AA'aa'}(\mathbf{r}', \mathbf{r}', \mathbf{r}')$  are expressions composed according to the type of the density matrix and having a rather cumbersome form. The explicit form is derived in Appendix II. Making use of the expression (2.11) for the exchange operator, and setting

$$2U_{AA'a} = V_{AA'a}, \qquad (2.13)$$

we get Eq. (2.10) in the form

$$(\Delta + k_{Aa}^2) F_{Aa} = \sum_{A'} V_{AA'a} F_{A'a}$$

$$+ \sum_{A'a'} \int W_{AA'aa'}(\mathbf{r}', \mathbf{r}) F_{A'a'}(\mathbf{r}') d\mathbf{r}'.$$
(2.14)

## 3. TRANSFORMATION TO INTEGRAL EQUATIONS. SEPARATION OF THE ANGULAR VARIABLES

We transform the set of integro-differential equations (2.14) to a set of integral equations. For this purpose, in the case of the collision of an electron with a neutral atom we make use of the Green's function

$$G_{Aa}\left(\mathbf{r}, \mathbf{r}'\right) = \frac{\exp\left(ik_{Aa} \mid \mathbf{r} - \mathbf{r}'\mid\right)}{4\pi \mid \mathbf{r} - \mathbf{r}'\mid},$$

which satisfies the equation

$$(\Delta + k_{Aa}^2) G_{Aa}(\mathbf{r}, \mathbf{r}') = -\delta(\mathbf{r} - \mathbf{r}').$$

In the case of the collision of an electron with an ion of charge  $z_0$ , we must choose a Green's function which possesses the specific asymptoticity of the wave functions of the continuous spectrum of the Coulomb field. This condition is satisfied by  $G_{Aa}$  which is defined by the equation

$$(\Delta + k_{Aa}^2 + z_0 / r) G_{Aa}(\mathbf{r}, \mathbf{r}') = -\delta(\mathbf{r} - \mathbf{r}')$$

In order to consider both cases at once, we write

$$(\Delta + k_{Aa}^2 - V_0(\mathbf{r})) G_{Aa}(\mathbf{r}, \mathbf{r}') = -\delta(\mathbf{r} - \mathbf{r}');(3.1)$$

 $V_0 = 0 \text{ or } - z_0 / r.$ 

We are interested in the  $F_{Aa}$  which possesses as an asymptotic expression (for large r)

$$F_{Aa} \sim \exp\left(i\mathbf{k}_{Aa}\mathbf{r}\right)\,\delta_{AA_{o}}\delta_{aa_{o}} \tag{3.2}$$

$$+ q_{Aa}r^{-1}\exp(ik_{Aa}r)$$

or, in the case of a collision with an ion,

$$F_{Aa} \sim \exp i \left[ \mathbf{k}_{Aa} \mathbf{r} + \gamma \ln \left( \mathbf{k}_{Aa} \mathbf{r} - \mathbf{k}_{Aa} \mathbf{r} \right) \right] \quad (3.3)$$
$$+ q_{Aa} r^{-1} \exp i \left( k_{Aa} r + \gamma \ln 2 k_{Aa} r \right);$$
$$\gamma = z_0 / k_{Aa}.$$

Taking (2.14) and (3.2)-(3.3) into account, we get

$$F_{Aa} (\mathbf{r}) = \varphi_{Aa} (r) \delta_{AA_{\bullet}} \delta_{aa_{\bullet}}$$
(3.4)  
$$- \sum_{A'} \int [V_{AA'a} (\mathbf{r}') - V_{0} (r') \delta_{AA'}]$$
$$\times G_{Aa} (\mathbf{r}, \mathbf{r}') F_{A'a} (\mathbf{r}') d\mathbf{r}'$$
$$- \sum_{A'a'} \int G_{Aa} (\mathbf{r}, \mathbf{r}') d\mathbf{r}'$$
$$\times \int W_{AA'aa'} (\mathbf{r}'', \mathbf{r}') F_{A'a'} (\mathbf{r}'') d\mathbf{r}'',$$

where  $\varphi_{Aa}$  is a regular solution of the equation

$$\Delta \varphi_{Aa} + (k_{Aa}^2 - V_0(r)) \varphi_{Aa} = 0.$$
 (3.5)

For  $V_0 = 0$ ,

$$\varphi_{Aa} = \exp\left(i\mathbf{k}_{Aa}\mathbf{r}\right). \tag{3.6}$$

For  $V_0 = -z_0/r$ ,  $\varphi_{Aa}$  has the asymptotic form

$$\varphi_{Aa} \sim \exp\left[i\mathbf{k}_{Aa}\mathbf{r} + \gamma \ln\left(\mathbf{k}_{Aa}\mathbf{r} - k_{Aa}r\right)\right].$$
 (3.7)

$$+ q_{Aa}^{(0)} r^{-1} \exp i (k_{Aa} r + \gamma \ln 2k_{Aa} r),$$

 $q_{Aa}^{(0)}$  is the scattering amplitude in a Coulomb field.

