

OPTIMAL SYSTEM OF BASIS FUNCTIONS IN THE THEORY OF COLLISIONS  
BETWEEN ELECTRONS AND ATOMS

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Solution of collision problems by expanding the wave function of the system in a set of eigenfunctions of the Hamiltonian of the unperturbed atom is not optimal with respect to rapid convergence of the series. A set of equation is obtained for the optimal basis and for the coefficients of the expansion of the  $\Psi$ -function in terms of the basis. Specific calculations of phase shifts are made for the elastic scattering of low-energy electrons by a hydrogen atom.

### 1. INTRODUCTION

LET an electron with energy  $k^2$  (in Hartree units) collide with an arbitrary atom. The wave function of such a system is customarily sought in the form of an expansion in a complete set of functions  $u_i$ , describing all possible states of the unperturbed atom<sup>[1-3]</sup>

$$\Psi = \sum_i F_i u_i. \quad (1.1)$$

This method leads to an infinite system of integro-differential equations, solution of which determines, in principle, the exact solution of the problem. In practical calculations it is necessary to use the first terms of the sought expansion. In view of the slow convergence of the series, such a cutoff is unsatisfactory, and calculations based on it are for the most part estimates. This is clear from several papers<sup>[4-6]</sup> in which account is taken of the virtual 2s and 3s states in the calculation of elastic scattering of electrons by a hydrogen atom. The approximate scattering lengths obtained thereby exaggerate the maximum estimates given in the article by Rosenberg, Spruch, and O'Malley<sup>[7]</sup>. An account of the 2p level greatly improves the situation,<sup>[8]</sup> but the computation accuracy, particularly for inelastic processes<sup>[9,10]</sup>, is still far from satisfactory.

Thus, the calculations based on expansion (1.1) can hardly be considered optimal. An analogous situation arises also in problems with a discrete energy spectrum. In fact, an attempt could be made to calculate the bound state of the helium atom by expanding the sought wave function in a

complete set of the hydrogen-atom wave functions. It is clear that such a series would have exceedingly slow convergence and the computation accuracy would be low. The shortcomings of the method lie in the fact that the system of hydrogen functions is not optimal for the helium atom from the point of view of rate of convergence of the series. By using a variational principle for the energy it is easy to obtain equations defining an optimal basis. The rate of convergence then increases to such an extent that in the overwhelming number of applications the single-electron approximation is sufficient. The equations for this approximation are called the Hartree-Fock equations.<sup>[11]</sup>

We can therefore hope to increase noticeably the rate of convergence of series (1.1) by correct choice of the system basis functions. This assumption was verified earlier<sup>[12]</sup> and it was shown in particular that to calculate the cross section for the elastic scattering of an electron by a hydrogen atom, at least for low energies  $k^2$ , the single-electron approximation is already sufficient.

In the present paper we obtain a system of equations for the optimal basis, for arbitrary  $k^2$  smaller than the ionization potential of the atom. All possible inelastic processes are taken into account. Specific calculations are made for the scattering of an electron by a hydrogen atom. The generalization to include an arbitrary atom does not entail any difficulties in principle.

We begin with the case of the scattering of an electron of infinitesimally low energy, the analysis of which is facilitated by the presence of a functional that is extremal with respect to the scattering length.

## 2. SCATTERING OF AN ELECTRON OF INFINITESIMALLY LOW ENERGY ( $k^2 = 0$ )

Let an electron with energy  $k^2 = 0$  be scattered by a hydrogen atom in the ground state. We consider the triplet case. We seek the unknown wave function in the form

$$\Psi(\mathbf{r}_1, \mathbf{r}_2) = \sum_{i=1}^n \Psi_i(\mathbf{r}_1, \mathbf{r}_2),$$

$$\Psi_i(\mathbf{r}_1, \mathbf{r}_2) = 2^{-1/2} (1 - P) F_i(\mathbf{r}_1) g_i(\mathbf{r}_2) \quad (2.1)$$

under the condition

$$g_i(\mathbf{r}) = u_i(\mathbf{r}), \quad F_i(r) \approx 1 + \alpha/r \quad (r \rightarrow \infty); \quad (2.2)$$

where  $u_i(\mathbf{r})$  — wave function of the hydrogen-atom ground state,  $\alpha$  — scattering length, and  $P$  — operator of electron permutation.