Changing the order of integration in the latter integral of Eq. (3.4), and assuming

$$K_{AA'aa'}(\mathbf{r}, \mathbf{r}') \tag{3.8}$$

$$= -G_{Aa} (\mathbf{r}, \mathbf{r}') [V_{AA'a} (\mathbf{r}') - V_0 (r') \delta_{AA'}] \delta_{aa'}$$
$$- \int G_{Aa} (\mathbf{r}, \mathbf{r}'') W_{AA'aa'} (\mathbf{r}', \mathbf{r}'') d\mathbf{r}'',$$

we get a system of integral equations

$$F_{Aa} (\mathbf{r}) = \varphi_{Aa} (\mathbf{r}) \,\delta_{AA_{o}} \delta_{aa_{o}}$$

$$+ \sum_{A'a'} \int K_{AA'aa'} (\mathbf{r}, \mathbf{r}') \,F_{A'a'} (\mathbf{r}') \,d\mathbf{r}'.$$
(3.9)

We go on to the spherical system of coordinates and carry out a separation of the angular variables. We shall assume that the center of the coordinate system lies in the nucleus, while the Z axis is directed along the electron stream, incident on the atom. We expand  $F_{Aa}$ ,  $\varphi_{Aa}$  and  $G_{Aa}$  in the spherical harmonics  $Y_{lm}$   $(\theta, \varphi)$ , normalized to unity,

$$F_{Aa} = \sum_{l} a_{l} r^{-1} f_{Aal}(r) Y_{lm}(\theta, \varphi), \qquad (3.10)$$
$$a_{l} = [4\pi (2l+1)]^{l/2} i^{l};$$

$$\varphi_{Aa}\left(\mathbf{r}\right) = \sum_{l} a_{l} r^{-1} u_{Aal}\left(r\right) Y_{l,0}\left(\theta\right). \tag{3.11}$$

In the expansion of (3.10), the summation is not carried out over *m*. By virtue of the conservation of the *Z* component of the momentum of the system "atom + electron", the dependence of  $F_{Aa}$  on the angle  $\varphi$  is determined by the dependence of  $\psi_{Aa}$ on  $\varphi$  implicit in the index *A*. The functions  $u_{Aal}$ satisfy the equation

$$\frac{d^2 u_{Aal}}{dr^2} + \left(k_{Aa}^2 - \frac{l(l+1)}{r^2} - V_0\right) u_{Aal} = 0, \quad (3.12)$$

where  $u_{Aal}(0) = 0$ . For  $V_0 = 0$ :

$$u_{Aal} = (\pi r / 2k_{Aa})^{1/2} J_{l+1/2} (k_{Aa}r).$$

For  $V_0 = -z_0/r$ :  $r^{-1}u_{Aal}$  is a regular radial function of the Coulomb field. Further,

$$G_{Aa}\left(\mathbf{r}, \mathbf{r}'\right) \tag{3.13}$$

$$=\sum_{lm} (rr')^{-1} \Gamma_{Aal}(r, r') Y_{lm}(\theta, \varphi) Y_{lm}^*(\theta', \varphi'),$$

 $\Gamma_{A\,a\,l}$  is a one-dimensional Green's function which satisfies the equation

$$\left(\frac{d^2}{dr^2} + k_{Aa}^2 - \frac{l(l+1)}{r^2} - V_0\right) \Gamma_{Aal}(r, r') \qquad (3.14)$$
$$= -\delta(r - r').$$

As is well known, this function can be expressed by  $u_{Aal}$  and the second independent solution of Eq. (3.12), which we denote by  $v_{Aal}$ :

$$\Gamma_{Aal}(r, r') = \begin{cases} -u_{Aal}(r) v_{Aal}(r') / \omega & \text{for } r \leqslant r' \\ -u_{Aal}(r') v_{Aal}(r) / \omega & \text{for } r \geqslant r' \end{cases}$$

 $w \{ u_{A a l}; v_{A a l} \}$  is the Wronski determinant.

Corresponding to the asymptotic expressions (3.2)-(3.3),  $v_{Aal}$  ought to have the form of a diverging wave for  $r \to \infty$ . We choose  $v_{Aal}$  so that w = 1. For  $V_0 = 0$ , we have

$$v_{Aal} = i^{-1} \left( \frac{\pi}{2} k_{Aa} r \right)^{1/2} H_{l+1/2}^{(1)}(k_{Aa} r).$$

We introduce the notation

$$V_{\omega\omega'}(\mathbf{r}') \qquad (3.16)$$

$$= \int Y_{lm}^{*}(\theta',\varphi') V_{AA'a}(\mathbf{r}') Y_{l'm'}(\theta'\varphi') d\Omega' \delta_{aa'},$$

$$W_{\omega\omega'}(\mathbf{r}',\mathbf{r}'') = \mathbf{r}'\mathbf{r}'' \int Y_{lm}^{*}(\theta''\varphi'')$$

$$\times W_{AA'aa'}(\mathbf{r}',\mathbf{r}'') Y_{l'm'}(\theta'\varphi') d\Omega' d\Omega'',$$

where  $\omega = (Aal)$ . Because of the presence of the term  $|\mathbf{r} - \mathbf{r}'|^{-1}$  in (2.12),  $\mathbb{W}_{\omega\omega}$ , (r, r') will have a

different form for  $r \leq r'$  and  $r \geq r'$ . In order to consider this circumstance, we shall write  $W^{(1)}_{\omega\omega}(r',r'')$  for  $r' \leq r''$  and  $W^{(2)}_{\omega\omega}(r',r'')$  for  $r' \geq r''$ . Further, let us set