To find the optimal system of basis functions we use the Hulthen functional

$$J = -\alpha + \frac{1}{4\pi} \int \Psi(\mathbf{r}_1, \mathbf{r}_2) (H - E) \Psi(\mathbf{r}_1, \mathbf{r}_2) d\mathbf{r}_1 d\mathbf{r}_2, \quad (2.3)$$

which has an extremum (minimum) for triplet scattering at  $k^2 = 0$  under the boundary conditions (2.2) [12].

Substituting (2.1) in (2.3) and varying with respect to  $F_i(\mathbf{r})$  ( $i = 1, 2, \dots, n$ ) and  $g_i(\mathbf{r})$  ( $i = 2, \dots, n$ ), we obtain a system of equations for these functions. The main consequence of the obtained equations is that the system  $g_i(\mathbf{r})$ , being the best (as follows from the extremal nature of the functional), does not consist of the eigenfunctions of the hydrogen atom. Consequently, it becomes necessary to deform at least the energetically unattainable levels during the course of the solution.

Further improvement of the system  $g_i(\mathbf{r})$  is based on the following remark. In the exact formulation of the problem it is necessary to solve the equation

$$H\Psi = E\Psi$$

under the boundary condition

$$\Psi(r_i, r_j) \rightarrow (-1)^i 2^{-1/2} g_i(r_i) (1 + \alpha/r_j), \quad r_j \rightarrow \infty$$

$$(i, j = 1, 2; \quad i \neq j)$$

and for the minimally possible  $E$ . It is important that the form of  $g_i(\mathbf{r})$  and the value of  $E$  need not be specified beforehand, for they are determined during the course of the solution (and naturally coincide with the hydrogen values). It follows therefore that the values of  $g_i(\mathbf{r})$  and  $E$  can differ from their exact values in the approximate solution of the problem and for the optimal value of  $\alpha$ . A shortcoming of the functional (2.3) is that it does not admit of variation of these quantities. A possible modification for it, free of these short-

comings, was proposed by one of the authors [14].

We shall not present the explicit form of the system of equations for  $k^2 = 0$ . It will be obtained later as the particular case of a more general analysis.

## 3. SCATTERING OF AN ELECTRON OF ARBITRARY ENERGY ( $k^2 \neq 0$ )

Let the initial state of the atom be determined by an energy  $E_0$ , a momentum  $l_1^0$ , a momentum projection  $m_{1l}^0$ , and a spin projection  $m_{1s}^0$ . The incident electron is described by a plane wave with wave vector  $\mathbf{k}_0$ . The wave function of the system has an asymptotic form ( $r_2 \rightarrow \infty$ ):

$$\Psi_{\mu_0}(\mathbf{r}_1, \mathbf{r}_2) \approx \frac{1}{V^2} \sum_{\mu} \Phi_{\mu}(1, 2) [\delta_{\mu_0\mu} \exp(ik_n r_2) + A_{\mu_0\mu}(\mathbf{n}_0, \mathbf{n}) \exp(ik_n r_2)/r_2] \quad (3.1)$$

Here  $\mu$  is the set of quantum numbers  $(nl_1 m_{1l} / m_{1s} m_{2s})$ , and

$$\Phi_{\mu}(1, 2) = g_{nl_1}(r_1) r_1^{-1} Y_{l_1 m_{1l}}(\Omega_1) \eta_{m_{1s}}(1) \eta_{m_{2s}}(2),$$

where  $g_{nl_1}(r_1) r_1^{-1} Y_{l_1 m_{1l}}(\Omega_1)$  — wave function of the hydrogen atom,  $\eta_{m_{1s}}(i)$  — spin functions of two electrons, and  $A_{\mu_0\mu}(\mathbf{n}_0, \mathbf{n})$  — scattering amplitude corresponding to the transition from state  $\mu_0$  to state  $\mu$  with change in electron direction from  $\mathbf{n}_0$  to  $\mathbf{n}$ .