$$S_{\boldsymbol{\omega}\boldsymbol{\omega}'}(\boldsymbol{r}, \boldsymbol{r}') = [v_{\boldsymbol{\omega}}(\boldsymbol{r}) \, u_{\boldsymbol{\omega}}(\boldsymbol{r}') \qquad (3.17)$$

$$- v_{\omega}(r') u_{\omega}(r)] [V_{\omega\omega'}(r') - V_{0}(r') \delta_{\omega\omega'}]$$

$$+ \int_{r'}^{r} [v_{\omega}(r) u_{\omega}(r'') - v_{\omega}(r'') u_{\omega}(r)]$$

$$\times [W^{(1)}_{\omega\omega'}(r', r'') - W^{(2)}_{\omega\omega'}(r', r'')] dr'';$$

$$T_{\boldsymbol{\omega}\boldsymbol{\omega}'}\left(\boldsymbol{r},\ \boldsymbol{r}'\right) \tag{3.18}$$

$$= \int_{0}^{r} \left[ v_{\omega}(r) \, u_{\omega}(r'') - v_{\omega}(r'') \, u_{\omega}(r) \right] W^{(2)}_{\omega\omega'}(r', r'') \, dr''$$

$$c_{\nu} = \delta_{\nu\nu} \delta_{\nu} + \sum_{i}^{\infty} N_{\nu} (r') \delta_{\nu}(r') \, \delta_{\nu}(r') \, dr' \qquad (3.19)$$

$$c_{\omega} = \delta_{AA_{\bullet}} \delta_{aa_{\bullet}} + \sum_{\omega'} \int_{0}^{1} N_{\omega\omega'}(r') f_{\omega}(r') dr', \qquad (3.19)$$

$$N_{\omega\omega'}(r') = v_{\omega}(r') \left[ V_{\omega\omega'}(r') - V_0(r') \delta_{\omega\omega'} \right]$$
$$+ \int_0^\infty W_{\omega\omega'}(r', r'') v_{\omega}(r'') dr''$$

(We note that  $S_{\omega\omega}$  , and  $T_{\omega\omega}$  , do not change under the transformation

$$v_{\omega} \rightarrow \lambda v_{\omega} + \mu u_{\omega}; \ u_{\omega} \rightarrow \lambda^{-1} u_{\omega},$$

where  $\lambda$  and  $\mu$  are constants.)

With the help of (3.17)-(3.19) we obtain\*

$$f_{\omega}(r) = c_{\omega}u_{\omega}(r)$$

$$+ \sum_{\omega'} \int_{0}^{r} S_{\omega\omega'}(r, r') f_{\omega'}(r') dr'$$

$$+ \sum_{\omega'} \int_{0}^{\infty} T_{\omega\omega'}(r, r') f_{\omega'}(r') dr'$$
(3.20)

<sup>\*</sup> The integrals entering into (3.17)-(3.19) converge. The convergence is guaranteed by the behavior of  $V_0$ ,  $V_{\omega\omega}$ , and  $W_{\omega\omega}$ , for large values of their arguments, and also by the fact the expressions of the type

 $V_{\omega\omega'(r)}v_{\omega}(r)f_{\omega}(r)$  and  $W_{\omega\omega'}(r', r)v_{\omega}(r)$  are finite for  $r \to 0$ .

Equation (3.20) can be simplified in this case if the wave functions of the atom,  $\psi_{Aa}$ , are approximated by one-electron wave functions. Then  $W_{\omega\omega}$ , will be expressed in the form of the sum of products of functions of r' and functions of r''. Consequently,  $T_{\omega\omega}$ , will have the form

$$T_{\omega\omega'}(r, r') = \sum_{i} R_{\omega\omega'i}(r) Q_{\omega\omega'i}(r'). \qquad (3.21)$$

For simplification of the calculation, we consider the case in which only one term enters into the sum over i in (3.21). Generalization to the case of several terms is trivial.

Substituting Eq. (3.21) in Eq. (3.20), and assuming

$$\mathcal{L}_{\omega\omega'} = \int_{0}^{\infty} Q_{\omega\omega'}(r') f_{\omega'}(r') dr', \qquad (3.22)$$

we put Eq. (3.20) in the form

$$f_{\omega}(r) = c_{\omega}u_{\omega}(r) + \sum_{\omega'}c_{\omega\omega'}R_{\omega\omega'}(r) \quad (3.23)$$
$$+ \sum_{\omega'}\int_{0}^{r}S_{\omega\omega'}(r, r')f_{\omega'}(r')dr'.$$

We now pass over from unknown f to the new unknown x by means of a linear transformation

$$f_{\omega} = \sum_{\omega'} c_{\omega'} x_{\omega\omega'}(r) + \sum_{\omega'\omega''} c_{\omega'\omega''} x_{\omega\omega'\omega''}(r). \quad (3.24)$$

Substituting (3.23) into (3.24), we get a system of Volterra integral equations

$$x_{\omega\omega'\omega''} = R_{\omega'\omega''}\delta_{\omega\omega'} \tag{3.25}$$

$$+\sum_{\omega''}\int_{0}^{r}S_{\omega\omega''}(r, r') x_{\omega''\omega'\omega''}(r') dr',$$
$$x_{\omega\omega'} = u_{\omega}\delta_{\omega\omega'} + \sum_{\omega''}\int_{0}^{r}S_{\omega\omega''}(r, r') x_{\omega''\omega'}(r') dr'.$$

As is seen from (3.25), the system of equations for  $x_{\omega\omega}$ , and  $x_{\omega\omega'\omega''}$  is developed in a series of independent subsystems.

If the system of equations (3.25) is solved, then we can determine the unknown constants  $c_{\omega}$  and  $c_{\omega\omega}$ . For this purpose, we must substitute the values of  $x_{\omega\omega}$ , and  $x_{\omega\omega'\omega'}$ , which have been found, in Eq. (3.24), and substitute the resultant expression in (3.19) and (3.22). A system of algebraic equations in  $c_{\alpha}$  and  $c_{\alpha\alpha'}$  is obtained:

$$\sum_{\omega''} c_{\omega''} L_{\omega\omega'\omega''} \qquad (3.26)$$

$$+ \sum_{\omega''\omega'''} c_{\omega''\omega''} (L_{\omega\omega'\omega''\omega''} - \delta_{\omega''\omega}\delta_{\omega'''\omega'}) = 0;$$

$$\sum_{\omega''} c_{\omega''} [M_{\omega\omega''} - \delta_{\omega''\omega}]$$

$$+ \sum_{\omega''\omega'''} c_{\omega''\omega'''} M_{\omega\omega''\omega'''} + \delta_{AA_{\bullet}}\delta_{aa_{\bullet}} = 0;$$

where

$$L_{\omega\omega'\omega''} = \int_{0}^{\infty} Q_{\omega\omega'} x_{\omega'\omega''} dr; \qquad (3.27)$$

$$L_{\omega\omega'\omega''\omega'''} = \int_{0}^{\infty} Q_{\omega\omega'} x_{\omega'\omega''\omega''} dr;$$

$$M_{\omega\omega''} = \sum_{\omega'} \int_{0}^{\infty} N_{\omega\omega'} x_{\omega'\omega''} dr;$$

$$M_{\omega\omega''\omega'''} = \sum_{\omega'} \int_{0}^{\infty} N_{\omega\omega'} x_{\omega'\omega''\omega''} dr.$$

We note that some of the quantities  $c_{\omega}$  and  $c_{\omega\omega}$ , can be equated to zero in certain cases. Actually, at the end of Sec. 1, it was pointed out that in the use of approximate expressions of  $\psi_{Aa}$  in terms of one-electron functions, we can change  $F_{Aa}$ , leaving unchanged the wave function of the entire system. This possibility can be used to impose on  $f_{\omega}$ the additional condition of orthogonality to some of the  $N_{\omega\omega}$ , or the  $Q_{\omega\omega}$ . The number of these additional conditions depends on the spin of the system and also on the number of different oneelectron functions used in the calculation.

## 4. ASYMPTOTIC EXPRESSIONS. EFFECTIVE CROSS SECTIONS.

Let us consider the asymptotic expressions for  $F_{Aa}[(3.2) \text{ and } (3.3)]$ . We represent  $q_{Aa}$  in the form

$$q_{Aa} = \sum_{l} i^{-l} a_l q_{Aal} Y_{lm}(\theta, \varphi) . \qquad (4.1)$$

The quantities  $q_{Aal}$  can be expressed by integrals containing the functions  $x_{\omega\omega}$ , and  $x_{\omega\omega}$ , w''.

For this purpose we consider the integral equations (3.20). Taking into account (3.17)-(319.) and (3.23), we can write, for large r:

$$f_{\omega}(r) \sim u_{\omega}(r) \,\delta_{AA_{\circ}} \,\delta_{aa_{\circ}} + B_{\omega} v_{\omega}(r); \quad (4.2)$$

where

$$B_{\omega} = \sum_{\omega''} c_{\omega''} \int_{0}^{\infty} \sum_{\omega'} \mathcal{E}_{\omega\omega'} x_{\omega'\omega''} dr' \qquad (4.3)$$

$$+ \sum_{\omega''\omega'''} c_{\omega''\omega'''} \int_{0}^{\infty} \sum_{\omega'} \mathcal{E}_{\omega\omega'} x_{\omega'\omega''\omega''} dr';$$

$$\mathcal{E}_{\omega\omega'} (r') = u_{\omega} (r') (V_{\omega\omega'} - V_0 \delta_{\omega\omega'})$$

$$+ \int_{0}^{\infty} u_{\omega} (r'') W_{\omega\omega'} (r', r'') dr''.$$

For  $\mathcal{V}_0 = 0$ , the asymptotic expressions for  $u_{\omega}$  and  $v_{\omega}$  have the form:

$$u_{\omega} \sim k_{Aa}^{-1} \sin \left( k_{Aa}r - l\pi/2 \right),$$
  

$$v_{\omega} \sim -\exp i \left( k_{Aa}r - l\pi/2 \right).$$
(4.4)

Consequently,

$$q_{\omega} = -B_{\omega}. \tag{4.5}$$

For  $V_0 = -z_0/r$ , the asymptotic expressions for  $u_{\omega}$  and  $v_{\omega}$  will be

$$u_{\omega} \sim k_{Aa}^{-1} e^{i\eta_{\omega}} \sin\left(k_{Aa}r - \frac{l\pi}{2}\right)$$

$$+ \eta_{\omega} + \gamma \ln 2 k_{Aa}r ,$$

$$v_{\omega} \sim -\exp i\left(k_{Aa}r - \frac{l\pi}{2} + \gamma \ln 2k_{Aa}r\right)$$
(4.6)

where  $\eta_{\omega} = \arg \Gamma(l + 1 - i\gamma)$ . Then we get for  $q_{\omega}$ 

$$q_{\omega} = q_{\omega}^{(0)} \delta_{AA_{\circ}} \delta_{aa_{\circ}} - B_{\omega}. \tag{4.7}$$

We now return to the asymptotic behavior of the wave function of the system "electron + atom", when any of the large r are large, for example,  $r_{n+1}$ .