We seek the function  $\Psi_{\mu_0}(\mathbf{r}_1, \mathbf{r}_2)$  in the form of an antisymmetrical combination

$$\Psi_{\mu_0}(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{V^2} \times \sum_{\Gamma} [(1 - P) \frac{1}{r_1} g_{\Gamma}^{\mu_0}(r_1) \frac{1}{r_2} F_{\Gamma}^{\mu_0}(r_2) Y_{l_1^{\mu_0} m_{1l}^{\mu_0}}(1, 2) Y_{S M_S}(1, 2)], \quad (3.2)$$

where

$$Y_{l_1^{\mu_0} m_{1l}^{\mu_0}}(1, 2) = \sum_{m_{1l}, m_{2l}} (l_1 m_{1l} l_2 m_{2l} | l_1 l_2 L M_L) Y_{l_1 m_{1l}}(1) Y_{l_2 m_{2l}}(2)$$

is the eigenfunction of the total orbital momentum operator,  $(\dots | \dots)$  are Clebsch-Gordan coefficients, and  $\Gamma$  is the set of indices  $(nl_1 l_2 L M_L S M_S)$ .

It follows from (3.1) and (3.2) that  $(\nu = \{nl_1 l_2\})$

$$B_{\Gamma}^{\mu_0}(r) \rightarrow \sum_{\substack{l_2^0, m_{2l}^0 \\ l_2^0, m_{2l}^0}} B_{\Gamma}^{\mu_0} \{ \delta_{\nu\nu_0} \exp[-i(k_n r - \pi l_2/2)] - S_{\nu\nu_0}^{LS} \exp[i(k_n r - \pi l_2/2)] \} \quad (r \rightarrow \infty),$$

$$B_{\Gamma}^{\mu_0} = (l_1^0 m_{1l}^0 l_2^0 m_{2l}^0 | l_1^0 l_2^0 L M_L) 2\pi i^{l_2^0+1} k_0^{-1} Y_{l_2^0 m_{2l}^0}^*(\mathbf{n}_0). \quad (3.3)$$

The scattering matrix  $S_{\nu\nu_0}^{LS}$  determines the

cross section of all the processes. In particular, the total atom excitation cross section for the transition  $n^0 l_1^0 \rightarrow n l_1$  is equal to

$$\sigma(n^0 l_1^0 \rightarrow n l_1) = \frac{\pi}{4k_0^2} \sum_{LSl_2 l_2^0} \frac{(2L+1)(2S+1)}{(2l_1^0+1)} |S_{\nu\nu_0}^{LS} - \delta_{\nu\nu_0}|^2.$$

To derive a system of equations for the radial functions  $F_{\Gamma}^{\mu_0}(r)$  and  $g_{\Gamma}^{\mu_0}(r)$  we use the functional

$$\begin{aligned} J = & A_{\nu_0 \mu_1}(\mathbf{n}_0, \mathbf{n}_1) - \frac{1}{4\pi} (-1)^{m_{1l}} \int dq_1 dq_2 \\ & \times \left\{ \int d\Omega_1 d\Omega_2 \Psi_{\nu_0}(-\mathbf{n}_0) (H - E) \Psi_{\nu_1}(\mathbf{n}_1) \right. \\ & - \sum_{i=1}^2 \sum (-1)^{l_i+l_2-L+M_L} \delta_{l_i l_i'} \delta_{l_2 l_2'} \chi_i^{\mu_0} \\ & \left. \times (-\mathbf{n}_0) (H_i - E) \chi_i^{\mu_1}(\mathbf{n}_1) \right\}; \end{aligned} \quad (3.4)$$

$$H = -\nabla_1^2 - \nabla_2^2 - 2/r_1 - 2/r_2 + 2/r_{12},$$

$$H_i = -\nabla_{r_i}^2 - \nabla_{r_j}^2 + l_j(l_j+1)/r_j^2 \quad (i, j = 1, 2; i \neq j),$$

$$\chi_i^{\mu}(\mathbf{n}) = (-1)^{l_i} 2^{-l_i/2} r_i^{-1} g_{\Gamma}^{\mu}(r_j) r_i^{-1} Q_{\Gamma}^{\mu}(r_i). \quad (3.5)$$

Here  $Q_{\Gamma}^{\mu}$  has the form (3.3),  $\Omega$  is the solid angle determining the position of the electrons,  $q$  the aggregate comprising the radial coordinate and the spin variable, and  $E$  is the total energy of the system. The summation is over  $L, S, M_L, M_S, \nu,$  and  $\nu'$ . The functions  $\Psi_{\mu_0}(-\mathbf{n}_0)$  and  $\Psi_{\mu_1}(\mathbf{n}_1)$  differ in the initial state of the atom and in the initial direction of motion of the free electron.