We substitute (1.13) in (1.6) and make use of Eq. (1.7) for  $\chi$ . (Consequently, we consider the spin of the system directed along z.) In view of the presence of transformation operators, there enter into the expression for  $\Phi$ [in addition to terms  $\psi_{Aa} F_{Aa} (\mathbf{r}_{n+1})$ ] terms in which the argument  $r_{n+1}$  enters into  $\psi_{Aa}$ . If we now let  $r_{n+1} \rightarrow \infty$ , then the terms, in which the  $\psi_{Aa}$  belonging to the discrete spectrum contain  $r_{n+1}$ , disappear. Similar terms, in which  $\psi_{Aa}$  belong to a continuous spectrum, remain finite but will play no role whatever in the following. Therefore, considering  $\Phi$  for large  $r_{n+1}$ , we take into consideration only those terms in which  $r_{n+1}$  enters into  $F_{Aa}$ .

Carrying out some transformations and neglecting the factor in front of  $\Phi$ , which is not essential in what follows, we get

$$\Phi \sim \sum_{A} \Phi_{A1} F_{A1} (\mathbf{r}_{n+1}) \alpha_{n+1}$$

$$+ k^{1/2} \sum_{A} \Phi'_{A_2} F_{A_2} (\mathbf{r}_{n+1}) \alpha_{n+1}$$

$$- (n - 2k + 2) k^{1/2} (n - k + 1)^{-1/2}$$

$$\times \sum_{A} \Phi_{A2} F_{A2} (\mathbf{r}_{n+1}) \beta_{n+1}.$$
(4.9)

Here  $\Phi_{A1}$  is the atomic wave function with spin  $s - \frac{1}{2}$ , composed, according to (1.6), of  $\psi_{A1}$  and  $\chi = \beta_1 \dots \beta_k \alpha_{k+1} \dots \alpha_n$ ,  $\Phi_{A2}$  is the atomic wave function with spin  $s + \frac{1}{2}$ , composed, by (1.6), of  $\psi_{A2}$  and  $\chi = \beta_1 \dots \beta_{k-1} \alpha_k \dots \alpha_n$ ,  $\Phi'_{A2}$  is composed also of  $\psi_{A2}$ , but  $\chi$  in this case has the form

$$\chi = (n - k + 1)^{-1/2} \tag{4.10}$$

$$\times \Big(1 + \sum_{j=k+1}^n P_{k,j}\Big)\beta_1 \dots \beta_k \alpha_{k+1} \dots \alpha_n.$$

 $\Phi'_{A2}$  corresponds to the spin  $s + \frac{1}{2}$ , but the value of the projection of the spin on the Z axis for this function is equal not to  $s + \frac{1}{2}$  but to  $s - \frac{1}{2}$ . Substituting the asymptotic expressions (3.2) or (3.3) for  $F_{Aa}$  in (4.9), calculating the vector current and summing over the spins, we can obtain, in the

usual way, the expressions for the effective cross sections.

We now consider, as an example, the case of the collision of an electron with an atom which has spin 0 before collision.

Taking (1.2) into consideration, and omitting the index n + 1, we get from (4.9):

1. . . .

$$\Phi \sim \Phi_{A_{01}} \exp(i\mathbf{k}_{A_{0}1}\mathbf{r}) \alpha \qquad (4.11)$$

$$+ \sum_{A} \Phi_{A_{1}}q_{A_{1}}r^{-1} \exp(ik_{A_{1}}r) \alpha$$

$$+ \left(\frac{n}{2}\right)^{1/2} \sum_{A} \Phi'_{A_{2}}q_{A_{2}}r^{-1} \exp(ik_{A_{2}}r) \alpha - 2\left(\frac{n}{n+2}\right)^{1/2} \times \sum_{A} \Phi_{A_{2}}q_{A_{2}}r^{-1} \exp(ik_{A_{2}}r) \beta.$$

Hence, the differential effective cross section of collision with no change in the spin of the atom is

$$d\sigma_{A_1,A_{\bullet 1}} = (k_{A_1} / k_{A_{\bullet 1}}) |q_{A_1}|^2 d\Omega, \qquad (4.12)$$

but with a change in the value of the spin of the atom,

$$d\sigma_{A_2,A_01} = (k_{A_2}/k_{A_01}) [n/2]$$

 $+ 4n/(n+2) |q_{A2}|^2 d\Omega.$ 

If the atom had spin differing from zero before the collision, say, s<sub>0</sub>, then there would be two possible values of the spin of the system:  $s = s_0 + \frac{1}{2}$ 

and  $s = s_0 - \frac{1}{2}$ . Therefore, there are two different problems. In the first of these the initial state of the atom is described by the functions  $\Phi_{A \circ 1}$ , in

the other, by the functions  $\Phi_{A\ 0\ 2}$ .