If we use for  $g_{\Gamma}^{\mu}(r)$  the wave functions of the hydrogen atom, then the functional (3.4) loses the last term and coincides with Kohn's functional<sup>[15]</sup>. In the general case it admits of individual variation of all the basis functions. For fixed  $E$ , the functional  $J$  is stationary with respect to  $A_{\mu_0 \mu_1}(\mathbf{n}_0, \mathbf{n}_1)$ , i.e.,  $\delta J = 0$ .

In the general case, allowing for the possibility of varying  $E$ , we have

$$\begin{aligned} \delta J = & \frac{1}{4\pi} (-1)^{m_{1l}} \sum_{\Gamma, \Gamma'} \delta E^{\nu LS} [I_{\nu\nu'}^{LS} \delta_{nn'} - \delta_{\tau; \tau'} \\ & \times (-1)^{1-S+l_1+l_2-L} \Delta(F_{\Gamma}^{\mu_0}, g_{\Gamma}^{\mu_1}) \Delta(F_{\Gamma'}^{\mu_1}, g_{\Gamma'}^{\mu_0})] (-1)^{l_1+l_2-L+M_L}, \\ I_{\nu\nu'}^{LS} = & \delta_{\tau; \tau'} \int_0^{\infty} (F_{\Gamma}^{\mu_0} F_{\Gamma'}^{\mu_1} - Q_{\Gamma}^{\mu_0} Q_{\Gamma'}^{\mu_1}) dr, \quad \Delta(A, B) = \int_0^{\infty} AB dr, \end{aligned} \quad (3.6)$$

where  $\tau = (l_1 l_2 LS)$ . The parameter  $E$  is assigned an index  $\nu$  because this parameter can be varied independently before each term of the sum (3.2). In practice it is necessary to vary only those  $E^{\nu LS}$  for which  $n \leq m$ , where  $m$  is the principal

quantum number of the last energetically attainable level.

The functional (3.4) leads in general form to a set of equations that determine two functions  $\Psi_{\mu_0}(-\mathbf{n}_0)$  and  $\Psi_{\mu_1}(\mathbf{n}_1)$ , so that this set is exceedingly complicated. A simplification is possible for elastic scattering of an electron by a spherically symmetrical atom, owing to the relation

$$\Psi_{\mu}^{\#}(-\mathbf{n}_0, \mathbf{r}_1, \mathbf{r}_2) \stackrel{\cdot}{=} \Psi_{\mu}(\mathbf{n}_1, D\mathbf{r}_1, D\mathbf{r}_2)$$

(here  $D$  is the operator of rotation by the angle between the vectors  $\mathbf{n}_1$  and  $\mathbf{n}_0$ ), and also for the case of elastic scattering forward. The latter case is of great interest in view of the existence of the optical theorem, which relates the imaginary part of the amplitude of elastic forward scattering with the total observed cross section:

$$\langle \text{Im} A_{\nu_0 \mu_1}^{\#}(0) \rangle_{m_{1l}^0 m_{1s}^0 m_{2s}^0} = (k_0/4\pi) \sigma_{n_0 l_1^0}.$$

In varying the functional it is necessary to take into account the supplementary conditions

$$\delta_{l_1 l_1'} \delta_{l_2 l_2'} \int_0^{\infty} g_{\nu LS}(r) (H^{l_1} - E_{\nu LS}) g_{\nu LS}(r) dr = 0, \quad (3.7)$$

$$\delta_{l_1 l_2'} \delta_{l_2 l_1'} \int_0^{\infty} F_{\nu LS}(r) (H^{l_2} - E_{\nu LS}) g_{\nu LS}(r) dr = 0. \quad (3.8)$$