In order to obtain the observed cross section, we must carry out an averaging over the spins.

I express my gratitude for discussions to V. A. Fock and Iu. N. Demkov.

#### APPENDIX I

We show that the expressions  $\boldsymbol{\Psi}_1$  and  $\boldsymbol{\Psi}_2$  satisfy

the conditions (1.3)-(1.4). Let us first consider  $\Psi_1$ . 1. Condition of antisymmetry up to the vertical bar is evidently satisfied, inasmuch as the arguments in  $\Psi_1$  and  $\psi_1$  are identical up to the bar.

2. Antisymmetry after the bar. We apply the operator  $(1 + P_{i,i})$ . Making use of Eq. (1.11), we get

$$(1+P_{i,j})\Psi_{1} = \begin{cases} \left(1-\sum_{l=k+1}^{n} P_{l,n+1}\right)(1+P_{i,j})\psi_{1}F & \text{for } i, j \neq n+1, \\ -\sum_{i\neq l} P_{i,n+1}(1+P_{i,l})\psi_{1}F & \text{for } j=n+1, \end{cases}$$
(1)

(2)

which vanishes since  $(1 + P_{i,l})\psi_1 = 0$ .

3. Condition of cyclic symmetry. Making use of (1.11), we can show that

$$\left(1 - \sum_{j=k+1}^{n+1} P_{k,j}\right) \left(1 - \sum_{i=k+1}^{n} P_{i,n+1}\right)$$
  
=  $\left(1 - \sum_{j=k}^{n} P_{k,j}\right) \left(1 - \sum_{i=k-1}^{n} P_{k,i}\right),$ 

inasmuch as

$$\left(1 - \sum_{i=k+1}^{n} l_{k,i}\right)\psi_{1} = 0,$$
  
consequently,

$$\left(1-\sum_{\substack{j=k+1\\j=k\neq 1}}P_{k,j}\right)\Psi_1=0.$$

Let us now consider  $\Psi_2$ .

1. Antisymmetry after the vertical bar.

$$(1+P_{i,j})\Psi_{2} = \begin{cases} \left(1-\sum_{t=1}^{n-1}P_{t,k}\right)\left(1-\sum_{j=k+1}^{n}P_{j,n+1}+\right) + \left(n-2k+2\right)P_{k,n+1}\right)\left(1+P_{i,j}\right)\psi_{2}F & \text{for } i, j \neq n+1, \\ \left(1-\sum_{t=1}^{k-1}P_{t,k}\right)\left[\left(n-2k+2\right)P_{k,n+1}\left(1+P_{i,k}\right)-\right) + \left(1-\sum_{t=1}^{k-1}P_{t,n+1}\left(1+P_{i,l}\right)\right)\psi_{2}F & \text{for } j=n+1, \end{cases}$$
(3)

which vanishes, since

$$(1 + P_{i,j})\psi_2 = (1 + P_{i,k})\psi_2 = 0.$$

2. Antisymmetry up to the bar. For  $i, j \neq k$ , the condition is evidently satisfied. For j = k,

$$(1 + P_{i,k}) \Psi_{2} = -\sum_{t \neq i} P_{t,k} \left( 1 - \sum_{i} P_{i,n+1} \right)$$
(4)  
+  $(n - 2k + 2) P_{k,n+1} (1 + P_{t,i}) \psi_{2} \dot{F},$   
hich vanishes, since  $(1 + P_{t,i}) \psi_{2} = 0.$ 

3. Condition of cyclic symmetry. Making use of

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the properties of  $\psi_2$ , we get, after some transformations,

$$\left(1 - \sum_{j=k+1}^{n+1} P_{k,j}\right) \Psi_{2}$$

$$= \left(1 + \sum_{j=k}^{n} P_{j,n+1}\right) \left[\left(1 - \sum_{j=k+1}^{n} P_{k,j}\right) - \sum_{t=1}^{k-1} P_{t,k}\left(1 - \sum_{j=k+1}^{n} P_{t,i}\right) - (n - 2k + 2)\right] \psi_{2}F.$$
(5)

Furthermore, we can show that by virtue of the properties of  $\psi_2$ , the equality

$$\left[\left(1-\sum_{j=k+1}^{n}P_{k,j}\right)\right)$$
(6)  
$$-\sum_{t=1}^{k-1}P_{t,k}\left(1-\sum_{j=k+1}^{n}P_{t,j}\right)\right]\psi_{2} = (n-2k+2)\psi_{2}$$

exists. Consequently,

$$\left(1 - \sum_{j=k+1}^{n+1} P_{k,j}\right) \Psi_2 = 0$$

### APPENDIX II

We derive expressions for the quantities

 $\rho_{AA'a}(\mathbf{r}'), \rho_{AA'aa}(\mathbf{r}', \mathbf{r}) \text{ and } \rho_{AA'aa}(\mathbf{r}'', \mathbf{r}', \mathbf{r}).$ In order to write down these expressions in the most compact form, we introduce the notation for the integral of the product  $\psi_{Aa}^*\psi_{A'a'}$  over all variables except certain exclusions. For example, the integral of the product  $\psi_{Aa}^*\psi_{A'a'}$  over all variables except  $\mathbf{r}_i$ , entering into  $\psi_{Aa}^*$ , and  $\mathbf{r}_j$  entering into  $\psi_{A'a'}$ , we denote by the symbol  $(r_i)_{Aa}(r_j)_{A'a'}$ =  $\int \psi_{Aa}^*\psi_{A'a'} d\mathbf{r}_1 \dots d\mathbf{r}_{i-1}d\mathbf{r}_{i+1}\dots d\mathbf{r}_{i-1}d\mathbf{r}_{i+1}\dots d\mathbf{r}_n$ . If, after integration,  $\mathbf{r}_i$  is replaced by  $\mathbf{r}$ , and  $\mathbf{r}_j$  by  $\mathbf{r}'$ , then we can describe this case by