Otherwise the sought equations turn out to be incompatible with required boundary conditions of the problem. The condition (3.8) must be regarded as a limitation on  $F_{\nu LS}(r)$ . In (3.7) and (3.8)  $\nu$  runs through all possible values, and  $\nu'$  only through those for which the corresponding  $k_{\Gamma}^2$  are positive. We use here the notation

$$\begin{aligned} H^l = & -d^2/dr^2 + l(l+1)/r^2 - 2/r, \\ E_{\nu LS} = & \int_0^{\infty} g_{\nu LS}(r) H^l g_{\nu LS}(r) dr = E^{\nu LS} - k_{\Gamma}^2. \end{aligned}$$

We require also that

$$\delta_{l_1 l_1'} \delta_{l_2 l_2'} \int_0^{\infty} g_{\nu LS}(r) g_{\nu' LS}(r) dr = \delta_{\nu\nu'}. \quad (3.9)$$

These orthogonality conditions, for a finite number of terms in (3.2), restrict somewhat the class of functions in which the solution is sought. Nonetheless, we retain this requirement in order to simplify the sought-for equations.

As a result we obtain the following system of equations:

$$\begin{aligned} \sum_{\nu, \lambda} f_{\nu\nu'}^{\lambda} \left\{ \delta_{\lambda 0} \right. \\ \left. \times \left[ (H^{l_1} + \lambda_{\nu\nu'}^{LS}) I_{\nu\nu'}^{LS} + \int_0^r F_{\nu LS}(r') \left( \frac{2}{r} - \frac{2}{r'} \right) F_{\nu LS}(r') dr' \right] \right\} \end{aligned}$$

$$\begin{aligned}
& + 2(1 - \delta_{\lambda 0}) y_{\lambda}(F_{\nu LS}, F_{\nu LS} | r) \} g_{\nu LS}(r) \\
& - (-1)^{1-S} \sum_{\nu', \lambda} g_{\nu \nu'}^{\lambda} \{ \delta_{\lambda 0} (H^{\lambda} - k_n^2) \Delta (g_{\nu LS}, F_{\nu LS}) \\
& + \delta_{\lambda 0} \Delta [F_{\nu LS} (H^{\lambda} - E_{\nu LS}) g_{\nu LS}] \\
& + 2y_{\lambda}(F_{\nu LS}, g_{\nu LS} | r) \} F_{\nu LS}(r) + \\
& \times \sum_{\nu'} \alpha_{\nu \nu'}^{LS} f_{\nu \nu'}^0 (H^{\lambda} - E_{\nu LS}) g_{\nu LS}(r) = 0, \quad (3.10)
\end{aligned}$$

$$\begin{aligned}
H^{\lambda} F_{\nu LS}(r) - k_n^2 F_{\nu LS}(r) = \\
& - \sum_{\lambda, \nu'} f_{\nu \nu'}^{\lambda} \{ \delta_{\lambda 0} \Delta [g_{\nu LS} (H^{\lambda} - E_{\nu LS}) g_{\nu LS}] \\
& + 2y_{\lambda}(g_{\nu LS}, g_{\nu LS} | r) \} F_{\nu LS}(r) \\
& - (-1)^{1-S} \sum_{\lambda, \nu'} g_{\nu \nu'}^{\lambda} \{ \delta_{\lambda 0} \Delta [g_{\nu LS} (H^{\lambda} - E_{\nu LS}) F_{\nu LS}] \\
& + \delta_{\lambda 0} \Delta (g_{\nu LS}, F_{\nu LS}) H^{\lambda} - 2y_{\lambda}(g_{\nu LS}, F_{\nu LS} | r) \} g_{\nu LS}(r) \\
& - \sum_{\nu'} \beta_{\nu \nu'}^{LS} g_{\nu \nu'}^0 (H^{\lambda} - E_{\nu LS}) g_{\nu LS}(r). \quad (3.11)
\end{aligned}$$

Here  $\alpha_{\nu \nu'}^{LS}$ ,  $\beta_{\nu \nu'}^{LS}$ , and  $\lambda_{\nu \nu'}^{LS}$  are the Lagrange multipliers determined by the conditions (3.7)–(3.9), and  $f_{\nu \nu'}^{\lambda}$  and  $g_{\nu \nu'}^{\lambda}$  are the matrix elements of the multipole interaction operators ( $\lambda$  is the order of the multipole):

$$\begin{aligned}
f_{\nu \nu'}^{\lambda} &= (l_1 l_2 L | P_{\lambda} (\cos \vartheta_{12}) | l_1' l_2' L), \\
g_{\nu \nu'}^{\lambda} &= (-1)^{l_1 + l_2 - L} (l_1 l_2 L | P_{\lambda} (\cos \vartheta_{12}) | l_1' l_2' L).
\end{aligned}$$