$$(r_i)_{Aa} \langle r_j \rangle_{A'a'}$$
  
The expressions of interest to us have the form:

$$\begin{split} \rho_{AA'1}\left(\mathbf{r}'\right) &= k \begin{pmatrix} r' \\ r_{1} \end{pmatrix}_{A'1} \begin{pmatrix} r' \\ r_{1} \end{pmatrix}_{A'1} + (n-k) \begin{pmatrix} r' \\ r_{n} \end{pmatrix}_{A_{1}} \begin{pmatrix} r' \\ r_{n} \end{pmatrix}_{A'_{1}}; \\ \rho_{AA'2}\left(\mathbf{r}'\right) &= (k-1) \begin{pmatrix} r' \\ r_{n} \end{pmatrix}_{A_{2}} \begin{pmatrix} r' \\ r_{n} \end{pmatrix}_{A'_{2}} + (n-k+1) \begin{pmatrix} r' \\ r_{n} \end{pmatrix}_{A_{2}} \begin{pmatrix} r' \\ r_{n} \end{pmatrix}_{A'_{2}}; \\ \rho_{AA'11}\left(\mathbf{r}',\mathbf{r}\right) &= q_{11} \begin{pmatrix} r' \\ r_{n} \end{pmatrix}_{A_{1}} \begin{pmatrix} r \\ r_{n} \end{pmatrix}_{A'_{1}}; \\ \rho_{AA'21}\left(\mathbf{r}',\mathbf{r}\right) &= q_{21} \begin{pmatrix} r' \\ r_{n} \end{pmatrix}_{A_{2}} \begin{pmatrix} r \\ r_{n} \end{pmatrix}_{A_{2}} \begin{pmatrix} r \\ r_{n} \end{pmatrix}_{A_{2}}; \\ \rho_{AA'21}\left(\mathbf{r}',\mathbf{r}\right) &= q_{22} \begin{pmatrix} r' \\ r_{n} \end{pmatrix}_{A_{2}} \begin{pmatrix} r \\ r_{n} \end{pmatrix}_{A_{2}} \begin{pmatrix} r' \\ r_{n} \end{pmatrix}_{A_{2}} + \rho_{22} \begin{pmatrix} r' \\ r_{1} \end{pmatrix}_{A_{2}} \begin{pmatrix} r \\ r_{n} \end{pmatrix}_{A'_{2}}; \\ \rho_{AA'11}\left(\mathbf{r}^{"},\mathbf{r}',\mathbf{r}\right) &= q_{12} \begin{bmatrix} k \begin{pmatrix} r'' & r' \\ r_{n} \end{pmatrix}_{A_{2}} \begin{pmatrix} r' \\ r_{n} \end{pmatrix}_{A_{2}} + \rho_{22} \begin{pmatrix} r' \\ r_{1} \end{pmatrix}_{A_{2}} \begin{pmatrix} r \\ r_{n} \end{pmatrix}_{A'_{2}}; \\ \rho_{AA'12}\left(\mathbf{r}^{"},\mathbf{r}',\mathbf{r}\right) &= q_{12} \begin{bmatrix} k \begin{pmatrix} r'' & r' \\ r_{n-1} & r_{n} \end{pmatrix}_{A_{1}} \begin{pmatrix} r'' & r \\ r_{n-1} & r_{n} \end{pmatrix}_{A_{1}} + (n-k-1) \\ \times \begin{pmatrix} r'' & r' \\ r_{n-1} & r_{n} \end{pmatrix}_{A_{1}} \begin{pmatrix} r'' & r' \\ r_{n-1} & r_{n} \end{pmatrix}_{A_{1}} + (n-k-1) \\ \times \begin{pmatrix} r'' & r' \\ r_{n-1} & r_{n} \end{pmatrix}_{A_{1}} \begin{pmatrix} r'' & r' \\ r_{n-1} & r_{n} \end{pmatrix}_{A_{1}} \begin{pmatrix} r'' & r' \\ r_{n-1} & r_{n} \end{pmatrix}_{A_{1}} \\ + (n-k-1) \begin{pmatrix} r'' & r' \\ r_{k} & r_{n} \end{pmatrix}_{A'} + (n-k-1) \begin{pmatrix} r'' & r' \\ r_{1} & r_{n} \end{pmatrix}_{A_{2}} \begin{pmatrix} r'' & r' \\ r_{1} & r_{n} \end{pmatrix}_{A_{1}} \\ + (n-k) \begin{pmatrix} r'' & r' \\ r_{k} & r_{n} \end{pmatrix}_{A'} + (n-k-1) \begin{pmatrix} r'' & r' \\ r_{1} & r_{n} \end{pmatrix}_{A_{1}} \begin{pmatrix} r'' & r' \\ r_{1} & r_{n} \end{pmatrix}_{A_{1}} \\ + (n-k) \begin{pmatrix} r'' & r' \\ r_{n-1} & r_{n} \end{pmatrix}_{A_{2}} \begin{pmatrix} r'' & r' \\ r_{1} & r_{n} \end{pmatrix}_{A_{2}} \begin{pmatrix} r'' & r' \\ r_{1} & r_{n} \end{pmatrix}_{A_{2}} \begin{pmatrix} r'' & r' \\ r_{1} & r_{n} \end{pmatrix}_{A_{2}} \\ + (n-k) \begin{pmatrix} r'' & r' \\ r_{1} & r_{n} \end{pmatrix}_{A_{2}} \begin{pmatrix} r'' & r' \\ r_{1} & r_{n} \end{pmatrix}_{A_{2}} \begin{pmatrix} r'' & r' \\ r_{1} & r_{n} \end{pmatrix}_{A_{2}} \begin{pmatrix} r'' & r' \\ r_{1} & r_{n} \end{pmatrix}_{A_{2}} \begin{pmatrix} r'' & r' \\ r_{1} & r_{n} \end{pmatrix}_{A_{2}} \begin{pmatrix} r'' & r' \\ r_{1} & r_{n} \end{pmatrix}_{A_{2}} \begin{pmatrix} r'' & r' \\ r_{1} & r_{n} \end{pmatrix}_{A_{2}} \begin{pmatrix} r'' & r' \\ r_{1} & r_{n} \end{pmatrix}_{A_{2}} \begin{pmatrix} r'' & r' \\ r_{1} & r_{n} \end{pmatrix}_{A_{2}} \begin{pmatrix} r'' & r' \\ r_{1} & r_{n} \end{pmatrix}_{A_{2}} \begin{pmatrix} r'' & r' \\ r_{1} & r_{n} \end{pmatrix}_{A_{2}} \begin{pmatrix} r'' & r' \\ r_{1} & r_{n} \end{pmatrix}_{A_{2}} \begin{pmatrix} r'' & r' \\ r_{1} & r_{n} \end{pmatrix}_{A_{2}} \begin{pmatrix} r'' & r' \\ r_{1} & r_{n$$

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# Inelastic Scattering of Photons by Indium-115 Nuclei

O. V. BOGDANKEVICH, L. E. LAZAREVA AND F. A. NIKOLAEV
P. N. Lebedev Physical Institute, Academy of Sciences, USSR (Submitted to JETP editor April 4, 1956)
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The yields of the reactions  $\ln^{115}(\gamma, \gamma') \ln^{115m}$  and  $\ln^{115}(\gamma, 2n) \ln^{113m}$  and the yield of neutrons accompanying the photodisintegration of indium were measured at various maximum energies of x-rays from 5 to 27 mev. Cross sections were calculated by the photon difference method.

T HE yield of the reaction  $\ln^{115}(\gamma, \gamma') \ln^{115m}$  at various maximum x-ray energies  $E_{max}$  from 5 to 27 mev was measured on the 30 mev synchrotron. The number of isomeric states of  $\ln^{115m}$ , formed after the irradiation, was measured by a scintillation counter which registers the  $\gamma$ -radiation emitted during the transition from the metastable level to the ground level ( $h\nu = 335$  kev, T = 4.5 hours).

If the conversion coefficient is not very large, this method of registration of metastable states seems to be more effective than the measurement of the induced activity by means of soft conversion electrons, since it makes possible a considerable increase in the number of counts at the expense of increasing the effective thickness of the sample, and simplifies the corrections for absorption and scattering of the radiation which is being registered. The photo-excitation cross sections of the metastable state of  $\ln^{115m}$  so obtained give a lower bound for the cross section of the reaction  $\ln^{115}(\gamma, \gamma')$ .

In reducing the  $\gamma$ -decay curves of the activity induced in the indium sample, the yield curve of the reaction  $\ln^{115}(\gamma, 2n) \ln^{113m}$  was also obtained. For simultaneous comparison of radiative and neutron width at various energies of x-rays, neutron fields during photodisintegration of indium were measured.

# 1. YIELD CURVE OF THE REACTION $\ln^{115}(\gamma, \gamma') \ln^{115m}$

The sample of indium (95.8%  $\text{In}^{115}$ ; 4.2%  $\text{In}^{113}$ ), 2.55 gm/cm<sup>2</sup> thick, was irradiated at a distance of 60 cm from the target of the synchrotron. In order to decrease the  $\gamma$ -activity arising as a result of capture of slow neutrons [ $\text{In}^{115}(n, \gamma) \text{In}^{116m}$ , T = 54 min], the sample of indium was placed during irradiation in a cadmium case (wall thickness 0.5 mm) wrapped in rhodium foil 0.4 mm thick.

The flux of  $\gamma$ -quanta falling on the sample was measured with an ionization chamber with thick aluminum walls (7.5 cm). The ionization in the air spaces of such a chamber for bremsstrahlung was calculated in Ref. 1. The measurement of the x-ray flux was made by placing the chamber at the position of the sample each time before and after irradiation. In order to avoid having to make a correction for the distribution of the  $\gamma$ -quanta flux over the

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