The explicit form of these coefficients follows from the theory of irreducible tensor operators and is contained in the paper of Percival and Seaton<sup>[2]</sup>. If we assume in (3.11) that  $g_{\nu LS}(r)$  is a complete system of hydrogen functions, then we return to the system obtained by Percival and Seaton<sup>[2]</sup>. The quantities  $y$  are given by

$$\begin{aligned}
y_{\lambda}(A, B | r) &= \frac{1}{r^{\lambda+1}} \int_0^r A(r_1) B(r_1) r_1^{\lambda} dr_1 \\
&+ r^{\lambda} \int_r^{\infty} A(r_1) B(r_1) r_1^{-\lambda-1} dr_1.
\end{aligned}$$

When  $k^2 = 0$ , confining ourselves to the single-electron approximation, we obtain the system previously obtained in <sup>[12]</sup>. We note that the agreement will be incomplete. In <sup>[12]</sup> there is no factor corresponding to  $\beta_{\nu \nu'}^{LS}$ , so that the equation that follows from (3.10) with  $k^2 = 0$  must be regarded as more correct.

When the number of terms in expansion (3.2) is increased, the functions  $g_{\nu LS}(r)$ , which describe the really excitable levels, tend to the hydrogen functions as a result of (3.7) and (3.8), and the asymptotic value of the wave function  $\Psi_{\mu_0}(\mathbf{r}_1, \mathbf{r}_2)$

takes on the form (3.1). When the number of terms is finite, (3.1) is not satisfied. Consequently, in any approximation it is advisable to modify somewhat the boundary conditions of the problem for an optimal determination of the scattering amplitude.

The parameters  $E_{\nu LS}$  are in general complex, and their imaginary parts tend to zero with increasing number of terms in (3.2).

The amplitude  $A_{\mu_0 \mu_0}(\mathbf{n}_0, \mathbf{n}_1)$  obtained from the system (3.10)–(3.11) can subsequently be improved by substituting the solutions of (3.10) and (3.11) in the functional (3.4), in which the parameter  $E$  must be equated to the exact value of the energy of the system under consideration.

#### 4. ESTIMATES OF THE PHASE SHIFTS FOR ELASTIC SCATTERING OF SLOW ELECTRONS BY HYDROGEN ATOMS

We confine ourselves in (3.2) to the zeroth approximation, i.e., we represent the  $\Psi$  function in the form

$$\Psi_S(\mathbf{r}_1, \mathbf{r}_2) = 2^{-1/2} (1 - P) r_1^{-1} g_S(r_1) r_2^{-1} F_S(r_2) Y_S(1,2) \quad (4.1)$$

(the indices  $M_S$ , which are immaterial in this problem, are omitted). Such an approximation is equivalent to account of s-scattering in the framework of the self-consistent-field method.

The functional (3.4) is of the form

$$\begin{aligned}
J &= -\frac{2\pi}{k} \text{tg } \eta_{\pm} - 2\pi \int_0^{\infty} \left[ F_S(r) \frac{d^2}{dr^2} F_S(r) - Q_S(r) \frac{d^2}{dr^2} Q_S(r) \right] dr \\
&- 2\pi \int_0^{\infty} [F_S^2(r_1) - Q_S^2(r_1)] dr_1 \int_0^{\infty} g_S(r_2) \left\{ \frac{d^2}{dr_2^2} + \frac{2}{r_2} \right\} g_S(r_2) dr_2 \\
&+ 4\pi \int_0^{\infty} \left[ U_0(r_1, r_2) - \frac{1}{r_2} \right] F_S^2(r_1) g_S^2(r_2) dr_1 dr_2 \\
&- 4\pi (-1)^{1-S} \int_0^{\infty} U_0(r_1, r_2) g_S(r_1) g_S(r_2) F_S(r_1) \\
&\times F_S(r_2) dr_1 dr_2 + 4\pi (-1)^{1-S} \int_0^{\infty} F_S(r_1) g_S(r_1) g_S(r_2) \\
&\times \left\{ \frac{d^2}{dr_2^2} + \frac{2}{r_2} \right\} F_S(r_2) dr_1 dr_2 \\
&- 2\pi (E_0 + k^2) \int_0^{\infty} [F_S^2(r) - Q_S^2(r)] dr \\
&- (-1)^{1-S} \left[ \int_0^{\infty} F_S(r) g_S(r) dr \right]^2. \quad (4.2)*
\end{aligned}$$

\*tg = tan.

Here

$$U_0(r_1, r_2) = \begin{cases} r_1^{-1}, & r_1 > r_2 \\ r_2^{-1}, & r_2 > r_1 \end{cases},$$

$E_0$  is the energy of the ground state of the H atoms, and  $\eta$  is the phase shift.

For the functions  $F_S(r)$  and  $g_S(r)$  we use the following approximations:

$$F_1(r) = k^{-1} \sin kr + (k^{-1} \operatorname{tg} \eta_- \cos kr + \gamma e^{-2\beta r}) (1 - e^{-2\beta r}),$$

$$Q_1(r) = k^{-1} \sin kr + k^{-1} \operatorname{tg} \eta_- \cos kr, \quad g_1(r) = 2\beta^{3/2} r e^{-\beta r}; \quad (4.3)$$

$$F_0(r) = k^{-1} \sin kr + k^{-1} \operatorname{tg} \eta_+ \cos kr (1 - e^{-2\beta r}) + 2\gamma\beta^{3/2} r e^{-\beta r},$$

$$Q_0(r) = k^{-1} \sin kr + k^{-1} \operatorname{tg} \eta_+ \cos kr, \quad g_0(r) = 2\beta^{3/2} r e^{-\beta r}. \quad (4.4)$$

As the zeroth approximation we use for the parameters  $k^{-1} \tan \eta$ ,  $\beta$ , and  $\gamma$  the data of a previous paper<sup>[12]</sup> for  $k^2 = 0$ . Substituting (4.4) and (4.3) in the right half of (4.1) we obtain the corrected values of  $k^{-1} \tan \eta$ . The results of the calculation are listed in the table, which shows for comparison also the data of the latest paper by Temkin<sup>[16]</sup>.

$k$	0.01	0.05	0.1
$\eta_-$	3.124	3.052	2.955
$\eta_-^*$	3.1237	3.046	2.942
$\eta_+$	3.084	2.855	2.565
$\eta_+^*$	3.086	2.86	2.59

$\eta$  — calculated values of the phase shifts,  $\eta^*$  — phase shifts as given by Temkin.<sup>[16]</sup>

The agreement between Temkin's calculations and ours offers evidence that even in the simplest approximation the proposed method ensures sufficient accuracy. At the same time, it was deemed interesting to check the reliability of Temkin's calculations, in which an approximation based on different principles was used.

## 5. CONCLUSION

The system (3.10)–(3.11), obtained above from an analysis of the elastic scattering of an electron by a spherically symmetrical atom (or forward scattering), actually has a wider range of applicability. It remains valid also in the presence of inelastic processes. This follows from the fact that the sought system of equations can be obtained from Schrödinger's equation by substituting in the

latter the expansion (3.2), multiplying from the left in succession by

$$r_1^{-1} g_{\nu LS}(r_1) Y_{l l_z}^{L M L}(1, 2) Y_{S M_S}(1, 2),$$

$$r_2^{-1} F_{\nu LS}(r_2) Y_{l l_z}^{L M L}(1, 2) Y_{S M_S}(1, 2)$$

and integrating over the corresponding angular, spin, and radial variables. The subtraction procedure with the use of the  $\chi$ -functions is quite easy to realize in this case.

A simplified variant of the system (3.10)–(3.11) can be obtained from a separate examination of the real and imaginary parts of the functional (3.4). This lets us confine ourselves to real  $g_{\nu LS}(r)$ . The resultant two independent systems of equations determine the real and imaginary parts of the scattering amplitude, respectively. The latter of these systems is of independent interest, in view of the optical theorem.

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<sup>1</sup> N. F. Mott and H. S. W. Massey, *Theory of Atomic Collisions*, Oxford Univ. Press, 1963.

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